2026 Southwest Regional Meeting Abstracts

SWRM 2026 SW01

Employing hypervalent iodine(III) compounds in the synthesis of nitrogen-rich energetic polymers and materials

***Nicolay V. Tsarevsky**, nvt@smu.edu. Department of Chemistry, Southern Methodist University, Dallas, Texas, United States*

Hypervalent iodine(III) compounds with the general structure $ArIL_2$ (Ar = aryl, L = caboxylate or halide) participate in ligand-exchange reactions with nucleophiles such as azide or tetrazolate (RCN_4^-) anions, yielding compounds with N-based ligands attached to the central iodine atom. They can serve in the functionalization of various unsaturated or saturated substrates or to initiate radical polymerizations. The products of these reactions contain one or more azide or tetrazole functionalities and are often energetic compounds. While compounds of the type $ArI(N_3)_2$ are unstable and must be generated and used *in situ*, several tetrazolate-based hypervalent iodine(III) compounds were isolated, characterized, and studied, including compounds with linear N-I-N fragment(s), such as $ArI(N_4CR)_2$ and the oligomeric μ-oxo compounds with the generic structure RCN_4-I(Ph)-[O-I(Ph)]$_n$-N_4CR (n = 1, 2, …), pseudocyclic *N*-heterocycle-(tetrazolate-)stabilized λ^3-iodanes, and heterocyclic compounds with fused benziodazole and tetrazole rings. They are typically stable at ambient conditions but often decompose violently at elevated temperatures and can plausibly find applications as constituents of energetic materials. The methods of preparation, the structural, spectroscopic, and thermal stability studies, as well as some synthetic uses of members of this class of hypervalent iodine(III) compounds will be presented.

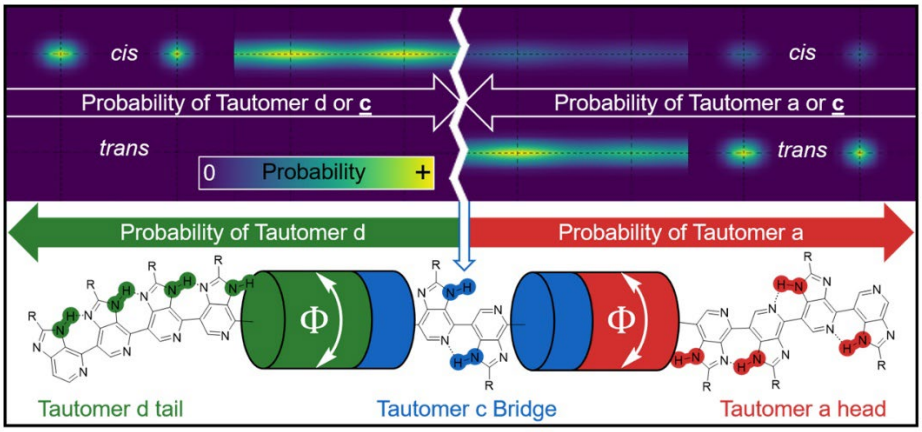
SWRM 2026 SW02

Novel imidazopyridine oligomers with manipulable backbone conformation evaluated under a probabilistic Bayesian framework

***Octavio Miranda**, om0213@tamu.edu. Chemistry, Texas A&M University System, College Station, Texas, United States*

π-Conjugated backbones depend on torsional coplanarity for efficient charge transport and strong intermolecular coupling, yet most conformational-control strategies lock a backbone into a single geometry, requiring a redesigned monomer for every new conformation. Herein hydrogen bonded imidazopyridine oligomers (HIPO) are introduced in which a single repeat unit carries both a hydrogen-bond donor and acceptor, and whose imidazole tautomerism gives access to two distinct coplanar geometries, a six-membered *trans* and a seven-membered *cis* hydrogen-bonded ring. Density functional theory on an imidazopyridine dimer reveals four tautomeric states with two coplanar minima, and the resulting Boltzmann torsional distributions are propagated along a polymer chain through a Bayesian belief-propagation model built on a tautomer transition network. Because the forward and reverse transition matrices are non-reversible, the model predicts a directional, chain-length-dependent funneling towards mostly *trans* at one chain end and fully *cis* at the other, bridged by a topologically required intermediate tautomer. Variable-temperature and solvent-dependent UV-Vis and fluorescence spectroscopy of the oligomers allow the evaluation of the model within the

context of steric and intermolecular interactions: HIPO-a (branched sidechain) behaves as a rigid, all-*trans* J-aggregate, while HIPO-b (linear sidechain) shows significant solvatochromic and thermochromic behavior consistent with interconversion between *cis*/*trans* conformers along the oligomer conjugated backbones. These results suggest tautomer-encoded, directional conformational control as a design principle for conjugated backbones, moving beyond the binary choice of torsional rigidity or free rotation.



SWRM 2026 SW03

Thermo-responsive desiccants for energy efficient building dehumidification

***Chengqian Huang**, chengqian.huang@utdallas.edu, Shuang Cui. The University of Texas at Dallas, Richardson, Texas, United States*

Proper humidity levels in buildings are essential for occupant comfort, moisture-sensitive manufacturing (e.g., semiconductors), and food preservation. Humidity control in buildings mainly relies on heating, ventilation, and air-conditioning (HVAC) systems, which are responsible for 600 million tons of CO_2 emissions annually. Conventional cold-surface condensation dehumidification requires cooling the air to very low temperatures, leading to overcooling and additional energy consumption for reheating. Desiccant wheels using hygroscopic materials such as silica gel (SG) can avoid overcooling by directly adsorbing moisture from the air. However, a high thermal energy input is required to overcome the enthalpy of vaporization (~2400 J/g) during the desiccant regeneration. Thermo-responsive polymer (TRP) desiccants offer a promising energy-efficient alternative through temperature-dependent water sorption. TRPs with lower critical solution temperatures (LCSTs) of 45–60 °C allow moisture uptake below the LCST and water release in liquid form above it. This approach bypasses the high enthalpy of vaporization and enables desiccant regeneration using low-grade heat sources, including industrial waste heat, solar energy, and condenser heat from HVAC systems, thereby further enhancing sustainability. In this work, the molecular structure of TRP was specially designed to incorporate functional moieties, creating high-performance TRP desiccants. The resulting desiccant materials exhibit high moisture-uptake capacity and tunable LCSTs within a moderate temperature range of 32 to 60 °C, enabling the desiccant regeneration under mild heating. In addition, the introduction of acrylate functional moieties improves interfacial adhesion between TRP and metal substrates, which is expected to enhance coating durability during fabrication, repeated dehumidification-regeneration cycles, and prolonged operational use in desiccant-wheel-based systems. The Python-based modeling further demonstrated that using TRP desiccants improves

energy efficiency by up to 40.6% compared with SG in dehumidification. This work represents a significant advance toward reducing energy use and greenhouse gas emissions in building dehumidification, contributing to sustainability and climate resilience.

SWRM 2026 SW04

N-oxyl radical-mediated electrochemical surface modification of nanocellulose toward polymer gel electrolytes for battery applications

Dong Hwan Nam[1]*, dhnam12@hanyang.ac.kr, Seongsu Park*[2]*, Chang Geun Yoo*[2]*, Hak-Yong Lee*[3]*, Gyu Leem*[1]*. (1) Department of Mechanical Engineering, The University of Texas Rio Grande Valley McAllen, McAllen, Texas, United States(2) Department of Chemical Engineering, SUNY College of Environmental Science and Forestry, Syracuse, New York, United States(3) Research Center for Bio-Based Chemistry, Korea Research Institute of Chemical Technology, Daejeon, Daejeon, Korea (the Republic of)*

Gel polymer electrolytes combine the mechanical stability of solid electrolytes with the ion-transport properties of liquid electrolytes. Nanocellulose is a material with a high aspect ratio, characterized by high specific strength, thermal stability, and the ability to modulate rheological properties; when used as a framework material for gel polymer electrolytes, it can enhance their mechanical properties. However, its intrinsic hydrophilicity can cause aggregation in organic electrolyte and acrylate monomer systems, limiting its dispersion and processability. To improve compatibility with organic systems, nanocellulose was modified through two independent strategies: N-oxyl-mediated oxidation to introduce carboxyl groups and cyano-functionalization to introduce polar CN-containing groups. These hydroxyl groups were cyanoethylated through alkaline activation followed by nucleophilic addition to acrylonitrile. The extent of cyanoethylation is evaluated through degree of substitution, while the effects of oxidative and nitrile-containing surface functionalities on charge density, dispersibility, and electrolyte compatibility are being systematically investigated. Furthermore, substitution of C2/C3 hydroxyl groups with functional moieties including epoxidation, esterification, and carbamation is investigated to improve compatibility with organic and/or aqueous media. These surface modifications of primary and secondary hydroxyl groups establish a mechanistic framework for controlling nanocellulose substitution, providing a pathway toward nanocellulose with tunable charge density, dispersibility, ion-transport properties and surface chemistry for next-generation gel electrolyte applications.

SWRM 2026 SW05

Elucidating the optical switching of electrochromic spiropyran copolymers

Robert M. Pankow*, rmpankow@utep.edu. Chemistry and Biochemistry, The University of Texas at El Paso, El Paso, Texas, United States*

Electrochromic technologies seek to provide a scalable, low-cost solution for thermal energy management, optical filtration, and electrochemical energy storage. Spiropyran (SP) is a stimuli responsive small-molecule capable of undergoing reversible isomerization to merocyanine (MC) following the application of chemical, photochemical, thermal, mechanical, or electrochemical stimulus. Recently, we have shown that the electrochemical isomerization of spiropyran to oxidized merocyanine (MC^+) can be employed in spiropyran-thiophene copolymers yielding semi-transmissive-

to-black electrochromic switching with desirable optical contrast (50%) and broad spectral coverage (400-1450 nm). To elucidate how the repeat unit structure influences this isomerization, a series of fluorene and carbazole copolymers with spiropyran were synthesized via Suzuki polymerization. The polymers are transmissive in their ground state (E_g = 2.88-3.34 eV), and when incorporated into electrochromic devices (ECDs) the polymers switch to dark coloration with optical absorption across the UV-visible wavelength range (350-750 nm). The mechanochemical isomerization (SP to MC) was then explored via sonochemical experiments, and these were monitored via ^{1}H-NMR confirming the formation of the MC isomer. Lastly, acid-induced isomerization (SP to MCH^+) was investigated to probe if this competing pathway occurs during electrochemical or mechanochemical isomerization. It was found that electrochemical, mechanochemical, and acid-induced isomerization pathways yield distinct optical absorption features, allowing for the deconvolution of these spectra. DFT and TD-DFT calculations were also performed to support these assignments and experimental trends. Overall, these findings establish key structural design guidelines for developing electrochromic spiropyran copolymers with targeted optical absorption and improved ECD performance metrics.

SWRM 2026 SW06

Salogels design strategies for development of shape stable thermal energy storage materials

Kartik Kumar Rajagopalan*, r2kkartik@tamu.edu, Ashik Abedin, Svetlana A. Sukhishvili. Materials Science and Engineering, Texas A&M University, College Station, Texas, United States*

Inorganic salt hydrates (ISHs) are promising phase change materials (PCMs) due to their high volumetric latent heat of fusion, high thermal conductivity, low cost, and non-flammability compared to organic PCMs. However, low viscosity in the molten state leads to leakage and phase segregation necessitating shape stabilization in thermal management applications. In this work, we demonstrate strategies for shape stabilization based on polymer networks called salogels which show on-demand reversible gelation yet provide shape stabilization at low polymer concentrations (<5wt%). The high salt (9-18 mol/kg) and low water concentration in ISHs resulting in incomplete hydration of ions and polymer leads to unusual polymer solubility and gelation behavior. Therefore, development of a broad strategy for using polymers which provide tunable, temperature-reversible shape stabilization of a variety of salt hydrates is hindered. In this work we first demonstrate that solubility and gelation of neutral, polar polymers strongly depend on ion type and water content using the case of a nitrate and a chloride salt hydrate. Dynamic boronate ester crosslinks are sufficient for the nitrate salt hydrate to produce thermo-responsive salogels with tunable gel-to-sol transition temperature (T_{gel}) in the range of 7-75 °C. Whereas the chloride requires the introduction of entanglements in addition to the boronate ester crosslinks where a synergistic effect resulted in hybrid salogels with tunable T_{gel}. While the boronate ester and hybrid salogels were suitable for shape stabilization of low-melting-point ISH PCMs (up to 50°C), temperature and creep-resistant salogels based on the thermo-reversible Diels-Alder (DA) chemistry shape stabilized ISH PCMs over a wide temperature range (up to 120 °C). The low overall polymer content (< 5 wt%) in salogels allows retention of >90 % of the heat of fusion of the PCM and shape stability with thermal cycling. Future work on salogel design using novel polymer architectures and gelation mechanisms is discussed.

SWRM 2026 SW07

Perovskite solar cells with dramatically suppressed photocurrent hysteresis through conjugated organic cations with carboxyl groups

***Xiong Gong**, xiong.gong@uta.edu. The University of Texas at Arlington, Arlington, Texas, United States*

Perovskite solar cells (PSCs) have been attractive in both academic and industrial sectors in the past years because of their easily scalable and cost-effective fabrication and the excellent optoelectronics of metal halide perovskites (MHPs) as well. As the strategy to improve the stability of three-dimensional (3D) MHPs, two-dimensional (2D) MHPs with different organic spacers were developed. However, most organic spacers used for 2D MHPs are insulating. While the impressive device performance has been reported by 2D/3D bilayer structure or 2D:3D mixed MHPs single layer structure, the insulating organic cations possess poor charge transport, restricting the device performance of PSCs. In this study, we use conjugated organic spacers and make the high-performance PSC devices based on the 2D:3D mixed MHPs. Compared to the 3D MHPs thin film, the 2D:3D mixed MHPs thin film possesses enhanced charge carrier mobilities and suppressed non-radiation charge carrier recombination. The 2D:3D mixed PSCs exhibit the highest power conversion efficiency of 26% and possess remarkably enhanced stability. Moreover, the carboxyl substitution on the organic spacer could further suppress the photocurrent hysteresis of PSCs. All these results demonstrate that the 2D:3D mixed PSCs based on the conjugated organic spacer are one of the facile ways to fabricate stable and high-performance PSCs.

SWRM 2026 SW08

Solar driven catalytic degradation of renewable materials to produce value-added chemicals under mild conditions

***Gyu Leem**, gyu.leem@utrgv.edu. The University of Texas Rio Grande Valley, Edinburg, Texas, United States*

Photocatalysis and electrocatalysis play crucial roles in organic reactions related to solar energy conversion, biomass processing, polymer degradation, and environmental sustainability. Here, we highlights synthetic molecular photoelectrochemistry for chemoselective C-C/C-O bond cleavage in renewable biomacromolecules (e.g., lignin) in the domains of carbon.A key challenge in these transformations is the chemoselective cleavage of C-C/C-O bond of aryl-ether linkages in lignin at room temperature, where precise oxidation control is essential for targeted value-added products. To address this, the Leem Research Group pioneers an aminoxyl radical-mediated (ARM) photoelectrocatalysis approach, integrating stable ARMs as electron-proton transfer mediators with heterogeneous photocatalysts. This method enables selective cleavage of C-C/C-O bond in lignin, a renewable aromatic biomacromolecule, facilitating its conversion into valuable low-molecular-weight chemicals via dye-sensitized photoelectrochemical cells. The ARM-catalyzed process extends to oxidative cleavage reactions and diverse chemical transformations under mild aerobic conditions, offering promising applications in synthetic organic chemistry and polymer depolymerization.

SWRM 2026 SW09

Oncogenic EGFR mutations differentially remodel receptor assembly and endocytic complex formation

***Adam W. Smith**, aw.smith@ttu.edu, Maryam Bello-Hassan, Pradeep K. Singh. Chemistry & Biochemistry, Texas Tech University, Lubbock, Texas, United States*

Activating mutations in the epidermal growth factor receptor (EGFR) are major drivers of non-small cell lung cancer, yet different oncogenic variants display distinct clinical responses to targeted therapies. While these mutations are generally viewed through the lens of kinase activation, their effects on receptor organization and assembly with downstream macromolecular complexes remain incompletely understood. Here, we combined pulsed interleaved excitation fluorescence cross-correlation spectroscopy (PIE-FCCS) with live-cell total internal reflection fluorescence microscopy to quantify receptor organization and engagement of the clathrin-mediated endocytic machinery in living cells.
We compared wild-type EGFR with the clinically prevalent L858R, E746–A750del, and L747–A750>P mutants. PIE-FCCS revealed mutation-specific differences in receptor assembly, with L858R and L747–A750>P exhibiting elevated basal receptor association, whereas the E746–A750 deletion retained predominantly ligand-dependent assembly. Following epidermal growth factor stimulation, wild-type EGFR and L858R underwent robust higher-order assembly, while the exon 19 deletion mutants exhibited more limited ligand-induced multimerization. These distinct organizational states were accompanied by corresponding differences in adaptor protein recruitment and receptor internalization, demonstrating that individual oncogenic mutations differentially influence the formation and progression of EGFR-associated endocytic complexes. These findings establish that clinically important EGFR mutations remodel receptor organization through distinct mechanisms beyond kinase activation alone. More broadly, this work highlights how quantitative measurements of membrane protein assembly can reveal mutation-specific regulation of macromolecular complexes that control receptor signaling and trafficking.

SWRM 2026 SW10

Investigating the RNA-binding landscape of thymine DNA glycosylase

***Victoria Shearer**, victoriashearer@tamu.edu, Jonathan T. Sczepanski. Chemistry, Texas A&M University System, College Station, Texas, United States*

Thymine-DNA glycosylase (TDG) is a member of the uracil DNA glycosylase superfamily involved in genetic and epigenetic regulation. TDG's canonical role is in DNA repair, where it recognizes mispairs, including G:T and G:U, and excises thymine or uracil, initiating base excision repair (BER). TDG performs the same excision chemistry during active DNA demethylation mediated by ten-eleven translocation (TET) enzymes. Here, TDG removes TET-oxidized 5-methylcytosine derivatives, 5-formylcytosine (5fC) and 5-carboxycytosine (5caC), initiating BER to restore unmodified cytosine. TDG additionally functions as a transcriptional coactivator, interacting with nuclear receptors such as ERα and RAR as well as the acetyltransferases CBP/p300. More recently, *in vitro* studies have established that TDG engages RNA in multiple contexts, acting catalytically within RNA-containing complexes and binding free RNA. TDG interacts with DNA/RNA hybrid species and can excise 5fC and 5caC from the DNA strand within them. It also binds single-stranded RNA directly, favoring G-rich oligonucleotides over other homopolymers, indicating that TDG binds RNA in the absence of DNA and discriminates among RNAs. Notably, RNA can compete with DNA duplexes for TDG binding. These interactions, however, were demonstrated *in vitro*, and whether TDG engages RNA in cells remains unclear. Herein, we profile TDG–RNA interactions at the cellular level; our results point to a direct and specific role for RNA in regulating TDG's function.

SWRM 2026 SW11

Oxidized 6-guanine mediated DNA-protein cross-links block DNA replication and induce mutations

***Peixin Wang**, pw8835@utexas.edu. The University of Texas at Austin, Austin, Texas, United States*

6-Mercaptopurine and azathioprine are prescribed for immunosuppressant and cancer treatment. Patients administrated with those drugs are prone to develop skin cancer, but the underlying mechanisms are not completely understood. Prior studies demonstrated that 6-mercaptopurine and azathioprine can induce the incorporation of 6-thioguanine into genomic DNA, which can be activated by ultraviolet A radiation that yields guanine-6-sulfonate (G_{SO3}), and G_{SO3} can further react with protein nucleophiles to form stable DNA-protein cross-links (G-DPCs). Here, we examined the effects of G-DPCs on DNA replication. We chemically synthesized site-specific G-DPCs and DNA-peptide cross-links (G-DpCs) by reacting G_{SO3} with four model proteins and four peptides containing a single nucleophile including a Cys, Lys, or N-term amine. We found that G- DPCs completely block all types of DNA polymerases (Pols) including e, b, h, i, k, and z, and G-DpCs can be efficiently bypassed by Polh and i. We further demonstrated that the lesion bypass is mutagenic and the nucleotide incorporation preference is dependent on the cross-linking chemistry and Pol identities. Specifically, Polh equally incorporates A and C opposite G-DpC at a Cys but inserts T to G-DpC at a Lys or N-term amine, whereas Poli incorporates T to G-DpCs regardless of the cross-linking chemistry. Finally, we found that unlike Poli that is only efficient for incorporation, Polh is capable of both incorporation and extension. Together, we demonstrated that G-DPCs are highly toxic and mutagenic, and Polh and i play vital roles in lesion bypass of G-DpCs. Our findings suggest that G-DPCs may contribute to the genome instability and cancer development in patients treated with 6-mercaptopurine and azathioprine.

SWRM 2026 SW12

Biochemical characterization of tousled-like kinase interactions with DNA sliding clamps

***Kirk West**, kwest@uams.edu. Biochemistry and Molecular Biology, University of Arkansas for Medical Sciences, Little Rock, Arkansas, United States*

Tousled-like kinases 1 and 2 (TLK1 and 2) are cell cycle-regulated serine/threonine kinases that have poorly characterized biological roles. Recent studies have demonstrated that TLK1 and 2 are involved in DNA repair. Our lab has recently identified a series of autophosphorylation events in TLK1's N-terminus surrounding a noncanonical proliferating cell nuclear antigen (PCNA) Interacting Protein (PIP)- box that negatively regulate TLK recruitment to sites of DNA damage. PCNA is a DNA sliding clamp that acts as a processivity factor in DNA replication helping proteins remain tethered to the DNA. Eukaryotes have two major DNA sliding clamps, PCNA and the RAD9A-HUS1-RAD1 (9-1-1) complex. Unlike PCNA, 9-1-1 is associated primarily with detecting and signaling DNA damage events to help maintain the G2/M checkpoint to prevent the spread of genomic instability and mutations to daughter cells. PCNA and 9-1-1 are highly similar in structure, with RAD9A having an extended intrinsically disordered C-terminal tail that is known to be phosphorylated by TLK1. We have previously shown that the TLK1 PIP box is required for TLK1-PCNA interaction and due to the similar structure of the two clamps we hypothesized that the TLK1 PIP box may also interact with the 9-1-1 complex. We have used recombinant TLK1 PIP peptides, purified PCNA and 9-1-1 in isothermal titration calorimetry experiments to confirm that a phosphomimetic containing TLK1 PIP mutant does in fact have lower affinity to PCNA than the wild-type sequence. We also show that neither the wild-type nor phosphomimetic PIP box bind to insect cell purified 9-1-1. In-vitro pulldowns of full-length TLK1 and TLK2 confirm interaction with 9-1-1, suggesting that although the clamps have similar

structures their interacting proteins have different modes of binding. Work is ongoing to identify the TLK/9-1-1 interaction domains.

SWRM 2026 SW13

MCM9 C-terminal extension is a portable regulatory module that reprograms damage specificity, RAD51 filament fate, and repair pathway choice

***Desmond Okafor**, desmond_okafor2@baylor.edu. Chemistry and Biochemistry, Baylor University, Waco, Texas, United States*

Mutations or deletions in MCM8/9 helicase complex cause premature ovarian failure and are associated with increased cancer risk in affected patients. We show that the MCM9 C-terminal extension (CTE) functions as a modular regulatory domain that helps direct interactions with specific repair factors to ultimately decide DNA repair pathway choice. Truncation of the CTE identified a minimal region required for damage-site localization that included a BRCv motif. Loss of MCM9 reduces crosslink induced RPA foci formation by more than threefold, and we verified that both the catalytic activity and an intact CTE are required for RPA loading. To test whether the CTE is functionally portable, we swapped it with CTEs from three other DNA repair helicases: RECQL5, ScSrs2, and FANCJ, in divergent repair pathways. Each chimera rescued damage induced MCM9 nuclear foci and RAD51 recruitment, but only the FANCJ chimera supported productive homologous recombination using a CRISPR-based reporter. RECQL5 and ScSrs2 chimeras formed abundant RAD51 foci, yet failed to complete repair, consistent with their anti-recombinase helicase activity that dismantles RAD51 filaments before strand invasion. CTE identity also reprogrammed downstream interactions: RECQL5 and ScSrs2 CTEs imported PCNA engagement through PIP box motifs absent from the native MCM9 CTE, while the FANCJ CTE recruited BRCA1 in a damage context-dependent manner. Taken together, our findings support a model in which the MCM9 CTE acts as a repair identity module necessary for fork protection and recombination, and CTE diversification among other DNA repair helicases generates distinct repair specializations directed through specific motifs to drive specific DNA remodeling activities.

SWRM 2026 SW14

Structural and biochemical basis of Rad34–Rad23–Rad33 in transcription-coupled repair of rDNA in yeast

***Meenuka Dalpathadu**[1], annmeenuka.dalpathadu@gmail.com, Jung Hyun Min[1], Linh Pham[2], Kenji Murakami[2]. (1) Chemistry and Biochemistry, Baylor University, Waco, Texas, United States(2) Department of Biochemistry and Biophysics, Perelman School of Medicine, University of Pennsylvania, Philadelphia, Pennsylvania, United States*

The nucleotide excision repair (NER) pathway is a conserved mechanism that maintains genome integrity by removing DNA helix-destabilizing lesions such as cyclobutane pyrimidine dimers and 6-4 photoproducts. A sub-pathway, the transcription-coupled NER (TC-NER), is initiated when a lesion stalls a transcribing RNA polymerase. In yeast, DNA damage removal in the transcribing strand (TS) of rRNA genes depends on Rad34 upon the arrest of RNA Polymerase I.This protein is a homolog to Rad4, the yeast ortholog of human XPC, a known damage sensor and initiator of NER. Although studies have shown that the TC-NER of the TS of rDNA is impaired in Rad34 mutant cells, the role of

this protein remains unclear. To assess Rad34's potential for identifying DNA damage, an electrophoretic mobility shift assay was performed, and the Rad34-Rad23 complex showed specific binding to damaged DNA, with a dissociation constant of 363 nM ± 9. Notably, the presence of Rad33 enhanced this specific binding by approximately two-fold. Fluorescence lifetime-based Förster resonance energy transfer (FLT-FRET) analyses further revealed that Rad34-bound damaged DNA adopts a more conformationally homogeneous state, and this is further increased in the presence of Rad33. A critical downstream event following damage recognition is the recruitment of the general transcription and repair factor, TFIIH, to the lesion site. To investigate this step, we assembled the Rad34–Rad23–Rad33 complex with damaged DNA and purified holo-TFIIH, enabling structural determination via cryo-electron microscopy (cryo-EM). Furthermore, in the assembly of Rad34 with Core TFIIH + TFIIK (reconstituted Holo TFIIH) and essential downstream NER factors, dual-incision products were generated, demonstrating that Rad34 can successfully assemble an active, incision-competent NER repair complex.

SWRM 2026 SW15

Structural and biochemical basis of holoTFIIH recruitment and activity in global genome nucleotide excision repair

Temilade Adeniran[1]*, temilade_adeniran1@baylor.edu, Linh Pham*[2]*, Kenji Murakami*[2,3]*, Jung Hyun Min*[1]*. (1) Chemistry and Biochemisty, Baylor University, Waco, Texas, United States(2) Biochemistry and Biophysics, University of Pennsylvania Perelman School of Medicine, Philadelphia, Pennsylvania, United States(3) Penn Center for Genome Integrity, University of Pennsylvania Perelman School of Medicine, Philadelphia, Pennsylvania, United States*

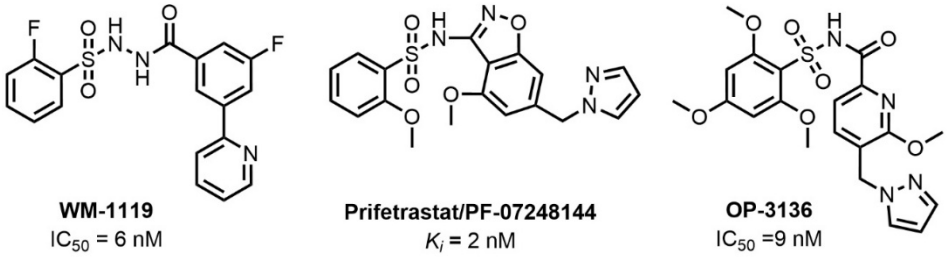
Nucleotide excision repair (NER) removes helix-distorting, bulky DNA lesions to safeguard eukaryotic genome stability. In global genome NER (GG-NER), the conserved Rad4 complex (human XPC) initiates damage recognition by recruiting the 10-subunit general transcription factor holoTFIIH, comprising the 7-subunit coreTFIIH and the 3-subunit TFIIK kinase module, for lesion verification and DNA unwinding before dual incision. While recent work has begun to visualize human repair intermediates, the structural organization, subunit architecture, and regulatory mechanisms governing the yeast holoTFIIH complex during lesion engagement remain unresolved.
Here, we combine single-particle cryo-electron microscopy (cryo-EM) and biochemical reconstitution to characterize yeast holoTFIIH recruitment during NER initiation. Cryo-EM reconstructions ranging from 4.12 Å to 10.07 Å define the architecture of intact holoTFIIH, resolving specific densities for the Tfb3, Kin28, and Ccl1 subunits of the TFIIK module. Notably, these reconstructions capture Rad4 directly recruiting holoTFIIH to damaged DNA, visualizing an early NER initiation state where TFIIK remains stably engaged. In both the holo- and core-TFIIH reconstructions, we also observe density corresponding to the ubiquitin-like (UbL) domain of Rad23, providing structural insight into the positioning of this previously unresolved domain during repair complex assembly.
To link these structural insights to repair activity, we reconstituted an *in vitro* dual-incision assay using a 94-bp DNA substrate containing a bulky internal Cy5 (iCy5) lesion. We demonstrate that intact holoTFIIH supports functional dual-incision, an activity stimulated by the regulatory factor Tfb6 and strictly dependent on the presence of both Rad1-Rad10 and Rad2 endonucleases. Our results define the structural organization of the yeast Rad4–holoTFIIH initiation complex, revealing how the early steps of nucleotide excision repair are coordinated.

SWRM 2026 SW16

KAT'ing edge biological activity and structural biology updates on lysine acetyltransferase (KAT) chemotypes

***David J. Leaver**, david.leaver@lcu.edu. Chemistry and Biochemistry, Lubbock Christian University, Lubbock, Texas, United States*

Lysine acetyltransferases (KATs) acetylate histones, which is an essential process for chromatin organization and function. KATs were considered undruggable until acylsulfonylhydrazides with nanomolar activity were reported with in vivo activity against KAT6A in 2018. The field of KAT6A chemotype inhibitors have since rapidly expanded as potential anticancer agents. Recent history of KAT6A inhibitors will be discussed including KAT inhibitors that have advanced to Phase I-III clinical trials as possible treatments for cancer patients.



SWRM 2026 SW17

Molecular orbital perspectives on relativistic effects in chemistry

***Chad E. Hoyer**, cehoyer@utep.edu. Chemistry and Biochemistry, The University of Texas at El Paso, El Paso, Texas, United States*

Relativistic effects play a central role in modern chemistry, from scalar-relativistic contributions that influence the catalysis of transition-metal complexes to spin-orbit coupling (SOC) that governs intersystem crossing. In actinide and other heavy-element compounds, both scalar relativity and SOC are essential. Scalar relativistic effects substantially modify the energies and radial distributions of the valence orbitals, bringing the 5*f* manifold closer to other valence orbitals, while SOC determines fine-structure splittings that govern many spectroscopic and chemical properties. We review commonly employed approximations for treating scalar relativity and SOC in quantum-chemical calculations and examine their relationship to the underlying Dirac-Coulomb Hamiltonian. Building on this framework, we present new relativistic quantum-chemical methodologies that incorporate effects beyond the conventional scalar-relativistic and SOC picture, and we discuss the circumstances under which these additional contributions become chemically significant.
Molecular orbitals remain one of the most successful conceptual tools in chemistry, yet their interpretation in the strong-SOC regime is underdeveloped. We present molecular-orbital analyses of linear actinide molecules and demonstrate projection-based approaches that recover chemically intuitive orbital pictures from fully relativistic wave functions. These representations provide a practical bridge between relativistic electronic-structure theory and the orbital concepts routinely used by chemists.

SWRM 2026 SW18

Chemical bonding guided orbital spaces for ORMAS and unitary cluster Jastrow wave functions

Nikolay V. Tkachenko[1,2,3]*, nikolay.tkachenko@ou.edu. (1) Department of Chemistry and Biochemistry, The University of Oklahoma, Norman, Oklahoma, United States(2) Materials Science and Engineering Program, The University of Oklahoma, Norman, Oklahoma, United States(3) Center for Quantum Research and Technology, The University of Oklahoma, Norman, Oklahoma, United States*

The construction of compact and physically meaningful orbital spaces remains a central challenge in multireference electronic-structure methods and quantum simulations of molecules. We introduce a bond-oriented orbital framework that transforms chemically intuitive bonding patterns obtained from Adaptive Natural Density Partitioning (AdNDP) into an orthonormal orbital basis suitable for correlated calculations. The resulting orbital basis (BOND) enables correlated orbital spaces to be designed directly in terms of chemically recognizable regions. We investigate this construction in occupation-restricted multiple active space (ORMAS) calculations, where BOND orbitals provide compact and balanced descriptions of electron correlation compared with conventional localized orbital choices. We further use the same bonding-guided orbital picture to construct compact unitary cluster Jastrow wave functions for quantum eigensolver applications. In this framework, chemical bonding information provides a natural way to organize the orbital space and reduce the depth the quantum ansatz. Together, these approaches connect chemically interpretable bonding patterns with compact classical and quantum many-electron models.

SWRM 2026 SW19

Towards reliable simulations of molecular quantum devices: Projected-interacting full configuration interaction density functional theory

Benjamin G. Janesko*, bjanesko@gmail.com. Texas Christian University, Fort Worth, Texas, United States*

Molecular quantum devices show promise for beyond-classical sensing, organic superconductivity, realizations of quantum computing circuits, and more. These devices' desirable properties often arise from electronic states involving large numbers of strongly correlated electrons. Designing and simulating these devices requires treating "the quantum and the chemistry", accurately predicting how large active spaces respond to temperature, pressure, structural changes, and more. I present projected-interacting full configuration interaction density functional theory as a solution for practical, formally exact treatments of huge active spaces. By combining near-exact wavefunction calculations on mulfiple partially-inteacting model systems, the approach can treat strong correlation in huge active spaces inaccessible to other methods. I present proof-of-principle calculations on a 300-electron active space, benchmark studies of polyradical spin state energies, and progress towards treatmentsof excited states, solids, and quantum materials.

SWRM 2026 SW20

Excited states and electric response properties with auxiliary field quantum Monte Carlo

***Leon W. Otis**, lo21@rice.edu, James Shee. Chemistry, Rice University, Houston, Texas, United States*

Electronic structure theory methods have historically been developed predominantly for the calculation of ground state energetics and many different high accuracy techniques including quantum Monte Carlo (QMC) methods are now regularly used for this problem. However, experimental measurements access energy differences and knowledge of the absolute ground state energy alone has limited chemical utility. Achieving a more direct connection between quantum chemical calculations and experimental measurements can pave the way to valuable physical and chemical insights, but requires computation of additional quantities including excitation energies and response properties. Phaseless auxiliary field quantum Monte Carlo (ph-AFQMC) is one promising approach for the accurate treatment of electronic correlation and our work examines the extension of ph-AFQMC to electronic excited states and electric response properties such as the dipole moment and static polarizability. We first focus on doubly excited states, which play an important role in the understanding of singlet fission and other photochemical processes. By systematically comparing multiple trial wave function protocols, we find that state-specific orbital optimization improves ph-AFQMC's accuracy for doubly excited states and is a useful approach for designing better ph-AFQMC trials. For response properties, we introduce a finite difference-based strategy that exploits noise cancellation from correlated sampling. This approach is scalable to large molecules and basis sets with a phaseless bias no worse than that of an energy calculation. The method obtains accurate dipole moments,[1] including in strongly correlated settings, and can be straightforwardly extended for computing polarizabilities. We also consider the role of the trial wave function and show that the limitations of mean field trials for strongly correlated cases can be overcome with relatively simple multi-determinant wave functions.

SWRM 2026 SW21

X-ray photoelectron spectra of halogen bonds in biochemically relevant systems

*Afifa Yousaf, **Daniel Devore**, ddevorecollege1@gmail.com, Devin Matthews. Chemistry, Southern Methodist University Dedman College of Humanities and Sciences, Dallas, Texas, United States*

Halogen-bond (XB) interactions are an increasingly important class of noncovalent interactions with applications in drug discovery and protein-ligand recognition. Herein, we investigate the amphoteric nature of halogen atoms, which enables the formation of halogen bonds and, where applicable, complementary hydrogen-bonding interactions with biologically relevant molecules, including alcohols, peroxides, and carboxylic acids. X-ray photoelectron spectroscopy (XPS) probes changes in elemental composition, chemical state, and local bonding environment at the atomic level. To investigate the spectroscopic signatures of XB complexes, we perform high-level equation-of-motion coupled cluster (EOM-CC) calculations to simulate XPS spectra for oxygen and, where applicable, chlorine atoms. Spectroscopic shifts associated with XB formation are analyzed alongside natural population analyses to identify relationships between
electronic structure and intermolecular interactions. This theoretical approach provides insight into how halogen-bond formation influences X-ray spectroscopic signatures and demonstrates the potential of XPS for probing molecular structure and noncovalent interactions.

SWRM 2026 SW22

Conductivity optimization of composite solid polymer electrolyte through additives for solid state sodium metal batteries

Tariq Bashir *[1,2], tbashir@xula.edu, Lamartine Meda[1,2]. (1) Department of Chemistry, Xavier University of Louisiana, New Orleans, Louisiana, United States(2) Energy Storage Research Alliance, Argonne National Laboratory, Lemont, Illinois, United States*

Composite solid polymer electrolytes (CSPEs) present an appealing method for fabricating solid-state batteries that are both mechanically robust and safer. Nevertheless, their relatively low ionic conductivity (~3.5x10^{-5} S cm^{-1}) continues to represent significant challenges to their commercialization. In this study, we explore a methodical additive-centric approach to improve Na ion mobility in a quasi-independent CSPE by the integration of glyme-based additives such as diglyme (G2), triglyme (G3), tetraglyme (G4), and plasticizer succinonitrile (S.N). Over a wide variety of compositions, the effects of additive type and concentration on the ionic conductivity, polymer segmental dynamics, and electrolyte structure are assessed. The integration of glymes provides additional ether-oxygen sites for coordination for Na ions and enhances the flexibility of the polymer matrix, whereas S.N is characterized as a plasticizer to reduce polymer rigidity and improve Na ion mobility in the polymer matrix. The conductivity response correlates with the concentration of the additive to determine the optimal formulation that maintains the mechanical stability of the CSPE while enhancing Na ions mobility. Electrochemical impedance spectroscopy is utilized to measure variations in bulk and interfacial resistance and to clarify the role of each additive in overall ion transport. This systematic enhancement elucidates the correlation among polymer architecture, additive–ion interactions, and Na ion mobility, presenting a viable approach for achieving highly conductive and mechanically robust CSPEs for future all-solid-state sodium-metal batteries.

SWRM 2026 SW23

Kinetic phase selection and defect-coupled ion transport in metastable Cu–B–Se nanocrystals

Progna Banerjee*[1,2], pb@pbanerjeelab.com. (1) Center for Nanoscale Materials, Argonne National Laboratory, Lemont, Illinois, United States(2) Chemistry and Biochemistry, Loyola University Chicago, Chicago, Illinois, United States*

Metastable nanocrystals provide access to compositions and local structures that are difficult to obtain under equilibrium conditions, but their electrochemical behavior also depends on how synthesis history is retained during assembly and consolidation. Here, we examine a composition- and time-resolved Cu–B–Se nanocrystal library to determine how non-equilibrium phase selection, copper deficiency, and interparticle contacts collectively govern transport. Variations in precursor stoichiometry and reaction time produce distinct diffraction signatures and nanoscale morphologies, which are tracked using powder and temperature-dependent X-ray diffraction, electron microscopy and diffraction, and thermal analysis. Nanocrystal-derived solids are subsequently evaluated by impedance spectroscopy as functions of applied load and temperature, allowing high-frequency transport to be distinguished from lower-frequency contact and interphase polarization. Across the library, nominal copper deficiency alone does not predict the measured conductivity. Instead, the transport response depends on the phase pathway selected during synthesis and the connectivity established during pellet consolidation. Optimized compositions exhibit apparent room-temperature conductivities approaching 10^(-5) S cm^(-1), while their pressure dependence reveals a substantial contribution from particle–particle contacts and associated interphases. Parallel chemical-lithiation experiments provide an additional perturbation for examining how cation incorporation and structural reorganization modify these networks. The results identify synthesis history and interphase topology

as coupled design variables for nanocrystal-derived solid electrolytes and provide a general framework for connecting metastable colloidal phases with measurable solid-state transport.

SWRM 2026 SW24

Discovery of selectively etched metastable materials for electrochemical energy storage

***Ruocun Wang**, ruocun.wang@unt.edu. Materials Science and Engineering, University of North Texas, Denton, Texas, United States*

Lithium-ion batteries have revolutionized wireless electronics and are now transforming the automotive and stationary energy storage industries. The next level of adoption demands lower cost, safer supply chains, and higher energy density. New materials can potentially tackle these challenges. Still, there has been a recent decline in the development of new intercalation materials, as decades of research have exhausted available material options. In this scenario, thermodynamically metastable phases have emerged as an underexplored materials space. One promising approach to exploring metastable materials is selective etching. Selective etching has enabled the synthesis of over 50 MXene materials by applying it to layered carbides and nitrides known as MAX phases. It opens a vast materials space and enables promising energy storage performance due to MXenes' layered structure. Here, we show that this method can be applied to oxides to discover new materials for energy storage, including bilayer tungsten oxide monohydrate. In an aqueous acidic electrolyte, the bilayer tungsten oxide monohydrate shows a capacity retention of ≈80% at 1000 mV s^{-1} (1.5-s discharge time) as compared to 1 mV s^{-1} (≈16-min discharge time) with cyclability for over 100,000 cycles. These results highlight the use of selective etching to synthesize metastable transition metal oxides for energy storage.

SWRM 2026 SW25

Unlocking materials insights with neutrons: Techniques, applications, and user opportunities

***Tianyu Li**, tianyu@latech.edu. Chemistry, Louisiana Tech University, Ruston, Louisiana, United States*

On behalf of the Oak Ridge National Laboratory Neutron Ambassador Program, this talk will promote the use of neutron characterization techniques to investigate the structure and dynamics of materials for energy applications. The presentation will briefly highlight the unique advantages of neutron-based characterization and introduce how different neutron techniques can provide complementary insights into material properties from different perspectives. Selected examples will be presented to illustrate how neutron characterization can be applied to a variety of materials systems and research questions.
Finally, the talk will introduce the neutron user facility program at Oak Ridge National Laboratory, including the various mechanisms through which researchers can access neutron facilities and capabilities **free of charge**. The goal is to provide researchers with an overview of available neutron techniques and resources and encourage broader use of neutron characterization in materials research.

SWRM 2026 SW26

Molecular insights into the MNene-electrolyte interphase for ammonia synthesis

David Kumar[1]*, davidky@tamu.edu, Abdoulaye Djire*[1,2]*. (1) Artie McFerrin Department of Chemical Engineering, Texas A&M University, College Station, Texas, United States(2) Department of Materials Science and Engineering, Texas A&M University, College Station, Texas, United States*

Ammonia is essential to global agriculture and is increasingly considered a potential carbon-free energy carrier, however, its conventional production remains highly energy- and carbon-intensive. Two-dimensional transition-metal nitride MXenes (MNenes) offer a promising pathway for electrochemical ammonia synthesis through the lattice-nitrogen-mediated (LNM) mechanism, in which lattice nitrogen is protonated to NH_3 and subsequently replenished by N_2. The effectiveness of this mechanism depends not only on lattice-nitrogen reactivity but also on the MNene-electrolyte interphase, where water organization, proton transport, and local pH govern the availability of protonating species, competition with the hydrogen evolution reaction (HER), and catalyst stability. Here, we investigate how the availability and transport of protonating species at the MNene-electrolyte interphase influence the reaction environment for LNM ammonia synthesis. Quasi-elastic neutron scattering, and ab initio molecular dynamics reveal that lattice C/N composition and surface terminations regulate confined-water mobility and hydrogen-bond networks in MNenes. Nitride-rich systems support thermally activated translational water diffusion, whereas mixed C/N lattices confine water to localized motion and carbide systems exhibit intermediate behavior, indicating these differences define the molecular environment through which proton transfer can occur. On the other hand, in situ Fourier-transform infrared spectroscopy, using phosphate speciation as a vibrational pH reporter, shows that cathodic polarization drives the MNene's interface strongly alkaline in nominally neutral electrolyte because proton consumption exceeds replenishment. Mildly acidic conditions partially moderate this pH rise by increasing proton availability, whereas strongly acidic conditions minimize interfacial pH variations but promote non-N_2-derived NH_3 release and destabilization of lattice nitrogen. Overall, these results indicate that interfacial water dynamics and proton availability are coupled design parameters for LNM ammonia synthesis. Controlling lattice composition, surface terminations, electrolyte proton-donating capacity, and operating current density offers a strategy to maintain sufficient proton delivery for lattice-N protonation while suppressing HER, excessive interfacial alkalization, and uncontrolled lattice-nitrogen depletion.

SWRM 2026 SW27

Metal-organic framework as a new platform for heterogeneous small molecule activation

Shengqian Ma*, shengqian.ma@unt.edu. University of North Texas, Denton, Texas, United States*

The activation of small molecules and their subsequent reactions have been considered as a fundamental pillar of modern catalysis and existing catalysts are dictated by transition metal-based compounds. This is particularly the case for heterogeneous small molecule activation, which primarily relies on precious metal-based catalysts (e.g. Pt, Pd, Rh, Ir) that are rare and costly. Over the past two decades, the rapid growth of metal-organic framework (MOF) that features tunable, designable, and functionalizable nanospace has provided plenty of opportunities for heterogeneous catalysis. Various design approaches will be discussed for the systematic development of MOF as a new and sustainable platform for heterogeneous small molecule activation including dihydrogen activation and carbon dioxide chemical transformations.

SWRM 2026 SW28

Tuning excitonic and photonic transport in cavity-coupled materials

***Arkajit Mandal**, mandal@tamu.edu. Texas A&M University System, College Station, Texas, United States*

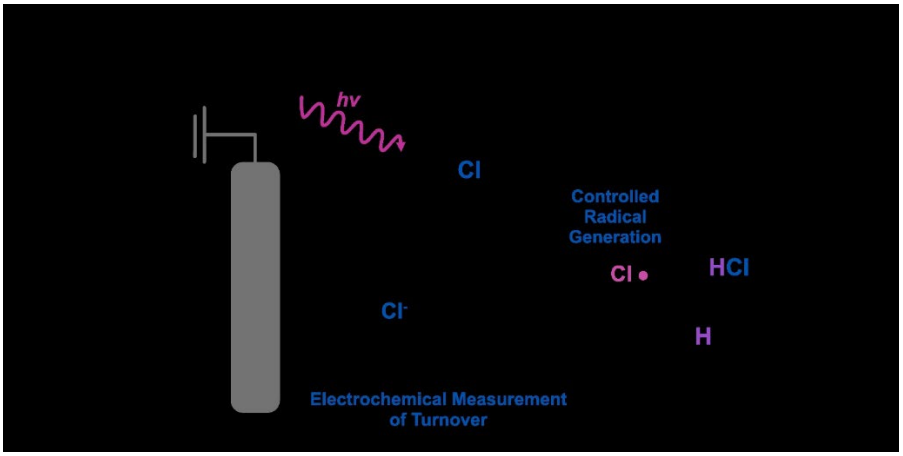
Quantum light-matter interactions between materials and confined quantized radiation inside an optical cavity have been experimentally suggested to have enabled a wide range of new exotic physical phenomena via the formation of polaritons, which are light-matter hybrid quasiparticles. However, many aspects of polariton physics remain elusive. In our recent works, we have focused on understanding how such light-matter interactions modify excitonic as well as photonic transport in materials. Using our custom quantum dynamical approaches and analytical theories, we show that quantum light-matter interactions can allow us to suppress phonon-induced decoherence, leading to ballistically propagating excitons (more precisely, exciton-polaritons) that remain coherent for extended periods of time even at room temperature. We show that the many-body multi-excitonic effects of exciton-polaritons can dictate exciton-polariton transport, relaxation, and localization. We also show how the same light-matter interactions can be leveraged to induce effective photonic interactions that enable spin-polarized photonic transport.

SWRM 2026 SW29

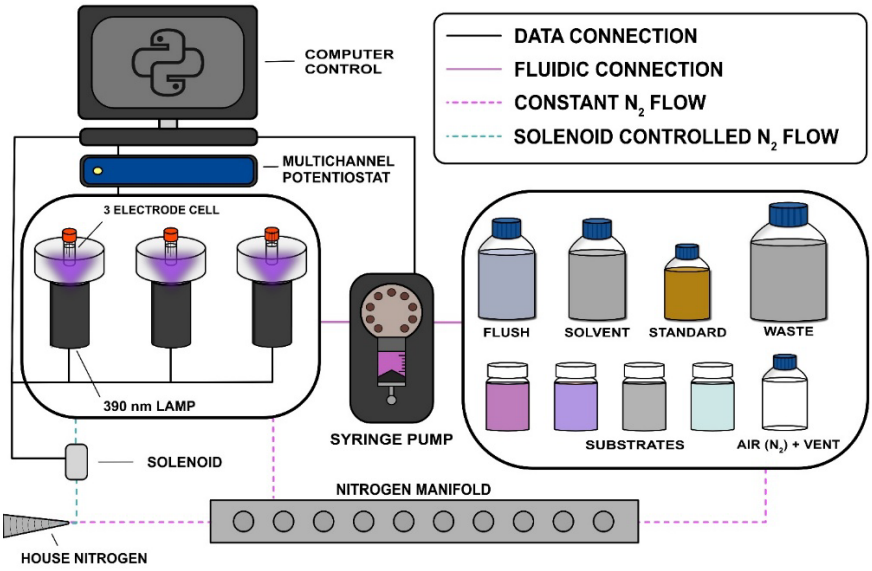
High-throughput cyclic voltammetry for assessment of photocatalytic C-H bond activation

***Sydney Noell**, sydney_noell1@baylor.edu. Chemistry and Biochemistry, Baylor University, Waco, Texas, United States*

Selective activation of C–H bonds is a longstanding challenge in the field of chemical synthesis, as their reactivity can be difficult to predict based on subtle differences in bond strength and steric accessibility. Molecular photocatalytic chlorine radical generation from earth-abundant transition-metal catalysts and chloride salts can be applied as a powerful and promising strategy for hydrocarbon functionalization. Cyclic voltammetry can be used as a quantitative measurement tool to assess molecular photocatalysis while capturing kinetic trends in hydrogen atom transfer reactions from various hydrocarbon substrates, revealing sensitivities to polarity, bond dissociation energies, and substrate structure. A new framework is proposed for measuring and directing chlorine radical C–H bond activation by utilizing electrochemistry as both an analytical tool and a synthetic control element. An autonomous, high-throughput electrochemical screening platform has been designed, created, and is being used to exhaustively map the kinetics and selectivity of photocatalytic C–H activation in the presence of diverse substrates, catalysts, and additives.



High Throughput Photocatalytic Cyclic Voltammetry Setup



SWRM 2026 SW30

Poly(3,4-ethylenedioxythiophene) (PEDOT)-modified microfluidic chip platform for electric- and magnetic-field-driven flow control at low ionic strength

Emma G. Nordstrom, *egn003@uark.edu, Ingrid Fritsch. Chemistry and Biochemistry, University of Arkansas, Fayetteville, Arkansas, United States*

Electric and magnetic fields can independently drive fluid motion in electrochemical microsystems via electrokinetic (EK) transport and redox-magnetohydrodynamic (R-MHD) flow, respectively. We investigate the interplay of these mechanisms in low-conductivity microfluidic systems (<5 mM ionic strength) using PEDOT-modified coplanar band electrodes (1.5 cm × 650 µm gold on a 5.08 cm × 2.54 cm chip, 0.3 cm gap) in a ~630 µm-high chamber containing 1–5 mM NaCl, under applied currents of 10–40 µA. With an external magnetic field (0.37 T), the ionic current generated by PEDOT electrodes produces R-MHD flow parallel to the electrodes (**j × B**); without a field, EK transport drives negatively charged tracer beads orthogonal to the electrodes, demonstrating two distinct, competing field-driven transport mechanisms within a single device. Unlike prior work at higher ionic strength, EK transport shows a strong inverse dependence on electrolyte concentration, explaining why EK effects are unobserved in conventional high-conductivity R-MHD systems. Chronoamperometry and

cyclic voltammetry show that the resulting PEDOT-mediated ionic current scales linearly with solution conductivity, while chronopotentiometric charge depletion scales linearly with the inverse of the applied current, consistent with an equivalent series RC model of the electrode–PEDOT–electrolyte interface, indicating that the PEDOT coating governs the effective charge transfer at low conductivity. Fluorescence microscopy and particle tracking velocimetry show that R-MHD velocities (~8.8–62.2 μm/s) scale primarily with applied current and device geometry, with minimal dependence on electrolyte concentration, consistent with literature R-MHD velocities (~1 μm/s per μA) once chamber dimensions and viscosity are accounted for. Flow is relatively uniform laterally and axially between the electrodes, driven directly by the Lorentz body force, while the vertical profile is parabolic, reflecting pressure-driven flow from viscous wall effects across the chamber height. EK bead velocities (0.4–11.5 μm/s) increase with applied current and decrease with increasing ionic strength. These results establish a direct link between PEDOT-mediated electrochemical processes, electric and magnetic field effects, and resulting fluid motion, providing fundamental insight into field-induced electrochemical transport and enabling the rational design of microfluidic systems.

SWRM 2026 SW31

Stereolithographic 3D-printed mold processing and PDMS microfluidic pump development for a portable microsampling backpack

Olivia Enietan[1]*, oenietan@uark.edu, Spencer Stutts*[2]*, Patrick M. Pysz*[1]*, Julie A. Stenken*[1]*. (1) Chemistry and Biochemistry, University of Arkansas, Fayetteville, Arkansas, United States(2) Physics, Hendrix College, Conway, Arkansas, United States*

Three-dimensional (3D) printing techniques such as stereolithography offer a rapid and low-cost route for producing miniaturized analytical devices and customized microfluidic systems. However, fabrication of polydimethylsiloxane (PDMS)-based microfluidic devices using 3D printed molds can be limited by resin-induced PDMS curing inhibition and poor fabrication reproducibility. Beyond fabrication, translation of these devices into portable sampling and analytical platforms requires efficient fluid handling and compact system integration and development of integrated detection systems allowing for in situ device assessment. This work addresses these fabrication and integration challenges for a long-term goal which is the development of portable systems for biological sampling and analysis on rodents. We developed a fabrication workflow for producing PDMS microfluidic devices from 3D-printed molds. A major limitation to this approach is the release and leaching of various compounds from the 3D printing resins resulting in inhibition of PDMS curing. We showed that resin chemistry choice, combined with a two-step post-treatment of UV exposure and thermal treatment of the printed molds, eliminates this curing inhibition problem. Extending the capabilities of this fabrication approach, PDMS microchannels were created as embedded peristaltic pumping elements to be applied to a portable micro sampling backpack intended for rat studies. Incorporating a PDMS-fabricated custom peristaltic tubing with ~200 μm channel dimensions resulting in a device volume of ~4 μL. This served to greatly reduce the dead volume for the microfluidic pump resulting in a decreased compression force further aiding in reduction of power needs and weight.
Finally, an automatic flow-imaging apparatus was tested and validated to enable rapid, real-time measurement of pump flow rates. This provides an instantaneous alternative to manual gravimetric flow measurements on-line and a practical platform for comparing and validating pump designs. This system images a droplet over time and is capable of sub-second flow rate measurement intervals.

SWRM 2026 SW32

High performance electrodialytic suppressor using 3D-printed gyroid channels for ion chromatography

***Kalpana Dumre**, kxd5658@mavs.uta.edu, Charles P. Shelor. Chemistry and Biochemistry, The University of Texas at Arlington, Arlington, Texas, United States*

Electrodialytic membrane suppressors are used in ion chromatography to neutralize an eluent acid or base thereby lowering the background conductance and enhancing analyte detection. For anion analysis, hydroxide eluents are preferred; the suppressor electrochemically generates H^+ which passes through a cation exchange membrane displace the eluent cation and neutralizing hydroxide in the process and converting the analyte into an acid which is measured using a conductivity detector. Increase the suppressor size increases the suppression capacity enabling more concentrated eluents to be used; however, the increased volume causing dispersion thus compromising separation. The suppressor design must therefore balance maintaining chromatographic efficiency with suppression capacity. To overcome these limitations, we are investigating low dispersion channels produced using high resolution stereolithographic 3D printing (~10-micron resolution). The channels were constructed of gyroids (a type of triply periodic minimal surface) to create a porous monolith with ordered morphology. This new design overcomes several shortcomings in previous suppressor designs including improved pressure tolerance, robustness, and dispersion. In resin packed suppressors, bed collapse may occur due to the pliable membranes distending under high pressure while rupture of the soft seals used with screen channels may also occur. The channel monolith is surrounded by and bonded to a smooth solid perimeter which serves as a hard sealing surface while the face exposed to the membranes remains open and may be used for detectors with high back pressure such as mass spectrometers. The gyroid channels have less dispersion (≤ 200 μL^2) than comparably sized commercial state of the art devices (≤ 970 μL^2) ; further, the dependence upon flow rate is essentially flat showing excellent mass transfer properties. Following printing, the device remains in an uncured state which permitted facile polymer grafting of ionic monomers to improve the overall ionic conduction. Suppressed chromatographic separations of 9 mM Na_2CO_3 had conductance noise of < 0.03 µS/cm and were comparable with the commercial devices. The device also showed ~50% lower pressure drops than devices of comparable efficiency consistent with monolithic stationary phases.

SWRM 2026 SW33

Advancing 3D printed microsampling probes for neuroscience applications

***Julie A. Stenken**[1], jstenken@uark.edu, Olivia Enietan[1], Julia Hoskins[2], MIn Zou[2], Patrick M. Pysz[1]. (1) Chemistry and Biochemistry, University of Arkansas, Fayetteville, Arkansas, United States(2) Mechanical Engineering, University of Arkansas, Fayetteville, Arkansas, United States*

Stereolithographic printing offers new opportunities for fabricating microsampling probes with geometries that are difficult to achieve using conventional microdialysis fabrication methods. Previous work from our group demonstrated a fully 3D-printed microsampling probe fabricated using two-photon polymerization (2PP) and masked stereolithography, including a 4 mm-long sampling needle with a microporous membrane. Current work extends this approach toward longer probes designed for neuroscience applications, with probe lengths now approaching 10 mm.
Extending the probe dimensions has revealed both the opportunities and challenges associated with 3D-printed microsampling devices. Fabrication failures become increasingly important as probe length dimensions increase, requiring evaluation of printing parameters, probe geometry, membrane formation, and post-print processing. Rather than treating these failures simply as fabrication limitations, we have used them to identify factors that influence probe integrity, reproducibility, and

fluidic performance. This presentation will describe the development of longer 3D-printed microsampling probes, including successful designs, failure modes, and lessons learned during the transition from proof-of-concept devices to probes suitable for neuroscience applications. These results provide practical guidance for the design and fabrication of 3D-printed microsampling devices and highlight both the potential and current limitations of additive manufacturing for in vivo chemical sampling.
Arkansas Biosciences Institute (ABI) and NIH NS140877 are acknowledged for support. The views expressed here are our own and not those of ABI or NIH.

SWRM 2026 SW34

Flagellin as an internal standard for absolute quantification and automated normalization in proteomics

***Vishal Sandilya**, vishal.sandilya@ttu.edu, Sarah Sahioun, Ronny Barrera, Abiodun Adewolu, Abderrahmane Koraich, Pelin Yildiz, Yehia Mechref. Chemistry and Biochemistry, Texas Tech University, Lubbock, Texas, United States*

Absolute quantification in bottom-up proteomics conventionally relies on isotopically labeled peptides, but their cost, incomplete labeling, and inability to account for sample-preparation losses limit adoption. Relative quantification is more accessible but does not provide abundances on an absolute scale. Here, we present a cost-effective alternative using bacterial flagellin from *Salmonella typhimurium* (FLA-ST) as an internal standard, selected for its lack of sequence homology with the human proteome. Because FLA-ST is spiked in prior to processing, it accounts for losses throughout the workflow that peptide-level standards cannot capture, and the same standard applies to both discovery and targeted analyses.
FLA-ST was spiked into human serum, homogenized brain tissue, and breast cancer cell samples. Proteins were reduced with dithiothreitol, alkylated with iodoacetamide, and digested with trypsin. Peptides were desalted using C18 TopTip cartridges and analyzed on a Vanquish Neo UHPLC coupled to an Orbitrap Fusion Lumos Tribrid mass spectrometer. Identification and quantification were performed using MSFragger against the human UniProt-Swiss-Prot database supplemented with the FLA-ST sequence. Quantified FLA-ST showed excellent linearity across the tested range (R^2 greater than 0.99), with multiple individual flagellin peptides also exceeding R^2 greater than 0.99 across matrices. No peptide-spectrum matches corresponding to FLA-ST were detected in unspiked samples, confirming orthogonality to the human proteome. Flagellin-based normalization was highly reproducible, with relative standard deviations below 15% across replicates, and increasing FLA-ST concentrations did not significantly reduce endogenous protein identifications.
To facilitate routine implementation, we developed a companion software tool that automates the workflow. It accepts peptide-level outputs from Proteome Discoverer, MSFragger, and MaxQuant, identifies robust FLA-ST peptides, calculates and applies correction factors, and reports normalized protein abundances with quality-control metrics. Support for multiple search engines and both targeted and untargeted acquisition enables straightforward integration into existing workflows. At approximately $1.36 per sample, this strategy provides a practical and economical approach for absolute quantification, normalization, and assessment of sample-preparation losses in bottom-up proteomics.

SWRM 2026 SW35

Advancing structural proteomics by mass spectrometry: Residue-specific covalent labeling, cross-linking, and AI analysis

*Sepideh Khaki Firooz, **Saiful M. Chowdhury**, schowd@uta.edu. Chemistry and Biochemistry, The University of Texas at Arlington, Arlington, Texas, United States*

The spatial arrangement and accessibility of amino acid residues determine the structure, function, and interactions of proteins. Although mass spectrometry (MS)-based covalent labeling and cross-linking offer powerful methods for investigating protein structure, conventional techniques have only allowed targeting of a limited number of residues. In this study, we have employed complementary residue-specific chemistries that act on tyrosine, acidic residues, and arginine ,and have combined chemoproteomics with protein language models to locate the reactive residues in inflammatory conditions. Tyrosine residues were selectively modified using 4-phenyl-3H-1,2,4-triazoline-3,5-dione (PTAD) under near-physiological conditions. Labeling patterns in model proteins were correlated with solvent accessibility derived from crystal structures and AlphaFold models, and their application to HeLa cell lysates demonstrated proteome-wide compatibility. A tyrosine-specific crosslinker further provided Tyr–Tyr distance constraints. Diphenyldiazomethane selectively modified aspartic and glutamic acid residues and enabled structural characterization of the Fel d 1 cat allergen complex. Cross-linking of Fel d 1 using dual-cleavable cross-linking technology identified the same structural region, providing complementary validation. Phenylglyoxal (PhG) labeling coupled with high-resolution LC–MS/MS was used to map arginine accessibility in lipopolysaccharide (LPS)-stimulated RAW 264.7 macrophages. ProtBERT-encoded peptide sequences were evaluated using supervised machine-learning models. Experimentally detected PhG-labeled residues were mapped onto three-dimensional structures of TLR4-MD2-LPS and IRAK4 kinase. The models correctly identified several experimentally modified arginine residues while also producing false-positive and false-negative predictions. These results indicate that sequence-derived features capture important determinants of arginine reactivity but do not fully account for structural and physicochemical influences. Incorporating solvent accessibility, residue depth, electrostatic environment, and interaction context may further improve predictive accuracy. Together, these studies establish a residue-diverse MS-based structural proteomics framework integrating chemoselective labeling, cross-linking, and AI-guided prediction to investigate protein accessibility, interactions, and conformational changes in purified proteins and complex biological systems.

SWRM 2026 SW36

Superficially porous particle-based stationary phases for fast LC separation of rare earths paired with direct vacuum ultraviolet detection

***Maria Olds**[1], mlo6134@mavs.uta.edu, Reza Salehi[1], Saba Aslani[1], Annika Dombrowski[2], Daniel W. Armstrong[1]. (1) Chemistry, The University of Texas at Arlington, Arlington, Texas, United States(2) VUV Analytics Inc, Cedar Park, Texas, United States*

Rare earth elements (REEs; lanthanides plus yttrium and scandium) are essential in high-technology materials, permanent magnets, catalysts, phosphors, and emerging energy and biomedical applications, driving a sustained demand for analytical methods that can both separate and quantify individual REEs in complex matrices with high selectivity, reasonable detection limits, and practical robustness. Due to the trivalent lanthanides having very similar ionic radii and coordination chemistry, chromatographic methods – particularly high- and ultra-high performance liquid chromatography (HPLC/UHPLC) and ion chromatography (IC) – have become central tools for REE analysis, often coupled to sensitive detection techniques such as UV–Vis spectrophotometry, fluorescence,

inductively coupled plasma–optical emission spectrometry/mass spectrometry (ICP-OES/MS), and radiometric detection. Further, the weak and narrow f-f absorption bands of REEs require the usage of post-column derivatization, increasing system dead volume and precluding spectroscopic characterization. Development and characterization of functionalized fully- and superficially- porous particles used as stationary phases for the chromatographic separation of REEs was conducted, with capabilities of baseline-resolution of the lanthanides in under 10 minutes, retention time precision demonstrated by replicate analyses, and continuous spectral information provided by a recently developed vacuum-ultraviolet (VUV) detector. Direct spectral data obtained from VUV detection provides both qualitative characterization for identification and the potential for deconvolution of co-eluting peaks for enhanced quantitative capabilities, and does not require post-column reagents. Method optimization, analysis of calibration curves and estimation of limits of detection (LODs), and analysis of real-world samples will also be discussed.

SWRM 2026 SW37

Chemometric visualization of mixed-mode chromatographic selectivity induced by kosmotropic and chaotropic ions

***Siddharth Jaya Sajeevan J**, sjj7510@mavs.uta.edu, Daniel W. Armstrong. University of Texas at Arlington Research Institute, Fort Worth, Texas, United States*

Mixed-mode/hydrophilic interaction liquid chromatography (HILIC) provides multiple retention mechanisms that can be exploited to alter chromatographic selectivity. However, the effects of mobile-phase ions on these interactions across different stationary-phase chemistries remain difficult to predict. Here, kosmotropic and chaotropic salt ions were systematically evaluated on eight stationary phases using 14 probe analytes representing eight chromatographic interactions. Retention data obtained with five mobile-phase additives were analyzed using hierarchical clustering and principal component analysis to identify conditions producing the greatest selectivity differences. Changing only the mobile-phase additive while maintaining all other chromatographic parameters produced substantial changes in selectivity. The magnitude of these changes varied among stationary phases, and the additive pair producing the greatest selectivity difference depended on stationary-phase chemistry. Electrostatic interactions and shape selectivity were most frequently affected. The practical utility of this approach was demonstrated using biologically relevant dipeptides and stimulant drugs, where additive-induced selectivity improved challenging separations. When baseline resolution was not achieved, derivative spectrum chromatogram analysis was used to extract information from overlapping signals. Overall, combining mobile-phase ion selection with chemometric analysis provides a practical strategy for identifying complementary chromatographic conditions and reducing redundant method-development experiments.

SWRM 2026 SW38

Nondestructive means for the reocovery of latent text from historical or damaged documents

***Donald C. Ballew**, donaldballew@my.unt.edu, Emily R. Carrizales, Teresa Golden. Chemistry, University of North Texas College of Science, Denton, Texas, United States*

The recovery of information from charred or destroyed documents is of particular importance to forensic scientists. These documents are delicate and difficult to work with due to exposure at high

temperatures. Also, preservation techniques used to stabilize documents can hinder the recovery process of important data. Here we present research in the recovery of information contained within heat damaged or aged documents by nondestructive means using novel techniques, newly designed instrumentation, and software analysis. First, we have modified standard DSLR cameras, by removing the hot mirror filter to utilize the full spectrum for recovery purposes. Circuits were then developed using LEDs of specific regions in the IR and near-UV spectrum (940 and 395 nm, respectively). A stage and enclosure were manufactured to act as light flags using Musou Black acrylic paint which absorbed 99.4% of all visible wavelengths. This reduced the amount of unwanted stray light from reaching the camera sensor. Use of the LEDs along with camera settings (aperture, shutter speed, and film speed) gave varying contrasts of the text versus the background material. Types of writing implements tested with this setup included; printer ink, pens, and pencils allowing for the capture of latent text from the documents. With the use of software packages, data was analyzed comparing the number of recovered pixels to wavelength.

SWRM 2026 SW39

Monitoring of small-molecule pharmaceutical crystallization in microgravity with miniaturized Raman spectroscopy

Allison L. Stelling[1]*, antistokes@gmail.com, Pavel Matousek*[2]*, Stephen Tuma*[3]*. (1) Chemistry and Biochemistry, The University of Texas at Arlington, Arlington, Texas, United States(2) Rutherford Appleton Laboratory, Didcot, England, United Kingdom(3) Redwire Corporation, Jacksonville, Florida, United States*

The crystalline form of a small-molecule active pharmaceutical ingredient directly impacts its physicochemical charactoristics including solubility, dissolution rate, bioavailability, and long-term stability; with significant regulatory and commercial consequences. Crystallizations on Earth suffer from the convective forces of gravity, and a body of work has illustrated how performing crystallizations in microgravity aboard the International Space Station results in higher crystal quality and aids in the discovery of novel crystalline forms. Raman spectroscopy and X-ray powder diffraction are well-established terrestrial tools for polymorph detection and in-situ monitoring of the crystallization process. Translating these analytical capabilities to a microgravity environment, where such process control is even more imparitive, requires overcoming stringent spaceflight constraints on instrument mass, volume, power consumption, and mechanical robustness for the instrumentation. We present the adaptation and integration of a miniaturized Raman spectroscopic system within the Pharmaceutical In-space Laboratory Biocrystal Optimization eXperiment Small Molecule Accelerated Laboratory for Structure (PIL-BOX SMALS), a platform designed and built by Redwire specifically for the crystallization of small organic molecules aboard the International Space Station (ISS). Unlike protein crystallization systems, the PIL-BOX SMALS targets small-molecule pharmaceuticals, a compound class where polymorphism is a well-documented and commercially significant phenomenon. The integrated Raman system enables in-situ, real-time spectroscopic monitoring of crystallization events within a 0.3 mL reaction chamber under microgravity conditions, providing polymorph identification at the point of crystal formation rather than post-return to terrestrial laboratories. Analytical performance of the miniaturized system is presented alongside crystallization data from PIL missions conducted aboard the ISS. Results demonstrate the ability to discriminate polymorphic forms in situ under microgravity, representing a meaningful extension of established pharmaceutical Raman methodology to a uniquely challenging analytical environment. Implications for polymorph discovery, real-time process monitoring, and the development of analytical methods for in-space pharmaceutical manufacturing are discussed.

SWRM 2026 SW40

Chemistry meets art: Investigating solvent dynamics and temperature-dependent solubility of shellac for art conservation

Anthony Vo[1]*, axv223@SHSU.EDU, Adrian Villalta-Cerdas*[1]*, Gregory D. Smith*[2]*. (1) Chemistry, Sam Houston State University College of Science & Engineering Technology, Huntsville, Texas, United States(2) Conservation Science Lab, Indianapolis Museum of Art Galleries, Indianapolis, Indiana, United States*

Understanding how varnishes interact with solvents is essential for developing safe and effective approaches to the conservation of artworks. Shellac, a natural resin widely used as a coating and varnish, exhibits complex solubility behavior due to its heterogeneous chemical composition. This ongoing study investigates the influence of temperature on the solubility of shellac in two binary solvent systems: n-hexane–isopropyl alcohol and cyclohexane–2-butanone.
These solvent combinations were selected to examine how changes in solvent composition, polarity, and temperature affect shellac dissolution. Controlled experiments are being conducted at different temperatures and solvent ratios to characterize the conditions under which shellac dissolves most effectively. The study also considers whether temperature alters the relative contributions of each solvent in the mixtures during dissolution.
By comparing the behavior of shellac in mixtures containing solvents with contrasting chemical properties, this research seeks to improve the understanding of solvent–resin interactions relevant to varnish removal and surface cleaning. The findings may help inform the selection of solvent systems that provide sufficient solubility while reducing unnecessary exposure of artworks to aggressive solvents.

SWRM 2026 SW41 - Withdrawn

SWRM 2026 SW42

Influence of poly(3,4-ethylenedioxythiophene):poly(styrenesulfonate) (PEDOT:PSS) in organic electrochemical sensor channel

Javier Soliz-Martinez[1,2]*, javier.soliz01@utrgv.edu, Megha Shinde*[2]*, Abijeet Mehta*[2]*, Gyu Leem*[1]*. (1) Department of Mechanical Engineering, University of Texas Rio Grande Valley, Edinburg, Texas, United States(2) Department of Health & Biomedical Sciences, University of Texas Rio Grande Valley, Brownsville, Texas, United States*

Organic electro chemical transistor (OECTs) are three-terminal devices with a gate, source, and drain, where the source and drain are connected by a polymeric channel material, wherein the gate interacts with the channel through an electrolyte which allows ions to move in response to an applied voltage. OECTs are useful in bioelectronics since they operate at low voltages, work well in aqueous environments, and can amplify small ionic or biological signals into measurable electronic signals which makes them promise for wearable sensors, point-of-care diagnostics, and other biomedical applications. Here, we report on the fabrication and electrochemical characterization of a screen-printed OECT incorporating a poly(3,4-ethylenedioxythiophene): polystyrene sulfonate (PEDOT:PSS)

channel and evaluating its performance toward biosensing applications. The device exhibited well-defined gate-dependent output and transfer characteristics, with a transconductance exceeding 3 mS, demonstrating effective conversion of ionic gating into amplified drain-current modulation. Electrochemical characterization further confirmed the interfacial and charge-transport properties of the device. Cyclic voltammetry in ferricyanide over scan rates of 10–100 mV s-1 showed systematic changes in peak current with scan rate, with peak-current dependence on the square root of scan rate consistent with diffusion-controlled electrochemical behavior. Importantly, the OECT displayed measurable dose-dependent drain-current modulation as the H2O2:PBS ratio was varied, demonstrating sensitivity to changes in the chemical environment. The present study will improve device performance by identifying best channel conditions for biosensing devices.

SWRM 2026 SW43

Leveraging high molar mass block copolymers in salogels for thermal energy storage materials

Kevin Nguyen[1]*, kn702202@gmail.com, Ashik Abedin*[2]*, Emily Pentzer*[1]*, Svetlana A. Sukhishvili*[2]*. (1) CHEM, Texas A&M University System, College Station, Texas, United States(2) MSEN, Texas A&M University System, College Station, Texas, United States*

Energy storage technologies that integrate polymers with inorganic materials represent a promising pathway towards scalable thermal energy storage (TES) materials. Specifically, inorganic salt hydrates (ISHs) boast high thermal capacity and nonflammability at a feasible price but often leak out of containers and phase separate past a certain temperature, limiting manufacturing flexibility. By tailoring polymer chemistry and architecture, polymer-inorganic hybrid systems can serve as new TES materials and overcome ISH processing constraints while maintaining or enhancing their heat capacity. This work investigates a polymer-inorganic hybrid system to make solid-liquid phase change materials (PCMs) using lithium nitrate trihydrate (LNH) as the ISH. The hypothesis is that polymers with controlled architecture and tailored functionality entangle together via hydrogen bonding interactions and stabilize LNH as a solid past its melting point to store more heat.
Controlled radical polymerization techniques are employed to prepare multi-arm polymers of defined molar mass and physical properties to a certain extent. Amphiphilic star block copolymers (BCPs) are synthesized to have hydrogen-bonding interactions with water in LNH and physically gelate it, resulting in a class of TES PCMs called “salogels.” Furthermore, this work establishes a novel synthetic route to obtain a uniform distribution of higher-molar mass BCPs of two differing monomer classes. By systematically tuning the composition, number of arms, as well as molar mass, these BCPs can further maximize the threshold of LNH’s heat storage capacity, and other ISHs in the future for a more diverse collection of TES PCMs.

SWRM 2026 SW44

Improving light confinement in hydrogel optical fibers using absorbing molecules

Sagor Biswas*, sagor.biswas@utdallas.edu, Zihao Ou. The University of Texas at Dallas, Richardson, Texas, United States*

Hydrogel optical fibers have attracted significant interest for biomedical sensing and imaging applications because of their biocompatibility, flexibility, and high water content. However, their optical performance is often limited by the relatively low refractive indices achievable in hydrogel materials, a consequence of the large water fraction intrinsic to their composition. This constraint reduces light confinement and increases propagation loss. To address this challenge, we introduce strongly absorbing molecules into the fiber core. Through the Kramers-Kronig relationships, these molecules increase the refractive index of the hydrogel at selected wavelengths, thereby enhancing optical confinement without substantially altering the hydrogel structure. Experimental measurements demonstrate that fibers with doped cores exhibit significantly lower attenuation coefficients than undoped control fibers of comparable dimensions. These results highlight the potential of absorber-assisted refractive index engineering as a simple and versatile strategy for reducing loss and improving light guidance in hydrogel waveguides.

SWRM 2026 SW45

Polymeric micelles for theranostic applications: Impact of polymer architecture on doxorubicin and $MnFe_2O_4$ encapsulation

***Esmail Qasimi**, exq230005@utdallas.edu. Chemistry and Biochemistry, The University of Texas at Dallas, Richardson, Texas, United States*

Polymeric micelles have emerged as promising nanocarriers for the co-delivery of chemotherapeutic drugs and magnetic nanoparticles (MNPs) owing to their tunable physicochemical properties and enhanced colloidal stability. In this study, the influence of polymer architecture on the encapsulation of doxorubicin (DOX) and manganese ferrite ($MnFe_2O_4$) magnetic nanoparticles was investigated using two amphiphilic diblock copolymers: poly(ethylene glycol)-block-poly(ε-caprolactone) (PEG-b-PCL) and poly(ethylene glycol)-b-poly(N-propyl-N-benzyl-7-oxopane-4-carboxamide) (PEG-b-PBnPyCL). Micelles were prepared by self-assembly of the diblock copolymers in deionized water and were characterized in terms of particle size, polydispersity index, encapsulation efficiency, loading capacity, and colloidal stability.
The results demonstrated that polymer composition significantly affected both drug and nanoparticle loading. The PEG-b-PBnPyCL copolymer exhibited enhanced DOX encapsulation compared with PEG-b-PCL, which can be attributed to stronger hydrophobic and π-π stacking between the aromatic moieties of the polymer and the anthracycline structure of DOX. Furthermore, the modified polymer provided improved incorporation of $MnFe_2O_4$ nanoparticles within the micellar core, resulting in higher nanoparticle loading and improved colloidal stability. Dynamic light scattering measurements indicated that both formulations formed micelles smaller than 100 nm, which are suitable for passive tumor targeting; however, the functionalized polymer showed superior stability under physiological conditions, maintaining particle size and dispersity over prolonged incubation.
These findings highlight the critical role of polymer structure in governing the loading efficiency and stability of multifunctional micellar systems. The incorporation of aromatic functional groups within the polymeric core represents an effective strategy for improving the co-encapsulation of hydrophobic drugs and magnetic nanoparticles, thereby enhancing the potential of polymeric micelles as promising theranostic nanocarriers for future cancer therapy applications.

SWRM 2026 SW46

In-vitro studies on microplastic removal from human blood products using organic plant-based polysaccharides and hydrogels

***Addison Anderson**, addisonanderson@yahoo.com, Jaci Youngblood, Rajani Srinivasan. Department of Chemistry, Geosciences, and Physics, Tarleton State University, Stephenville, Texas, United States*

Microplastics (0.1–5,000 µm) and nanoplastics (1–100 nm) are emerging environmental and health concerns that accumulate in various human body systems, including cardiac and brain tissue, as well as neonatal vasculature. Research links microplastic contamination to increased risks of cardiac ischemia, myocardial infarction, cerebrovascular accidents, and certain cancers, such as colon cancer. Prior studies have identified effective microplastic removal from human blood using fenugreek, okra, and tamarind polymers, as well as solid polymers, polymer solutions, and fruit biomass. This study investigates and compares the effectiveness of tamarind polysaccharide hydrogels using alternate methods and contact times. Blood samples were treated with deionized water, EDTA, and 1% KOH solution, and then hemocytometer analysis was performed to identify microplastics before and after hydrogel treatment. These samples were then subjected to experimentation using two alternative methods: gravity filtration and direct contact in solution, with various hydrogel sample sizes.

SWRM 2026 SW47

Telechelic all-*cis* polycyclooctene via catalytic stereoretentive ROMP for the synthesis of polylactide-based ABA triblock copolymers

*Jake Nicholson, **Antoine Gravet**, antoine.gravet@tamu.edu, Quentin Michaudel. Chemistry, Texas A&M University System, College Station, Texas, United States*

Controlling polymer stereochemistry remains a great challenge despite its outsized influence on material properties. For example, the *cis* or *trans* geometries of the repeating alkenes largely dictate the crystallinity of polybutadiene and polyisoprene. Recent progress in stereoselective olefin metathesis has enabled access to precise stereodefined unsaturated polymers containing polar functional groups via stereoselective acyclic diene metathesis (ADMET) and ring-opening metathesis polymerization (ROMP). However, these processes require relatively high loadings of costly ruthenium catalyst, that would potentially prevent further industrial implementation. This presentation will discuss the synthesis of *cis*-polycyclooctene (PCOE) via catalytic stereoretentive ROMP of commercially available *cis*-cyclooctene (*cis*-COE) using a chain-transfer agent to access well-defined polyalkenamers with >99% *cis* contents and high molar masses, as well as deliberate introduction of functional chain ends. Subsequent post-polymerization modification of the chain ends delivered ABA triblock copolymers via ring opening polymerization of D,L-lactide and provided poly(lactic acid) (PLA) with a rubbery middle block of tunable length. The impact of this architecture over the thermomechanical performance of PLA will be highlighted.

SWRM 2026 SW48

Synthesis and optimization of thermoresponsive polymers for reducing building energy consumption

Hansani Sandamali Amarasuriya Amarasuriyage[1], *hsa210009@utdallas.edu, Marius S. Popa*[1], *Chengqian Huang*[2], *Mihaela C. Stefan*[1], *Shuang Cui*[2]. *(1) Chemistry and Biochemistry, The University of Texas at Dallas, Richardson, Texas, United States(2) Mechanical Engineering, The University of Texas at Dallas, Richardson, Texas, United States*

Buildings consume a large amount of energy for cooling and dehumidification. Growing demand for cooling and humidity control, especially in hot and humid areas, highlights the need for new materials and technologies to reduce this energy crisis. Thermoresponsive polymers (TRPs) are smart, versatile materials that change their properties upon heating and can be used in smart windows and as desiccants for energy-efficient thermal management and dehumidification. However, achieving application-specific control over transition temperature, transition sensitivity, reversibility, and water interactions remains challenging. This work focuses on poly(diethylene glycol methyl ether methacrylate) (PDEGMA), poly(triethylene glycol methyl ether acrylate) (PTEGA), and their P(DEGMA-*co*-TEGA) copolymers. Reversible addition-fragmentation chain-transfer polymerization was used to synthesize homopolymers and copolymers with controlled compositions and well-defined molecular weight distributions. This synthetic control will improve structural uniformity, sharpness and reproducibility of the transition behaviors. This copolymer combination can tune the lower critical solution temperature (LCST), hydrophilic-hydrophobic balance and resulting thermoresponsive behavior. The oligo(ethylene glycol) side chains provide hydrophilicity and water uptake for humidity-control applications. The polymers were characterized to evaluate composition, molecular properties, thermal stability, and thermoresponsive behavior. Varying the copolymer composition shifted the LCST from 29 °C to 60 °C. Polymers with LCST values around 29-40 °C are promising for smart-window applications because this range is close to building window operating temperatures. Above LCST, these polymers can switch their optical response reducing solar transmission and minimizing unwanted heat gain. Compositions with transitions around 45-60 °C are suitable for dehumidification and low-temperature regeneration because they remain hydrophilic below the LCST and promote moisture absorption under ambient conditions, while heating above the LCST promotes release of absorbed water at relatively low temperatures. The materials showed reversible and cyclable thermoresponsive behavior over repeated heating and cooling cycles. In summary, temperature-responsive switching, reversibility and controlled hydration/dehydration behavior can help relieve intensive energy demand for indoor air conditioning and for humidity management.

SWRM 2026 SW49

Efficient recovery of valuable chemicals from Kraft black liquor using thermo-responsive polymer absorbents

Leshi Feng, *lxf220001@utdallas.edu, Yuvraj Dangat, Krishna Dasari, Chengqian Huang, Hedieh Torabifard, Shuang Cui. The University of Texas at Dallas, Richardson, Texas, United States*

Chemical recovery from industrial wastewater is critical to improving resource efficiency and reducing environmental impacts in the pulp and paper industry. The Kraft pulping process generates a large volume of black liquor (BL), which contains valuable inorganic chemicals such as sodium hydroxide, sodium sulfide, and sodium carbonate, along with organic compounds such as lignin. Conventional recovery relies on multi-effect evaporation followed by combustion, which requires high thermal energy to overcome the latent heat of vaporizing water, leading to significant CO2 emissions and waste of valuable organic compounds. Therefore, alternative separation technologies are needed for efficient chemical recovery with reduced energy consumption.
In this work, we aim to recover valuable minerals from BL by selectively separating its components using thermo-responsive polymer (TRP) absorbents. The key contribution of this study is the

development of a lower critical solution temperature (LCST)-based separation strategy that enables selective recovery of inorganic salts without vaporization of water. Below the LCST (~37°C), the TRP absorbent is hydrophilic and absorbs the aqueous solution from BL while rejecting macromolecular organic compounds such as lignin. Above the LCST, the absorbent becomes relatively hydrophobic and releases the absorbed solution containing salts in liquid form. This LCST behavior enables the separation of inorganic salts and lignin, resulting in a salt-concentrated solution for potential reuse in the Kraft pulping process.
Our results demonstrate effective separation performance for both synthetic and real BL, with lignin removal rates above 70% and 50%, respectively. The absorbent exhibited excellent durability over 10 cycles, with less than a 5% loss in lignin removal rate. To further enhance lignin removal, a sequential treatment strategy was implemented using fresh absorbent after each cycle. The removal efficiency reached 87% after four cycles for synthetic BL and 86% after three cycles for real BL, approaching the performance of membrane-based filtration (~90%). In summary, our TRP absorbent-based approach eliminates pressure-driven operation and reduces the substantial thermal energy required by conventional evaporation-based recovery, offering a pathway toward reduced energy consumption and lower carbon emissions.

SWRM 2026 SW50

Self-adaptive thermal regulator for dynamic heating and cooling through coupled thermal energy storage and solar modulation

Jiaxiang Wen[1]*, dal716699@utdallas.edu, Bernadette Magalindan*[1]*, Lyu Zhou*[1,2,3]*, Chengqian Huang*[1]*, Shuang Cui*[1]*. (1) Mechanical engineering, The University of Texas at Dallas, Richardson, Texas, United States(2) Electrical and Computer Engineering, Texas Tech University, Lubbock, Texas, United States(3) National Wind Institute, Texas Tech University, Lubbock, Texas, United States*

Indoor climate control accounts for nearly half of global building energy consumption and can place substantial stress on power grids under extreme weather conditions. Developing energy-efficient thermoregulation technologies is therefore critical for reducing building energy demand and improving infrastructure resilience. While conventional insulation materials function as static thermal barriers, they are unable to adapt to changing environmental conditions and seasonal thermal demands. This work reports a heterostructure adaptable optical–thermal dual-mode thermoregulator (AOT-DTR) that integrates a thermo-responsive poly(N-isopropylacrylamide) (PNIPAM)-based top layer with a solar-absorptive phase change material (PCM)-based underlayer to achieve self-adaptive heating and cooling. The PNIPAM-based layer dynamically modulates solar energy utilization in response to ambient temperature, switching from a heating mode with a solar absorptivity of 86.4 % (below the critical solution temperature [LCST]) to a cooling mode with a solar reflectivity of 75.1 % (above the LCST). Meanwhile, the PCM-based underlayer provides thermal buffering through latent heat storage, exhibiting a melting enthalpy of up to 126.5 J/g with a melting temperature of 33 °C. This stored thermal energy can be released for passive nighttime heating, extending the thermal regulation capability beyond daytime operation. By coupling thermo-responsive solar modulation with latent heat storage, the heterostructure AOT-DTR achieves substantially enhanced thermal regulation performance compared with systems relying on either mechanism alone. More importantly, by strategically pairing the LCST of the PNIPAM layer for solar modulation with the solid–liquid phase change temperature (PCT) of PCM, our modeling based on a subtropical climate (Dallas, TX) reveals that the utilization efficiency of latent heat storage can be maximized to achieve all-season thermal regulation. This synergistic design establishes a self-adaptive thermal regulation strategy that integrates solar modulation and thermal energy storage within a single material platform, providing a

promising pathway toward sustainable and energy-efficient building envelopes and next-generation passive thermal management technologies.

SWRM 2026 SW51

Acid-promoted ring opening metathesis polymerization to access main-chain pyridine-containing cationic polymers

***Vaishak Bhat**, vaishak.bhat@tamu.edu, Quentin Michaudel. Chemistry, Texas A&M University, College Station, Texas, United States*

With the increased threats posed by antibiotic-resistant bacteria, the exploration of alternative strategies to design antibacterial treatments is crucial. Cationic polymers, inspired by host-defense peptides, have been shown to disrupt bacterial membranes in a non-specific manner, inducing cell lysis without causing resistance over time. Modular, well-controlled synthesis of these polymers can enable systematic tuning of structural parameters to achieve potent antibiotic activity. Among these structural parameters, the placement of cationic charge with respect to the polymer backbone, has been identified to influence the antibacterial activity of cationic polymers. Specifically, main-chain cationic polymers can have superior bioactivity when compared to the side-chain variants due to a potential increase in cation stability and ability to adopt favorable conformations for cooperative binding. This presentation will introduce a strategy to access cationic polymers derived from pyridine units incorporated directly in the main chain. First, the synthesis of pyrido[2,3-*b*]norbornadiene monomers for ring opening metathesis polymerization (ROMP) will be presented, as well as the challenges caused by the Lewis basic nitrogen in the ROMP process. Recognition of the deleterious nitrogen coordination to the propagating Ru-carbene prompted the development of acidic conditions to perform ROMP and promote controlled polymerization with predictable molar masses and narrow dispersities. Finally, diversification of the pyridine core via nitrogen quaternization affording cationic polymers with tunable hydrophobicity-to-charge ratios will be highlighted.

SWRM 2026 SW52

Non-native square packing and structural arrangement of ultrahigh molecular weight diblock copolymer from one-step solvent vapor annealing

***Yuheng Wang**[1], yuhengwang@my.unt.edu, aikhila Joy[1], Natalia Hnatchuk[1], Tejal Pawale[1], Tosin Orgunrinala[2], Vasanta Gurung[1], Diana Berman[1], Ying Bao[2], Xiao Li[1]. (1) Department of Material Science and Engineering, University of North Texas College of Engineering, Denton, Texas, United States(2) Department of Chemistry, Western Washington University College of Science and Engineering, Bellingham, Washington, United States*

Block copolymer (BCP) self-assembly provides a promising approach for fabricating periodic nanostructures for nanolithography. However, simple diblock copolymers generally favor thermodynamically stable morphologies such as hexagonally packed cylinders, making square-packed structures difficult to achieve. In this work, ultrahigh-molecular-weight (UHMW) PS-b-PMMA was used to form square-packed cylindrical arrays through a one-step solvent vapor annealing (SVA) process. By comparing solvents with different affinities and vapor pressures, trichloroethylene (TCE) was identified as an effective solvent for producing vertically oriented PMMA cylinders with square packing. Based on this solvent condition, film thickness and annealing time were further varied to

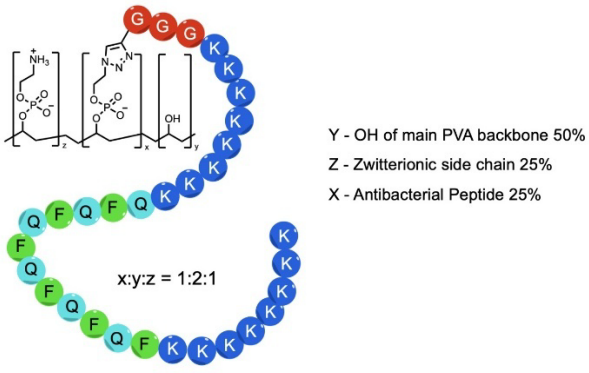
determine the processing window for square-array formation, with well-ordered structures obtained at approximately 0.5–0.75 L_0 after 40–50 min of annealing. Using this optimized square-packed structure as a basis, PMMA homopolymer was introduced to further improve structural ordering. The optimized polymer structure was subsequently converted into an inorganic nanostructure through sequential infiltration synthesis (SIS), where selective infiltration of the PMMA domains produced Al_2O_3 cylinders while preserving the original square arrangement. These results demonstrate a simple bottom-up strategy for controlling square-packed structures in diblock copolymer thin films and their subsequent conversion into inorganic nanostructures for potential nanolithography applications.

SWRM 2026 SW53

Zwitterionic PVA-peptide conjugate polymer (pEtN-PVA-Pep): Synthesis, characterization, and evaluation for biomedical applications with emphasis on biofilm inhibition

Md Tareque Hassan Mukut, *mxm9062@mavs.uta.edu. Chemistry, The University of Texas at Arlington, Arlington, Texas, United States*

The design of antimicrobial materials heavily depends on controlling biofilm formation, as biofilms contribute to both bacterial resistance and chronic infections. In our study, we synthesized phospho-azide-containing polyvinyl alcohol (pN_3-PVA) and then functionalized the pN_3-PVA with an antimicrobial peptide (Pep) followed by incorporation of zwitterionic properties. This will generate a bioactive material with zwitterionic properties, designed to prevent biofilm formation.
We labeled 50% of the hydroxyl groups of polyvinyl alcohol (PVA) with phospho-azide side chains and then 50% of the azide groups of pN_3-PVA labeled with the antimicrobial peptides (Pep) using Cu-catalyzed click chemistry, facilitating its integration onto the polymer. Following this, the remaining azide groups reduced to amino groups, introducing zwitterionic characteristics into the material. Analytical methods like UV-Vis, LC-MS, FTIR, NMR, and ICPMS were used to confirm how well the functionalization works.
We are evaluating the antimicrobial and biofilm-preventing properties of the modified material. The assessment involved biofilm-forming bacterial strains like *Escherichia coli* and *Staphylococcus aureus* with a focus on their impact on biofilm development, inhibition, and dispersal by biofilm assay. Additionally, scanning electron microscopy will be used to visualize biofilm architecture and bacterial adhesion on treated surfaces. This approach paves the way for the development of innovative biocompatible and biodegradable materials with dual applications in biomedicine and environmental research, specifically for antibacterial and anti-biofouling purposes.



SWRM 2026 SW54

Dual porphyrin-based two-dimensional π-extended covalent organic frameworks as photoactive materials

***Jishnu Chevayil Vasudevan**, cvjishnu98@gmail.com, Hong Wang. Chemistry, University of North Texas, Denton, Texas, United States*

π-Extended covalent organic frameworks (COFs) with customized electronic properties will give rise to novel materials with promising photoelectric properties. Herein we introduce a new family of two-dimensional (2D) π-extended porphyrin-based COFs , comprised of both porphyrin donor and acceptor units. These frameworks are synthesized by a [4+2] imide condensation reaction from a D_{2h} symmetrical *β*-functionalized *π*-extended porphyrin and D_{4h}-symmetrical 5,10,15,20-tetrakis(4-aminophenyl)porphyrin. In contrast to common porphyrin-based COFs, most of which employ *meso*-functionalized porphyrins, in our study we use *β*-functionalized porphyrins, which enable enhanced *π*-conjugation and electron delocalization within the frameworks. Structural studies have shown that the material possesses high crystallinity with a staggered AB stacking and porosity, which was characterized by BET surface area measurements. Thanks to the presence of *π*-conjugated backbone and *π*-*π* stacking interactions, these frameworks show a narrow optical bandgap. COFs derived from both free base and metalated porphyrin have been prepared and their optoelectronic properties were measured using various characterization techniques such as powder XRD, SEM , BET measurement, ^{13}C NMR spectroscopy and solid UV-vis absorption spectroscopy. THz and four-probe conductivity measurements revealed that both COFs exhibit long-lived photoconductivity and exceptionally high electrical conductivity.

SWRM 2026 SW55 – Withdrawn

SWRM 2026 SW56

Advanced material platforms of conductive polymer with ionic liquids for stretchable and flexible electronics

***Fatima Abbas**, fabbas@ualr.edu, Krishna KC, Noureen Siraj. University of Arkansas at Little Rock, Little Rock, Arkansas, United States*

Influenced by the hard–soft acid–base (HSAB) theory, different hard–soft cations and anions are used to investigate the counterion effects of ionic liquids (ILs) on electrical and mechanical characteristics of the conductive polymer commonly known as (PEDOT:PSS) and IL free-standing films. Two protic ILs, i.e., methylimidazolium dicyanamide and imidazolium dicyanamide , are synthesized and characterized for the first time. Six ions ranging from hard to soft (cations as protic imisazolium, protic methylimidazolium and ethyl methylimidazolium, and anions as tetrafluoroborate , tetracyanoborate , and dicynamide) are studied to investigate their impact on advancing conductive flexible films. Herein, PEDOT-PSS with protic ILs exhibited tremendous increase in electrical conductivity of 2730 S/cm and 3547 S/cm, respectively. Both protic ILs improved external strain of up to 11%, surpassing aprotic IL (7%) and pristine PEDOT:PSS (<4%). This study revealed that ILs containing hard cation and soft anion exhibited superior conductivity and flexibility in the composite films.

SWRM 2026 SW57

Studies of the anionic ring-opening polymerization of lipoates

Leonel Garcia[1]*, leonelg@smu.edu, Amman Nadeem*[2]*, Scott M. Grayson*[2]*, Nicolay V. Tsarevsky*[1]*. (1) Department of Chemistry, Southern Methodist University, Dallas, Texas, United States(2) School of Science & Engineering, Tulane University, New Orleans, Louisiana, United States*

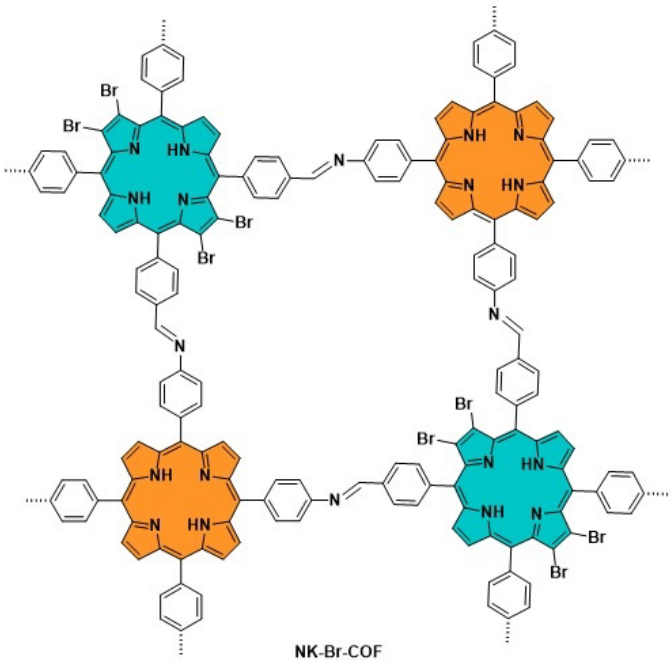
Ethyl lipoate, a 1,2-dithiolane-containing monomer, can undergo ring-opening polymerization under radical, anionic, and cationic conditions to afford reductively cleavable materials. Herein, it is shown that a moderate degree of polymerization control was achieved in anionic polymerizations conducted in the presence of cations that bind to the thiolate-type propagating chains. Polymerizations were conducted in *N,N*-dimethylacetamide, *N,N*-dimethylformamide, and acetone at 25 ^{o}C. MALDI-ToF analysis of the isolated polymers was utilized to elucidate the nature of the polymer chain ends. Anionic polymerizations were also conducted in the presence of isosorbide dilipoate, a cyclic disulfide crosslinker, to study the formation of branched and eventually crosslinked polymers. The reductive degradation of all synthesized polymers (linear, branched, and network) was accomplished with tributylphosphine. The photochemical degradation of the polymers was studied as well.

SWRM 2026 SW58

β-tetra-brominated functional porphyrinic covalent organic framework

Nikhil Kumar*, nikhilkumar2@my.unt.edu, Hong Wang. Chemistry, University of North Texas, Denton, Texas, United States*

Covalent organic frameworks(COFs) based on porphyrins have long range order, persistent porosity, and the capacity to harvest and interact with light. The primary methods of tuning porphyrin based porous materials have been metalation and meso-aryl group modification. In contrast, functionalization of the *β*-pyrrole positions, an established strategy in porphyrin chemistry, has received far less attention within these materials. Here, we present NK-Br-COF, an imine linked full porphyrinic COF with two porphyrin based building units: 5,10,15,20-tetrakis(4-aminophenyl)porphyrin(TAPP) and *β*-tetrabrominated tetrkis(4-formylphenyl) porphyrin (TFPP-t-Br). The incorporation of four bromine atoms at the *β*-positions of the porphyrin-aldehyde linker provides an electron withdrawing and heavy atom substitution in the COF skeleton, which functions as an optoelectronic modifier (red shift) and reagent for post-synthetic cross coupling (Suzuki-Miyaura reaction). Our goal with this *β*-brominated porphyrin COF is to investigate whether the presence of bromine atoms at the *β*-positions of the porphyrin linker improves intersystem crossing efficiency through the heavy atom effect, promoting triplet state and singlet oxygen formation, a well-known mechanism in molecular *β*-halogenated porphyrins. This makes NK-Br-COF fully porphyrin COF with the potential to act as a photosensitiser via the heavy atom effect.[1,2]



SWRM 2026 SW59

ROS-responsive gold nanoparticles for targeted methotrexate delivery

Niloofar Valizadeh Dana*, niloo.valizadeh_dana@okstate.edu, Elaina HEath, Jimmie D. Weaver, Yolanda Vasquez. Chemistry, Oklahoma State University The College of Arts and Sciences, Stillwater, Oklahoma, United States*

Rheumatoid arthritis is a chronic inflammatory disease in which elevated levels of reactive oxygen species (ROS) contribute to an oxidative environment in affected joints. This project aims to use that environment as a trigger for a responsive drug-delivery system based on gold nanoparticles. The system incorporates a thioketal (TK) linker, which is sensitive to ROS, and polyethylene glycol (PEG), which acts as a spacer and provides a thiol group for attachment to the gold surface. Methotrexate is the intended therapeutic payload for the final system. Two strategies were investigated for the synthesis of the TK–PEG conjugate. ^1H NMR characterization revealed signals corresponding to both TK and PEG, confirming the successful formation of TK–NH–PEG–SH. The conjugate was subsequently attached to citrate-stabilized gold nanoparticles and characterized using UV–Vis spectroscopy, dynamic light scattering (DLS), and zeta-potential measurements. In addition, ATR-FTIR spectroscopy confirmed the retention of the characteristic functional groups following conjugation. After successful MTX conjugation, the final Au–S–PEG–NH–TK–MTX system will be tested in RAW cells to evaluate its cytotoxicity and cellular effects, followed by further biological assays to assess its performance as a ROS-responsive drug-delivery platform.

SWRM 2026 SW60

Viscoelastic characterization of pore engineered hydrazone-linked covalent organic framework films

***Chamila S B Rajapaksha W M**, cxr230002@utdallas.edu, Milinda C. Senarathna, Ronald Smaldone. Chemistry and Biochemistry, The University of Texas at Dallas, Richardson, Texas, United States*

Covalent organic frameworks (COFs) with hydrazone linkages are a promising class of materials due to their excellent physico-chemical properties. However, lack of suitable processing techniques limits their applications. In this study we comparatively discuss three different approaches to process hydrazone linked materials and how the material properties vary with the processing technique and chemical structure. Further we discuss utilization of viscoelastic characterization by nanoindentation as a reliable mechanical property analysis method for covalent organic framework films to address the time-dependent response to loading and avoid over estimation of the moduli values by common time-independent methods. Synthesized COF films exhibit excellent mechanical properties, such as Young's modulus of up to 1 GPa range even after accounting for overestimation factors. This demonstrates the high potential of pore engineered hydrazone COFs as mechanically robust materials.

SWRM 2026 SW61

Acrylate-polyrotaxane double network hydrogels enabled by vat photopolymerization 3D printing

***Gaveshika Rajapaksha**, gxr230000@utdallas.edu, Ronald Smaldone. Chemistry and Biochemistry, The University of Texas at Dallas, Richardson, Texas, United States*

Double-network (DN) hydrogels are widely studied for their enhanced mechanical properties; however, their implementation in vat photopolymerization-based 3D printing remains limited. Here, we report a digital light processing (DLP)-printable DN hydrogel comprising a covalently crosslinked acrylic network interpenetrated with a polyrotaxane-based supramolecular network. The polyrotaxane network (PRH), which is contributed by the cyclodextrin crystalline domains provides an extra energy dissipation mechanisms compared to the traditional DN network hydrogels. These DN gels show a significant improvement in mechanical performance, including high fracture stress and extensibility, and allows the polyrotaxane network to be retained after washing. Additionally, our study shows that DLP printing provides access to otherwise unreachable monomer combinations by suppressing macroscopic phase separation in DN hydrogel systems that fail under traditional thermal polymerization. The polyrotaxane network is preserved within the printed constructs, as confirmed by PXRD and ^{1}H-NMR characterization. Together, this work establishes a general materials design strategy that integrates polyrotaxane chemistry, DN hydrogel mechanics, and vat photopolymerization, opening new avenues for the design of architected tough hydrogels for advanced soft-matter applications.

SWRM 2026 SW62

***In-vivo* plant-based polymers for microplastic removal from pigs**

***Jaci Youngblood**, jaci.youngblood@go.tarleton.edu, Brooke Nevans, Addison Anderson, Rajani Srinivasan. Tarleton State University, Stephenville, Texas, United States*

In 2020, global plastic production reached approximately 367 million metric tons. As these plastics break down through weathering and environmental exposure, they generate microplastics and

nanoplastics that have become a growing environmental and public health concern. These plastic particles have been detected in waterways, drinking water supplies, soils, plants, animals and even the human body. This highlights the widespread nature of plastic pollution and its potential impact on ecosystems and human health. These plastics have been linked to increased risk of vascular plaques and cancer. Prior studies have demonstrated the effectiveness of plant-based polymers for removing plastics from human blood and various water sources. This project demonstrates the effectiveness of the same polymers capturing and removing microplastics from the bloodstream of pig models. The blood samples were treated with EDTA, deionized water, and 1% potassium hydroxide solutions, followed by analysis using a hemocytometer to identify and quantify microplastics in each treatment group.

SWRM 2026 SW63

Visible light induced lignin degradation using Ir(III) polypyridyl complexes coated on metal oxide nanoparticles at room temperature

David M. Martinez[1]*, david.martinez25@utrgv.edu, Andrea Razo*[1]*, Mi-Hyun Lee*[1,2]*, Hye-Young Jang*[2]*, Gyu Leem*[1]*. (1) Department of Mechanical Engineering, The University of Texas Rio Grande Valley College of Engineering and Computer Science, Edinburg, Texas, United States(2) Department of Chemistry, Ajou University, Suwon-si, Gyeonggi-do, Korea (the Republic of)*

Lignin depolymerization is a challenging transformation that can generate valuable aromatic compounds for pharmaceutical, food, and chemical applications. In this work, we report visible light driven photocatalytic C-C/C-O bond cleavage of lignin model compounds (LMCs) using Ir(III) polypyridyl complex (IrP) as a homogeneous photocatalyst and IrP anchored on metal oxide nanoparticles (e.g., TiO2 and SiO2), as a heterogeneous photocatalyst. As part of a two-step fragmentation strategy, this study focuses on the second step following selective oxidation of the secondary benzylic alcohol moiety in lignin. More importantly, this work investigated the elucidation of intermolecular charge transfer between the IrP and phenolic LMCs containing β-O-4 linkages under visible light illumination in acetonitrile solution. The resulting intermolecular charge transfer enabled subsequent cleavage of C-C/C-O bonds in LMCs at room. This approach offers a promising alternative to conventional chemical degradation processes and represents a significant advancement toward controllable C−C/C−O sigma bond cleavage for sustainable lignin valorization and chemical transformations.

SWRM 2026 SW64 - Withdrawn

SWRM 2026 SW65

Harnessing RAFT-based glycopolymers for sustainable heavy metal sequestration

Mahak Chhabra*, mahakchhabra@utexas.edu, Cassandra E. Callmann. Chemistry, The University of Texas at Austin College of Natural Sciences, Austin, Texas, United States*

Rapid industrialisation has emerged as a major contributor to heavy metal pollution, posing a risk not only to human health but also to environmental sustainability. Traditional methods such as filtration,

precipitation, or ion exchange are effective methods to remove metals, but they lack long-term sustainability and reusability. Conversely, glycopolymers are promising candidates for developing sustainable materials due to their environmental friendliness and biodegradability. While polyvalent carboxylates such as EDTA and citrates have been extensively used as chelating agents for heavy metals, the superior binding affinity of glycopolymers indicates factors beyond multivalent interactions.
Our previous work using ROMP-based cation-trapping glycopolymers shows effective reversible sequestration of Cd^{2+} ions in the presence of other competing cations. We hypothesise that steric accessibility, macromolecular conformation, and solubility are integral to binding heavy metals effectively.
As such, the broad goal of this work is to identify molecular determinants to maximise chelation and, further, to make materials that remain soluble at the same time. This will provide insights into structure-function relationships that will help in designing bioinspired sustainable glycopolymers with tunable solubility and metal binding affinity. In this presentation, I will discuss our work on developing soluble RAFT polymers that bind heavy metals with high affinity as a function of structure, and our work on designing next-generation sustainable materials for water remediation and biomedical detoxification.

SWRM 2026 SW66

Anionic effect on the effective saccharide hydrolysis via modified noncovalent interactions to the pore environment

Amena Khatoon*, amenakhatoon@my.unt.edu. Chemistry, University of North Texas, Denton, Texas, United States*

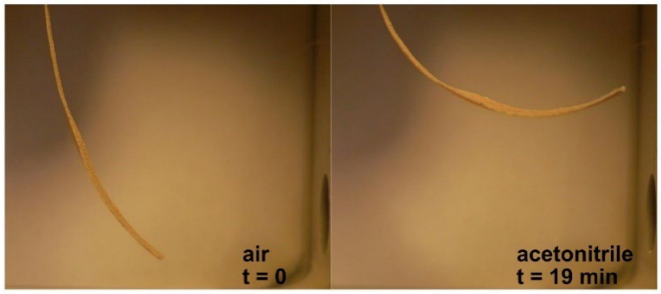
The catalytic depolymerization of lignocellulosic biomass into fermentable sugars remains a central challenge for sustainable biofuel production. Herein, we report the rational design of a functionalized covalent organic framework (COF) that mimics key features of glycoside hydrolases to enable efficient hydrolysis of glycosidic bonds under aqueous conditions. By integrating acidic sites within a confined porous architecture and engineering a synergistic network of hydrophilic and hydrophobic interactions, the COF provides a biomimetic microenvironment that promotes both substrate recognition and catalytic turnover. The resulting material exhibits high structural stability in water and demonstrates exceptional catalytic performance in the hydrolysis of cellobiose and related saccharides. Notably, glucose yields exceeding 90% are achieved under optimized conditions, highlighting the effectiveness of the designed catalytic platform in mimicking enzymatic function. Mechanistic insights suggest that the cooperative interplay between pore confinement, noncovalent interactions, and acid catalysis is critical for enhancing substrate binding and bond activation. This work establishes a versatile strategy for constructing enzyme-inspired COF catalysts and underscores their potential in advancing scalable biomass valorization processes, offering a promising pathway toward sustainable biofuel production and green chemical synthesis.

SWRM 2026 SW67

Actuation of polymer composites driven by the breathing of embedded metal-organic frameworks

***Jacob Baker**, jb79993@utexas.edu, Michael L. Aubrey. Chemistry, The University of Texas at Austin, Austin, Texas, United States*

Embedding flexible metal-organic frameworks, capable of large volume changes or breathing, within polymers has emerged as a means to fabricate actuating devices for applications in soft robotics, biomemetics, and sensors. By varying the density of MOF crystals through the composite thickness a differential stress gradient results as the MOF crystals breath in response to stimuli such as heat, pressure, or guest molecules. The MIL-53 family of flexible frameworks has remained sparingly used compared to other flexible MOFs despite being capable of up to 40% changes in unit cell volume. In this work a novel polymer composite film actuator composed of polyvinyl alcohol and MIL-53(Fe) is fabricated in which the gradient of MOF crystals results in bending a deformation as the crystals swell in response to organic solvent vapors. The actuation is attributed to MIL-53(Fe) through a combination of PXRD and beam bending modeling upon exposure to organic solvent vapors. This work further supports the the use of flexible breathing MOFs to drive actuation in polymer composites with potential for application in a variety of applications.



PVA-MIL-53(Fe) composite actuator. MOF loading is more dense on left side of film, upon exposure to acetonitrile MOF crystals expand and gradient results in net curling motion of clamped beam towards right side. Response to vapors occurs within seconds and is stable over long time periods.

SWRM 2026 SW68

Evaporation-induced assembly of paintable MXene organohydrogels for long-term skin-conformal bioelectronic interfaces

***AAMIR IQBAL**[1,2], aamir@tamu.edu. (1) Department of Chemical Engineering, Texas A&M University, College Station, Texas, United States(2) Empa Swiss Federal labortories for Materials Science & Technology, Dubendorf, Zurich, Switzerland*

Conductive hydrogels are promising interface materials for epidermic electronics in continuous health monitoring and clinical diagnostics. However, their intrinsically fluidic and weakly crosslinked structures hinder the formation of conformal and bioadhesive skin interfaces, typically requiring additional adhesives and insulating substrates that increase interfacial impedance and degrade signal fidelity. Herein, we report substrate-free, on-skin paintable conductive organohydrogels composed of highly conductive and stable $Ti_3C_2T_x$ MXene nanosheets dispersed in a glycerol-water-ethanol solvent mixture, with poly(vinyl alcohol) (PVA) serving as the polymer matrix and tannic acid (TA) as a multifunctional crosslinker. A solvent volatilization-driven gelation strategy transforms the liquid ink into a soft, self-supporting gel within 2 minutes after brushing or painting onto skin. Progressive evaporation induces multiple hydrogen bonding interactions among MXene surface terminations, PVA, and TA, while simultaneously promoting the close packing and percolation of highly crystalline $Ti_3C_2T_x$ nanosheets, yielding a mechanically compliant yet electrically continuous network. The in-situ

formed organohydrogel establishes intimate, gap-free epidermal contact with intrinsic adhesion, eliminating the need for external fixation. As a result, the organohydrogel electrode significantly suppresses motion-induced artifacts, interfacial impedance, and noise under both static and dynamic conditions, compared to conventional hydrogel electrodes. For long-term electrophysiological monitoring, the highly crystalline $Ti_3C_2T_x$ MXene organohydrogel enables stable, high-fidelity electrocardiogram (ECG) recording for over one month with enhanced signal-to-noise ratio relative to conventional MXene hydrogels and commercial gel electrodes. This study establishes an evaporation-assembled, user-adaptive, and long-term stable organohydrogel platform that integrates paintable processability, conformal biointerfaces, and durable electrical performance for next-generation wearable bioelectronics.

SWRM 2026 SW69

TEMPO-functionalized copolymers for electrochemical energy storage

*Christopher E. Van Pelt[1,2], **Bryn Jenkins**[1], bryn_jenkins@outlook.com, Minhchau Do[1], Mohd Avais[3], Alex Mirabal[4], Sandip Maurya[2], Benjamin L. Davis[2], Emily Pentzer[3]. (1) Materials Science and Engineering, Texas A&M University, College Station, Texas, United States(2) MPA-11: Materials Synthesis & Engineering, Los Alamos National Laboratory, Los Alamos, New Mexico, United States(3) Chemistry, Texas A&M University, College Station, Texas, United States(4) Sigma 2: Finishing Manufacturing Science, Los Alamos National Laboratory, Los Alamos, New Mexico, United States*

Non-aqueous redox flow batteries utilize organic solvents and redox active organic molecules which can be a cost-effective electrochemical energy storage system. However, this relatively young technology faces design challenges such as low solubility of redox species and active material crossover. Polymers containing both redox-active and solubility promoting pendant groups can address both issues. This work reports the synthesis and characterization of methacrylate copolymers bearing pendant redox-active units of 2,2,6,6-tetramethylpiperidinyl-N-oxyl (TEMPO) and the solubilizing group of di(ethylene glycol) methoxy ether methacrylate (DEGMEMA). Post polymerization modification was used to attach the TEMPO functional groups to the polymer backbone, i.e., using copper-catalyzed azide-alkyne cycloaddition (CuAAC) “click chemistry”. Copolymers with 1:3, 1:1, and 3:1 ratios of TEMPO: DEGMEMA were prepared. Electrochemical characterization of the copolymers using cyclic voltammetry experiments revealed that the polymers adsorbed to the electrode and that the amount of adsorbed polymer increased with TEMPO functionalization. We further observed that the electrolyte solvent dictates the electrochemical response of the polymer, but does not prevent the adsorption of the polymers. This work provides insight into the design of a modular platform for preparing polymers for electrochemical energy storage and highlights the impact of electroactive materials interacting with the electrode. Further studies could provide more evidence to the specific mechanism occurring to facilitate adsorption behavior.

SWRM 2026 SW70

Controlled nanostructuring of single-ion magnets using 2D covalent organic frameworks

***Noreen Mazhar**, nxm230047@utdallas.edu, Mario Wriedt. Chemistry, The University of Texas at Dallas, Richardson, Texas, United States*

Bulk magnetic materials play a crucial role in everyday life. Single molecule magnets (SMMs) and single ion magnets (SIMs), collectively known as molecular magnets (MMs), exhibit magnetic bistability and slow magnetization relaxation. Due to their large spin ground states and high axial magnetic anisotropies, MMs are gaining attention for potential molecular-level data storage and quantum computing applications. The discovery of the first known SMM, Mn12Ac, marked a breakthrough in magnetism for data storage devices. However, a significant challenge in molecular spintronics and MM design is their air sensitivity and functionality at ultralow blocking temperatures (TB < 10 K). While attaching MMs to surfaces like gold or graphene has been explored, this often results in a loss of symmetry and even destruction of their magnetic bistability. To enable reliable read/write functions, it is essential to organize MMs in a controlled manner that preserves their magnetic properties. In 2015, Wriedt et al. addressed this challenge by using 3D metal-organic frameworks (MOFs) as hosts for nanostructuring MMs. Building on this work, we aim to further explore MM behavior within 2D hosts such as covalent organic frameworks (COFs). We believe this approach could overcome many challenges related to encapsulating and separating individual MM domains. Ultimately, SIM@COF thin films have the potential for ultra-high data storage applications.

SWRM 2026 SW71

Sustainable drop-in alternative to PBAT: MDI chain-extended bio-based PPeAT for flexible film packaging

Mahdi Mazaheri*, mazaheri@ou.edu, Hesham Aboukeila, Onkar Singh, Brian P. Grady, John Klier. School of Sustainable Chemical, Biological and Materials Engineering, The University of Oklahoma, Norman, Oklahoma, United States*

The widespread use of linear low-density polyethylene (LLDPE) and low-density polyethylene (LDPE) in flexible film packaging poses significant environmental challenges due to their non-biodegradability and contribution to microplastic pollution. Although biodegradable alternatives such as poly(butylene adipate-co-terephthalate) (PBAT) have been commercialized, their relatively low stiffness, higher cost, and reliance on petroleum-based 1,4-butanediol limit broader adoption. Bio-based polyesters such as poly(pentylene adipate-co-terephthalate) (PPeAT), synthesized using 1,5-pentanediol derived from agricultural waste streams, offer a promising alternative. However, conventional PPeAT systems suffer from long synthesis times and undesirable coloration, which hinder their commercial viability. In this work, PPeAT synthesis was optimized through the incorporation of methylene diphenyl diisocyanate (MDI) as a chain extender, following strategies used in commercial PBAT production. Copolymers with varying adipic/terephthalic acid ratios were synthesized to tailor thermal properties for film applications. Gel permeation chromatography confirmed the formation of high molecular weight polymers with controlled polydispersity. Thermal analysis identified the 30:70 adipic/terephthalic composition (PPeAT70+MDI) as optimal, with glass transition and melting temperatures suitable for processing. The addition of a nucleating agent reduced the crystallization half-time from approximately 40 minutes to about 1 minute, enabling practical melt processing. Mechanical testing showed that the Young’s modulus of the synthesized materials falls between PBAT and LLDPE, while PPeAT70+MDI maintains elongation at break comparable to LLDPE. Additionally, preliminary barrier measurements indicate a water vapor transmission rate more than three times lower than PBAT. These improvements in processability, mechanical performance, and barrier properties, together with the use of a bio-based diol, enable the production of thinner films with reduced material consumption and cost. Overall, PPeAT70+MDI represents a promising drop-in alternative to PBAT for flexible packaging applications.

SWRM 2026 SW72

Investigating the effects of particle size on oxygen reduction reaction using MXene electrocatalysts

***Anthony Wiederkehr**, abwiederkehr7@tamu.edu. Chemical Engineering, Texas A&M University System, College Station, Texas, United States*

Pt/C currently serves as the benchmark catalyst for the Oxygen Reduction Reaction, however, it's high cost and scarcity motivate the search for alternatives. MXenes have been increasingly investigated as potential candidates due to their tunability and metallic conductivity. Herein, Ti_3CN MXene performance is investigated with controlled particle sizes to draw a relationship between size and electrocatalytic performance. Ti3CN is synthesized through a top-down process where its MAX phase (Ti_3AlCN) is MILD-etched with lithium fluoride and stirred for 24 hours. Then, it is acid washed with formic acid and centrifuged until a neutral pH is achieved. Lastly, our centrifuged vials are vacuum filtered onto a PES membrane (0.45 μm) which is vacuum dried overnight. Once, few layer Ti3CN MXene is achieved, particle size is varied using a bath sonicator (Branson 5800). Samples are divided into four sonication times: 5 mins, 1 hr, 2 hr, and 4 hr. Electrochemical characterization of the groups comes from using a PINE system and AfterMath software. Limiting current was greatest at one hour sonication or a median particle size of 12.73 μm, the largest of the four groups. However, chemical stability was best at a median of 0.021 μm, the smallest. No consistent relationship was observed between bath sonication time and particle size, indicating that this method cannot reliably reduce particle size. This highlights the need for a more controlled and effective size reduction technique to draw more confident conclusions between particle size and ORR performance.

SWRM 2026 SW73

3D-printed emulsion-templated foam composites with metal-organic frameworks for selective gas adsorption

***Lyndsay Ayers**, lyndsay.ayers@utdallas.edu, Ronald Smaldone. Chemistry and Biochemistry, The University of Texas at Dallas School of Natural Sciences and Mathematics, Richardson, Texas, United States*

Mixed-matrix membrane (MMM) materials are an approach for improving metal–organic framework (MOF) processability by incorporating MOF particles into polymeric matrices while preserving critical properties such as high surface area and selective affinity toward toxic gases; however, their performance depends heavily on maintaining accessible active sites and minimizing particle aggregation or pore blockage within the MOF. High internal phase emulsion polymers (polyHIPEs) are highly porous polymer materials formed by emulsifying an internal aqueous phase (water, W) within an external monomer or oil phase (O), followed by polymerization. An 80/20 W/O emulsion produces interconnected micro-, meso-, and macropores throughout the polymer matrix. The MOF used in this work, UiO-66-NH_2, consists of zirconium metal nodes connected by organic linkers containing reactive amine groups, providing high affinity for gas adsorption. By combining the high surface area and interconnected porosity of polyHIPEs with the adsorption and catalytic properties of UiO-66-NH_2, this work demonstrates the development of MMM composites with enhanced mass transfer and accessible adsorption sites for targeted gas capture. Digital light processing 3D printing further enables the fabrication of complex, customizable geometries, expanding the potential applications of these materials to wearable technologies and filtration systems. Excessive MOF loading can cause particle aggregation and pore blockage, limiting gas transport through the material;

this composite demonstrates high efficiency at a loading of only 15 wt% relative to the polymer. Overall, this research demonstrates a promising approach for designing customizable, mechanically resilient, and highly porous MMM-MOF composites for volatile gas filtration and other advanced gas adsorption applications.



SWRM 2026 SW74

Structuring metal-organic framework polymer composites via polymerization induced phase separation: Towards a predictive 3D printing strategy

Tien M. Tran, *tmtran1827@gmail.com. Chemistry, The University of Texas at Dallas, Richardson, Texas, United States*

This work investigates the role of resin polarity, crosslinker chain-length and metal-organic framework (MOF) particle size on polymerization-induced phase separation (PIPS) in digital light processing (DLP)-printed MOF-polymer composites. Three Zr based MOFs (UiO-66, UiO-66-NH_2 and MOF-808) were selected to determine whether formulation-phase separation trends are generalizable across different MOFs. To ensure that the MOF retained its crystallinity after the 3D printing process, the MOF-composites were characterized by powder x-ray diffraction (PXRD). MOF-composite distribution was measured by scanning electron microscopy/energy-dispersive x-ray spectroscopy (SEM/EDS) to quantify phase-separated domains. Hydrolysis of nitrophenyl acetate (NPA) was used to evaluate accessibility of MOF catalytic sites within the printed composites. The results established predictive structure-formulation-processing relationships governing PIPS-driven MOF redistribution in photopolymerization systems, providing design principles for catalytically active 3D-printed composites.

SWRM 2026 SW75

Effects of bio-based additives on the fire-retardant performance and environmental durability of phosphorus-based wood treatments

Chloe Qian[1,2]*, haiyue.qian@gmail.com, Chuang Shi*[2]*, Feng Gu*[2]*. (1) Orange County School of The Arts, Santa Ana, California, United States(2) School of Chemistry and Chemical Engineering, Yancheng Institute of Technology, Yancheng, Jiangsu, China*

Wood is a renewable structural material, but its combustibility creates a need for fire-retardant treatments that remain effective after environmental exposure. This study investigated whether cellulose-derived hydroxyethyl cellulose (HEC) and ammonium lignosulfonate (ALS) could improve the fire-retardant performance and environmental durability of a 10% ammonium phosphate (AP) wood treatment. HEC (0.1–1.0%) and ALS (0.25–2.0%) were first screened individually, followed by evaluation of combined formulation. Five replicate specimens were evaluated per treatment using after-flame time, specimen mass loss, char integrity, and char proportion. Compared with the water-treated negative control, 10% AP alone greatly reduced sustained burning. The combined addition of HEC and ALS further enhanced fire-retardant performance, with 10% AP + 1% HEC + 2% ALS providing the best overall baseline performance, including 0 s after-flame, approximately 0.3% mean specimen mass loss, and a char-integrity score of 5/5. Selected formulations were also challenged by heat stress and simulated rainfall to test durability. Simulated rainfall more clearly differentiated coating durability: mean coating retention was approximately 22% for AP alone and 59% for AP + HEC + ALS. Phytic acid (PA) was further explored as a bio-derived fire-retardant system, with coating retention after simulated rainfall increasing from approximately 62% for PA alone to 77% with chitosan (CS) and ALS additives. Overall, these findings demonstrate that bio-based additives can enhance the fire-retardant performance and environmental durability of phosphorus-based wood treatments and support further development of more sustainable bio-derived systems.

SWRM 2026 SW76

Investigating the repair of 3'-DNA-protein cross-links arising from abasic sites

Joel cepeda*, joelcepeda@utexas.edu. Chemical Biology and Medicinal Chemistry, The University of Texas System, Austin, Texas, United States*

DNA-protein cross-links (DPCs) are highly toxic DNA lesions that arise through various means, namely as byproducts of metabolic processes, from environmental hazards, and through chemotherapeutic induction. Persistence of these bulky adducts facilitates genomic instability and ultimately cell death if left unresolved. Complicating the efforts to elucidate DPC repair mechanisms arises from various chemical characteristics, namely protein identities, surrounding DNA structures, and specific chemical linkages. While previous work has investigated the formation and repair of a subset of DPCs, the formation of DPCs arising from abasic (apurinic/apyrimidinic, AP) sites at the 3′-end of DNA (3′-DPCs) and their subsequent repair mechanisms are less studied. Here we use a stable and site-specific 3′-aminooxylysine DNA-peptide cross-link (3′-OxyK-DpC) to investigate the role of APE1, TDP1, and TREX1/2 in repairing 3′-DpCs in cell extracts. Additionally, four types of 3′-DpCs arising from Michael addition or Schiff base formation via lysine-, histidine-, or cysteine-residues were synthesized to assess the influence of chemical linkages on DpC repair. Consequently, in reconstituted DpC repair in HEK293T cell nuclear extracts, APE1 primarily contributed to the 3′-DpC repair process, with TDP1 playing a minor role. Steady-state kinetics revealed that APE1 and TDP1 repair 3′-DpCs with different preferences. Notably, APE1 repairs the 3′-Lys(Michael addition)-DpC with the greatest catalytic efficiency, followed by the 3′-Lys(Schiff base)-DpC, 3′-His-DpC, and finally the 3′-Cys-DpC. For TDP1, the 3′-Cys-DpC was repaired most efficiently, followed by the 3′-Lys(Schiff base)-DpC, 3′-His-DpC, and finally the 3′-Lys(Michael addition)-DpC. Collectively, APE1 and TDP1 serve as the major and minor 3′-DpC repair enzymes, respectively, in HEK293T cell extracts. Additionally, 3′-DpC repair by APE1 and TDP1 is strongly affected by the chemical linkage.

SWRM 2026 SW77 - Withdrawn

SWRM 2026 SW78

Evaluating a rationally designed peptide and small-molecule compounds against *Clostridioides difficile*

***Juan F. Dominguez**, juandominguez1733@yahoo.com. School of Integrative Biological and Chemical Sciences, The University of Texas Rio Grande Valley, Edinburg, Texas, United States*

Clostridioides difficile is an important bacterial pathogen associated with healthcare-associated infections, and increasing antimicrobial resistance highlights the need for alternative therapeutic approaches. This study evaluated the antimicrobial activity of a rationally designed peptide according to C. difficile translational initiation factor 1 (Cd-IF1), and several molecular compounds, with the additional aim of investigating the synergistic effect of the peptide and caffeic acid or trans-caffeic acid. Vancomycin, niclosamide, polymyxin B sulfate, gossypol-acetic acid, and the CdIF1-derived peptide (NH2-HISGKLRMNFIRILEGDK-COOH) were evaluated against C. difficile ATCC 43543. The peptide was also evaluated in combination with caffeic acid and trans-caffeic acid. C. difficile was cultured anaerobically in BHI broth following growth on Brucella agar. Broth microdilution assays were performed in 96-well plates using two-fold serial dilutions and incubated anaerobically at 37°C for 48 h. Growth was assessed by visual observation, with vancomycin and DMSO serving as positive and vehicle controls, respectively. Vancomycin consistently demonstrated inhibition across the dilution series, while DMSO controls demonstrated growth. Gossypol-acetic acid showed apparent growth throughout the tested dilution range. Polymyxin B sulfate and niclosamide demonstrated inhibition across portions of their dilution series, although replicate variability was observed. The CdIF1-derived peptide and peptide combinations with caffeic acid or trans-caffeic acid demonstrated variable, non-monotonic patterns of apparent growth inhibition. Although further quantitative investigation of these molecular agents' minimum inhibitory concentrations (MICs) is necessary, these preliminary findings demonstrate promising potential for developing novel Clostridioides difficile inhibitors to combat infection and antibiotic resistance.

SWRM 2026 SW79

Watercress flavonoids as natural protectants of human serum albumin under oxidative stress: A molecular study

***Bidisha Sengupta**, bsgupta.tougaloo@gmail.com, Nkeiruka Aziekwu, Ken Fiffick, Michael Janusa. Chemistry and Biochemistry, Stephen F Austin State University, Nacogdoches, Texas, United States*

Oxidative stress can alter the conformation and integrity of proteins, making the development of naturally derived protective compounds of interest at the chemistry–biology interface. Watercress (*Nasturtium officinale*) is a flavonoid-rich plant that contains several kaempferol derivatives and has previously demonstrated antioxidant potential in our laboratory. In this study, we examined whether watercress-derived phytochemicals could preserve the structural characteristics of human serum albumin (HSA), a well-established model protein, under chemically induced oxidative conditions. HSA was exposed to an oxidative system generated by $FeSO_4$ and H_2O_2, followed by treatment with

watercress ethanol extract, kaempferol, or their combination. Changes in the protein were examined using circular dichroism, dynamic light scattering, SDS-PAGE, and biochemical measurements. UPLC–Orbitrap mass spectrometry was used to characterize the major constituents of the watercress extract and identified kaempferol, kaempferol-3-*O*-glucoside, kaempferol-3-*O*-rutinoside, and quercetin. Oxidative treatment markedly altered the secondary structure and physical characteristics of HSA, whereas watercress extract and kaempferol reduced these changes. The combined treatment provided greater preservation of protein structure than either treatment alone. These findings demonstrate the potential of watercress-derived phytochemicals to protect protein structure under oxidative conditions and provide a basis for further investigation of plant-derived compounds at the intersection of natural-product chemistry, protein biochemistry, and sustainable approaches to oxidative stress management.

SWRM 2026 SW80

Identification and characterization of a putative Fe^{2+}-ZIP transmembrane transporter in *Naegleria fowleri*

***Prakriti Budhathoki**, pxb220050@utdallas.edu, Temiloluwa Ogunsanya, Humera Gull, **Gabriele Meloni**, gabriele.meloni@utdallas.edu. Chemistry and Biochemistry, The University of Texas at Dallas, Richardson, Texas, United States*

Naegleria fowleri, also known as the brain-eating amoeba, causes a brain infection that leads to fatal meningoencephalitis. While colonizing the brain, the pathogen hijacks host cellular pathways to acquire essential micronutrients, thereby enabling its survival and replication. During infection, iron is a critical micronutrient and catalytic cofactor for key metabolic processes that must be taken up from the host, but the molecular processes involved in these nutritional immunity responses remain elusive. In this work, using bioinformatic approaches, we identified a novel putative iron transmembrane transporter (*Nf*FiT, ferrous iron transporter) belonging to the ZIP (Zrt-/Irt-like protein) family as a mediator of iron uptake in *N. fowleri*. The ZIP transporter family is known for facilitating the influx of biologically essential divalent metal cations including Zn^{2+}, Mn^{2+}, Fe^{2+}, and Cd^{2+} in all domains of life. However, the structure and function of Fe^{2+}-transporting ZIPs, in particular from unicellular eukaryotic protozoan pathogens, remain largely unexplored. To address this gap, we developed a platform to express, purify, and reconstitute *Nf*FiT in artificial lipid bilayers to provide mechanistic insights into its cargo selectivity, promiscuity, and mechanism of metal transport. By developing real-time metal proteoliposome-based transport assays followed by stopped-flow spectroscopy, we defined cargo selectivity and kinetic parameters associated with metal translocation. Upon encapsulating the fluorescent probes responsive to diverse stimuli (metals, pH, and transmembrane potential) in the proteoliposome lumen, we established that *Nf*FiT is a highly selective electroneutral $Fe^{2+}/2H^{+}$ antiporter with very fast translocation kinetics and high affinity, allowing it to compete with the host labile iron pool. Mutagenesis established residues involved in cargo selection and translocation across the lipid bilayer. These findings expand the current understanding of Fe^{2+} homeostasis in *N. fowleri* and provide mechanistic insight into Fe^{2+} translocation by the ZIP family, offering novel pathways to combat this lethal pathogen.

SWRM 2026 SW81

Mechanism of *Ostrinia furnacalis* PBP2 function: Role of the C-terminal tail

***AHMAD T. AZEEZ**, ahmad.t.azeez@okstate.edu. Chemistry, Oklahoma State University, Stillwater, Oklahoma, United States*

Ostrinia furnacalis, also known as Asian Corn Borer, a lepidopteran moth, is an agricultural pest found across Asia, Australia, Africa, and some regions of the United States. It is responsible for the destruction of over one-third of the total crops and food stored globally. The common use of pesticides is detrimental to the crops as well as the environment. Many produces contain as many as 30 different pesticide residues that are harmful to human health. The *O. furnacalis* pheromone-binding protein 2 (OfurPBP2) located in the male antennae is involved in detecting female-emitted pheromones, a crucial step in the mating process. The binding of pheromone to OfurPBP2 is the first step in the signaling events where a chemical signal translates into an electrical signal resulting in the behavioral response in the male. Two biological gates (His70-His95 and C- terminus) have been reported to be involved in the ligand release in several well-studied lepidopteran PBPs. In contrast OfurPBP2 contains an Arg70-His88 gate and a C-terminus containing additional charged residues. To investigate the role of the C-terminus in pheromone binding and release, we have deleted the C-terminal tail of OfurPBP2 generating the OfurPBP2DP129-Q144 truncated mutant. We will present the recombinant protein expression, refolding, and purification and the impact of the truncation on protein folding. Understanding the mechanism of pheromone binding and release would ultimately help in the development of sustainable pest management strategy.

SWRM 2026 SW82

Discovery of novel DNA–protein cross-links by mass spectrometry

***Bingru Li**, bingru.li@utexas.edu, Ying Peng, Kun Yang. College of Pharmacy, The University of Texas System, Austin, Texas, United States*

DNA-protein cross-links (DPCs) are highly toxic because they block DNA replication and transcription. The accumulation of DPCs has been linked to human diseases including cancer. Apurinic/apyrimidinic (AP) sites are the most abundant DNA lesions and can generate DPCs, however, their chemical structures and cellular formation are poorly characterized. We developed sensitive and accurate mass spectrometry approaches to characterize the DPCs derived from AP sites in vitro and in human cells. We discovered two novel AP-derived Michael addition 3′-DNA terminal DPCs formed at histidine and lysine residues. This study provides direct evidence of these DPCs and establishes a robust, quantitative workflow for their analysis, laying a foundation for future investigations into their formation, influence on DNA integrity, and contribution to understanding DPC repair mechanisms.

SWRM 2026 SW83

Design and synthesis of mitochondria-targeted antioxidants for improving myoglobin redox and meat color stability

***Prabir Kumar Gharai**[1], pkgiicb@gmail.com, Siddhartha Maji[2], Richard A Bunce[2], Ranjith Ramanathan[1]. (1) Department of Animal and food Sciences, Oklahoma State University Division of Agricultural Sciences and Natural Resources, Stillwater, Oklahoma, United States(2) Department of Chemistry, Oklahoma State University The College of Arts and Sciences, Stillwater, Oklahoma, United States*

Beef discoloration costs the beef industry $3.7 billion and results in 400 million pounds of beef waste. Plant-derived polyphenols are widely used in the food industry to limit oxidative deterioration during storage; however, their application is often restricted by poor stability, interactions with food biomolecules, and undesirable sensory effects. Development of new antioxidants may improve their stability and functionality in complex food systems. Therefore, the objective of this study was to synthesis of mitochondria-targeted antioxidants and evaluate their antioxidant activity in *invitro* (equine myoglobin), and meat systems. A series of antioxidants (SB-4Me, SB-4OMe, SB-5Me, SB-5OMe, and SB-5tBu) was synthesized through a three-step synthetic approach and characterized. The molecules were designed to contain a triphenyl-phosphonium cation to promote mitochondrial accumulation and a catechol moiety to scavenge excessive reactive oxygen species. Ascorbic acid was included as a positive control throughout antioxidant comparisons where appropriate experiments. Antioxidant capacity was initially evaluated using ABTS and DPPH radical-scavenging assays, together with ferryl myoglobin inhibition and fluorescence-based assessment of heme degradation. Among the synthesized compounds, SB-5Me exhibited the strongest overall antioxidant activity. The ability of these compounds to influence myoglobin redox stability was subsequently evaluated *in vitro*. Oxymyoglobin was treated with each antioxidant at 0.01% and 0.02% and incubated at 37 °C for 0, 3, and 6 h, followed by evaluation of metmyoglobin reduction. SB-5Me showed the greatest protective effect against myoglobin oxidation. The antioxidants were further evaluated for their potential to improve meat color stability and mitochondrial function in beef. Beef steaks obtained at 7 days postmortem (n = 5) were minced, treated with 0.01% and 0.02% antioxidant, and aged for 4 and 9 days. Sarcoplasmic fractions were isolated, and metmyoglobin percentage was determined as an indicator of discoloration. Consistent with the in vitro findings, SB-5Me showed the greatest ability to limit metmyoglobin accumulation among the tested compounds. Overall, these findings demonstrate that new synthesized mitochondria-targeting antioxidants can enhance antioxidant performance where SB-5Me emerged as the most promising candidate for reducing oxidative changes and improving myoglobin redox stability in meat system.

SWRM 2026 SW84

Analysis of the mammalian glutathione synthetase H-loop

***Michael Marks**, mb.marks1109@gmail.com, Mary E. Anderson. Chemistry and Biochemistry, Texas Woman's University, Denton, Texas, United States*

Glutathione (GSH) is an intracellular antioxidant tripeptide (L-γ-glutamyl-L-cysteinylglycine). GSH is found in every cell of most organisms and is crucial for supporting enzyme function, facilitating amino acid transport, and protecting against reactive oxygen species (ROS). Low GSH level has been associated with numerous diseases, including Parkinson's, Alzheimer's, Lou Gehrig's, diabetes, cystic fibrosis, HIV/AIDS and cardiovascular diseases. GSH is synthesized through two sequential enzymatic reactions. First, γ-glutamylcysteine synthetase (GCS) uses ATP to ligate glutamate to cysteine to form γ-glutamylcysteine (γ-GC). Glutathione synthetase (GS) then catalyzes the final step by using ATP to ligate γ-GC and glycine, forming GSH. Human GS (hGS) is a homodimer (~52 kDa each subunit) that displays negative cooperativity to γ-GC substrate, such that binding of γ-GC at one active site decreases the likelihood of GSH catalysis at the other active site. Protein loops of hGS often play important roles in substrate binding and in stabilizing or protecting reaction intermediates within the enzyme's active sites. Our group characterized G-, A-, and S-loops in hGS, and are seeing to the characterization of H-loop. We hypothesize that the Ser and Thr residues within the H-loop (147-TISASF-152) contribute to substrate binding and catalysis. H-loop variants were prepared by site-directed mutagenesis, expressed in E. coli, purified, and characterized. Preliminary results show that mutated enzymes exhibit reduced catalytic activity compared to wild type (WT = ~18.2 kcat),

along with variation in binding affinities (Km) and Hill coefficients (h) among the different variants. These findings will provide a better understanding of how the H-loop residues contribute to γ-GC substrate binding and catalytic function in hGS and gain insight into future strategies for targeting disorders associated with impaired glutathione homeostasis. (Supported in part by a Welch Foundation Grant to the Chem Dept Grant, TWU)

SWRM 2026 SW85

Circadian regulation of calcium uptake by cardiac mitochondria

Theodore Nguyen[1,2]*, tanguyen1@udallas.edu, Beverly Rothermel*[2]*. (1) Chemistry, University of Dallas, Irving, Texas, United States(2) Internal Medicine, The University of Texas Southwestern Medical Center, Dallas, Texas, United States*

The heart undergoes circadian changes to match its energy production with fluctuating demands throughout the day. Glucose oxidation, a major source of energy for the heart, is controlled by pyruvate dehydrogenase (PDH), an enzyme partly regulated by calcium uptake into the mitochondrial matrix during a “fight-or-flight” response. Calcium enters the mitochondrial matrix primarily through the mitochondrial calcium uniporter (MCU), a highly selective channel in the inner mitochondrial membrane. Once inside the matrix, calcium activates pyruvate dehydrogenase phosphatase (PDP), which dephosphorylates and activates pyruvate dehydrogenase, stimulating glucose oxidation. However, the time-of-day dependence of these regulatory inputs remains unclear. Herein, an assay was developed to measure oxygen consumption evaluate mitochondrial calcium uptake.

SWRM 2026 SW86

Investigation of redox-based post-translational modifications in *Arabidopsis thaliana* lipid metabolism

Cody King[1]*, codyking2@my.unt.edu, Patrick Horn*[2]*. (1) Chemistry, University of North Texas, Denton, Texas, United States(2) Biological Sciences, University of North Texas, Denton, Texas, United States*

Recent proteomics studies have revealed that many enzymes in plant metabolism undergo redox-based post-translational modifications (redox PTMs). Cysteine residues are particularly susceptible to redox PTMs under stress conditions. For example, sulfenylation alters the oxidation state which may act to regulate its activity level. Despite their abundance and potential impact on plant health, most redox PTMs, including sulfenylation, remain uncharacterized. Here we report on in vivo and in silico modeling approaches to characterize the structure and function of redox PTMs on key enzymes in plant lipid metabolism: stearoyl ACP-desaturase (SAD, produces unsaturated fatty acids, FAs), Ketoacyl ACP-synthase II (KASII, produces longer FAs), and glycerol-3-phosphate acyltransferase I (ATSI, helps assemble FAs into membrane and storage lipids). The cysteine residues on SAD, KASII, and ATS1, detected as sulfenylated, show a high rate of sequence conservation. We hypothesized that these PTMs serve as a form of both activity regulation and product turnover in response to environmental cues. Supporting this hypothesis, in vivo experiments show sustained or altered abilities of SAD, KASII, and ATS1 cysteine mutants (e.g., to mimic redox PTMs) to alter heterologous host lipid profiles in yeast or E. coli systems. Mutations in the SAD structure have been shown to cause increased levels of unsaturated fatty acid content in E. coli cells. Interactions with reactive

oxygen species (ROS) produced during times of plant stress could oxidize cysteine residues, resulting in alterations of activity levels. Investigations of these specific modifications will lead to a better understanding of redox conditions and the metabolic regulation that affects enzyme activity levels. Fatty acid molecules and their content in various marketed products are well founded in industrial uses. The potential understanding of the regulation of vital enzymes and their roles in the production and incorporation of fatty acids could have great economic benefits.

SWRM 2026 SW87

Biochemical characterization of Rad7-Rad16 in yeast global genome nucleotide excision DNA repair

Chathurika Ranmini Silva Hewa Bhashithage*, chathurika_hewabhas1@baylor.edu, Temilade Adeniran, JungHyun Min. Chemistry and Biochemistry, Baylor University, Waco, Texas, United States*

Nucleotide excision repair (NER) is a major cell DNA repair pathway to remove structurally diverse bulky DNA lesions. Defects in NER can lead to genomic instability, mutations, and cancers. Global genome NER (GG-NER) removes lesions from the transcriptionally inactive DNA. Since NER is conserved among eukaryotes, this study delves into understanding eukaryotic NER using yeast *Saccharomyces cerevisiae* as a model system. In yeast, Rad7-Rad16 is indispensable for initiation and, together with Abf1, for excision steps of GG-NER. However, the detailed molecular mechanism of how Rad7-Rad16 (-Abf1) roles are linked in lesion recognition and excision remains unknown. Here, we show that Rad7-Rad16 has a higher lesion specificity than Rad4-Rad23, which is known as the lesion recognizer in yeast. Damage-specific DNA binding of the purified Rad7-Rad16 complex was quantified using a competitive electrophoretic mobility shift assay (EMSA). The Cy5 end-labeled 24 bp long mismatched and matched DNA was used as the substrates. Rad7-Rad16 showed 67±5 nM specific binding and 8268±394 nM non-specific binding, which indicates ~123 times more specific binding of Rad7-Rad16 to mismatched DNA. Our results demonstrate that Rad7-Rad16 has 15x higher lesion specificity than Rad4-Rad23 without ATP. Other than that, Rad7-Rad16 showed ~22x higher binding to the 94 bp long internal iCy5 labeled DNA rather than Cy5 end labeled 94 bp DNA. This protein tends to prefer long DNA over short DNA for the ATPase activity assay. We will characterize the impact of Rad7-Rad16 on the recruitment of Rad4-Rad23 and lesion initiation in the future. We will also characterize the interaction between Rad7-Rad16 and Abf1 and the effect on excision. Our studies will pave the way for the structural characterization of Rad7-Rad16 in NER using Cryo-EM.

SWRM 2026 SW88

Impact of torsional restraint in coordinating nucleotide excision repair dual incision

Comfort O. Alex-Samuel*, comfort_alexsamuel1@baylor.edu, Temilade Adeniran, JungHyun Min. Chemistry and Biochemistry, Baylor University College of Arts and Sciences, Waco, Texas, United States*

DNA is often susceptible to damage from various endogenous and exogenous factors (such as reactive oxygen species, ultraviolet irradiation, and carcinogens). Nucleotide excision repair (NER) is an important repair system that removes bulky lesions that distort the DNA double helix, thereby maintaining genomic stability. The global genome NER (GG-NER) pathway operates across the

entire genome. While the catalytic roles of individual repair endonucleases have been well characterized, how the physical state of DNA influences the coordinated multi-protein machinery remains less understood. To determine how DNA topology affects repair efficiency, we constructed a topologically defined double-stranded minicircle (dsMC) substrate featuring an internal Cy5 (iCy5) label and a 26–31 nt mismatched poly-T bubble. The Cy5 label enabled sensitive detection and quantification of DNA cleavage products on denaturing gels. We evaluated the endonuclease activities of core yeast NER proteins (Rad1–Rad10 for 5′ incision and Rad2 for 3′ incision) and tested a fully reconstituted Global Genome NER (GG-NER) dual incision system across both topologically restrained dsMC substrates and relaxed double-stranded linear DNA (dsL). Our results demonstrated that dsMC and dsL with mismatched bubble DNA are good substrates for individual endonucleases, consistent with their known 3' and 5' overhang cleavage activity for Rad2 and Rad1-Rad10, respectively. However, dual-incision products were observed only with the relaxed linear DNA substrate lacking a pre-existing bubble, in the presence of all NER machinery. These results demonstrate that a static, pre-formed bubble is insufficient to trigger complete NER. Instead, productive dual incision requires sequential protein assembly and dynamic, step-by-step DNA unwinding. We propose that DNA torsion generated before and during the unwinding process is essential for the full NER protein complex to catalyze dual incision.

SWRM 2026 SW89

Can a biologically relevant Fe–oxygen intermediate drive aerobic C–C bond formation?

***Tahmina Afroz**, tahmina.afroz@tcu.edu, Kayla N. Green. Department of Chemistry, Texas Christian University, Fort Worth, Texas, United States*

Aerobic iron-catalyzed pyrrole arylation provides a sustainable route to C–C bond formation using molecular oxygen as the terminal oxidant, yet the oxygen-derived species responsible for the initial oxidative step remains unresolved. Preliminary studies suggest that catalysis proceeds through Fe(III)–oxygen intermediates rather than high-valent Fe–oxo species. Given the established roles of Fe(III)-peroxo and Fe(III)-hydroperoxo complexes in biological O_2 activation, elucidating their involvement in iron-mediated pyrrole arylation is of particular interest. Density functional theory (DFT) calculations are employed to define the Fe–O_2 intermediate landscape accessible to Fe–Me_2Cyclam and characterize the Fe(III)–oxygen species formed during catalysis. These studies investigate whether a common Fe(III)–oxygen intermediate lies at the crossroads of selective arylation to 2-phenylpyrrole and competing pyrrole polymerization, providing fundamental insight into how O_2 activation controls selectivity in aerobic iron-catalyzed C–C bond formation.

SWRM 2026 SW90

Chromatography-based investigation of the cytosolic labile iron pool of *Saccharomyces cerevisiae*

***Salina Aryal**, salina_aryal2023@tamu.edu, Paul A. Lindahl. CHEMISTRY, Texas A&M University, College Station, Texas, United States*

Iron is an essential micronutrient required for numerous cellular processes, including mitochondrial respiration, DNA synthesis and repair, and biosynthesis of iron-containing proteins1. However, excess or improperly coordinated iron can promote the formation of reactive oxygen species,

requiring cells to tightly regulate iron. A central component of cellular iron metabolism is labile iron pool (LIP), a dynamic collection of low molecular mass iron species that is thought to serve as an intermediate in intracellular iron trafficking, utilization and storage2. Despite its biologicalimportance, the chemical composition and properties of the LIP remain poorly defined.Conventional chelator-based probes can perturb endogenous iron equilibria, complicating characterization of native LIP species3,4. This study investigates the LIP in WT W303 budding yeast Saccharomyces cerevisiae using liquid chromatography coupled to inductively coupled plasma mass spectrometry (LC-ICPMS) and Mössbauer spectroscopy. Cells were cultured under different metabolic and oxygen conditions, and low molecular mass cellular extracts were analyzed to evaluate changes in speciation. Our results reveal changes in the abundance and distribution of labile iron species depending on cellular metabolic state. Labile iron pool was found elevated in hypoxically grown iron sufficient respiring yeast. Chromatographic features consistent with Fe Citrate and Fe-ATP complexes were observed, suggesting that these species may contribute to the cellular LIP. These findings provide insight into the chemical composition of LIP and establish a framework for understanding the regulation of intracellular iron trafficking.

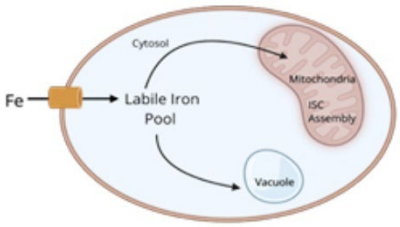


Figure 1. Iron trafficking in Saccharomyces cerevisiae

SWRM 2026 SW91

From Cu(II) thionitrite to N2O: Evidence for an HNO-mediated pathway

***Anagha Kuruvayil**, akuruvayil@mail.smu.edu, Saikat Mishra, Yasmina Said, Pokhraj Ghosh. Chemistry, Southern Methodist University Dedman College of Humanities and Sciences, Dallas, Texas, United States*

Nitric oxide(NO) and hydrogen sulfide(H2S) are biologically relevant gaseous signalling molecules. They undergo interconnected signalling pathways, and their crosstalk results in the formation of various S/N hybrid species. SNO (thionitrite), SSNO (perthionitrite) and HNO (nitroxyl) are proposed to be the key intermediates formed during the crosstalk of NO and H2S. However, their formation, reactivity and characterisation at biologically relevant transition metals are not clearly understood. Copper is particularly relevant in this context because of its accessible redox chemistry and strong interaction with S/N containing species. Despite the importance of SNO as a transient intermediate formed in NO/H2S crosstalk, structurally characterised metal-bound thionitrite complexes remain unprecedented. To date, only one structurally characterised metal-bound thionitrite species is known at a zinc centre. However, spectroscopic evidence for the metal-coordinated SNO/HSNO species has been identified. Here we report the isolation of the first structurally characterised Cu(II) bound thionitrite complex, as the platform for studying the NO/H2S crosstalk at a biologically relevant redox-active metal centre. Cu(II)SNO species was isolated using a sterically bulky tridentate 2,6-diisopropylpyridinediimine ligand and characterised using SC-XRD, UV-vis, ATR and ^{15}N NMR techniques. The reaction of Cu(II)SNO species with 0.5 eq. of HBF4.OEt_2 under UV-vis conditions

showed the SNO-SSNO conversion and resulted in the formation of N2O, confirmed by FTIR. To elucidate the N2O formation mechanism, HNO was trapped using triphenylphosphine; the resulting phosphine oxide(O=PPh3) and phosphine ylide(HN=PPh3) were characterised by 31P NMR and ESI-MS data. These reactions proved the acid-promoted conversion of Cu(II)SNO to SSNO and N2O generation. The present work explores the reactivity of rare Cu(II)SNO species as a molecular platform for understanding the potential NO/H2S crosstalk at a redox-active metal centre.

SWRM 2026 SW92

Hybrid copper ferrite nanomaterials for antibacterial control of *Xanthomonas* pathogens

*Benedict Muia, **Sharadie Liyanage**, shl012@shsu.edu, Tarek M. Trad. Department of Chemistry, Sam Houston State University, Huntsville, Texas, United States*

Xanthomonas plant pathovars are economically important crop pathogens that cause significant agricultural losses worldwide. Conventional management commonly relies on copper-containing compounds and antibiotics; however, prolonged use raises concerns regarding bacterial resistance and environmental accumulation of heavy metals. Therefore, alternative antibacterial strategies are needed. In this study, berberine-loaded, silica-encapsulated copper ferrite nanoparticles were investigated as potential antibacterial agents against Xanthomonas pathovars. Magnetic copper ferrite nanoparticles were synthesized from stearate precursors and annealed at 400, 600, and 800 °C to control crystallite size and magnetic properties. The nanoparticles were subsequently encapsulated with silica to provide a surface for berberine loading and facilitate controlled copper release. Powder X-ray diffraction (PXRD) confirmed the cupro-spinel phase, while dynamic light scattering (DLS) showed an average hydrodynamic diameter of approximately 60 nm. X-ray fluorescence (XRF) analysis yielded a Cu:Fe ratio of 29:60. FT-IR spectroscopy confirmed characteristic metal–oxygen and silica vibrations, and magnetic response was verified using a neodymium magnet. Antibacterial activity was evaluated against seven Xanthomonas plant pathovars and Stenotrophomonas maltophilia using colony-counting assays. Berberine (2.0 mg/mL) inhibited bacterial growth, while berberine-loaded silica-encapsulated copper ferrite nanoparticles at 2.0 mg/mL showed slightly lower inhibition. All tested antibacterial treatments significantly inhibited bacterial growth compared with the untreated LB broth control ($P \leq 0.0001$).

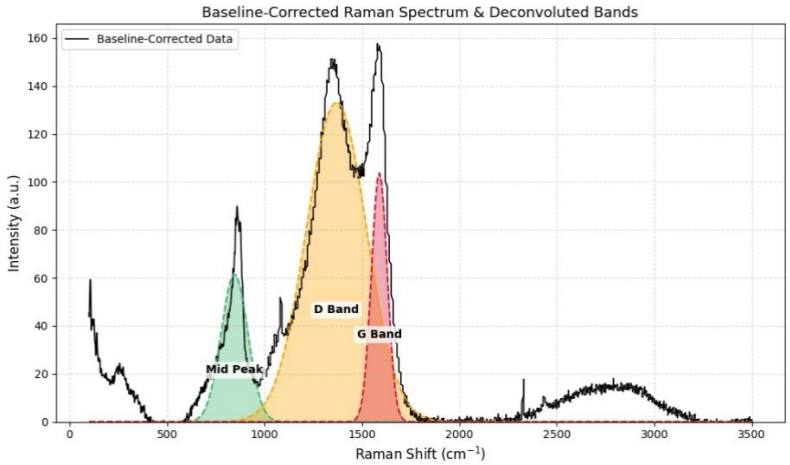
SWRM 2026 SW93

Electrochemical detection of gastric cancer VOC biomarkers using $Ca(OH)_2$ templated porous carbon electrodes

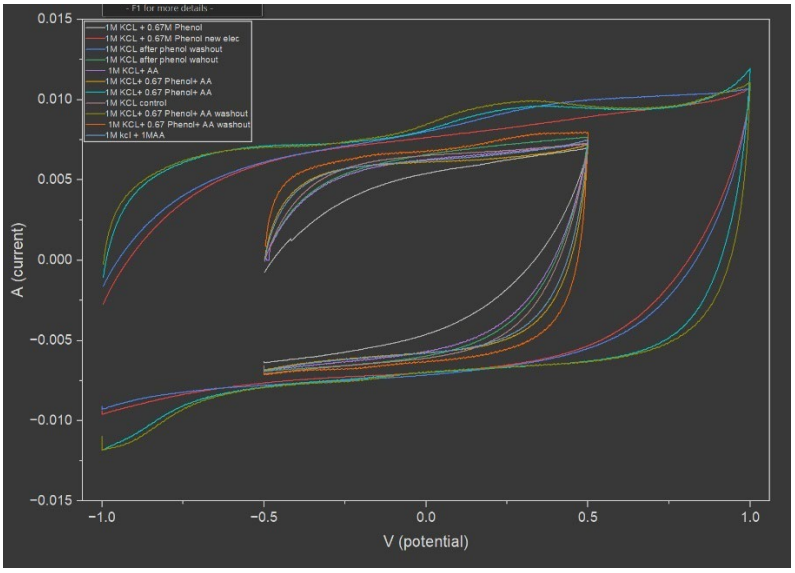
***Charles Asante**[1,2], asante.charlesa@gmail.com. (1) chemistry, The University of Texas at Dallas, Richardson, Texas, United States(2) Biomedical engineering, The University of Texas at Dallas, Richardson, Texas, United States*

Gastric cancer diagnosis often suffers from late-stage detection due to non-invasive screening limitations. Volatile organic compounds (VOCs) present in exhaled breath, such as phenol and acetic acid, serve as crucial non-invasive biomarkers for early-stage screening. In this work, we fabricated an electrochemical sensor platform using calcium hydroxide-templated porous carbon electrodes to detect target VOC analytes in aqueous electrolyte media. Structural characterization via Raman spectroscopy confirmed the graphitic nature of the synthesized material, displaying distinct D (~1350

cm^{-1}) and G (~1580 cm^{-1}) bands with a low I_D/I_G intensity ratio, demonstrating high structural ordering and enhanced electrical conductivity. The electrochemical behavior of the templated carbon was evaluated in a potassium chloride electrolyte system using both T-cell and coin cell architectures across potential windows of -0.5 V to 0.5 V and -1.0 V to 1.0 V at a scan rate of 100 mV/s. Cyclic voltammetry characterization revealed distinct current response variations upon the introduction of phenol and acetic acid, both individually and in combination. The template-derived porous carbon exhibited high double-layer capacitance alongside concentration-dependent modulation in capacitive current. Reusability trials demonstrated significant recovery of baseline current following washout steps, pointing toward reversible surface interaction mechanisms. These preliminary results highlight the potential of templated porous carbon electrodes as a reliable, cost-effective electrochemical sensing platform for monitoring gastric-cancer-associated VOCs.



Raman



CV

SWRM 2026 SW94

Switching the heme ligand switches the chemistry: First- and second-sphere control of peroxidase reactivity in sfh5

Chandradeep Ghosh*, chandradeepghosh@tamu.edu, Vytas Bankaitis, Paul A. Lindahl. Chemistry, Texas A&M University System, College Station, Texas, United States*

Sfh5 is an unusual heme-binding Sec14 homolog that exhibits dynamic proximal coordination between histidine and tyrosine, providing a rare platform to examine how first- and second-sphere interactions control heme reactivity. UV–Vis, EPR, resonance Raman, CO-binding, and pH-perturbation studies establish a reversible His↔Tyr coordination equilibrium in the active site. The His-biased Sfh5^{Y175H} variant preferentially forms highly reactive Compound I-like ferryl species and displays substantially enhanced TMB peroxidase turnover, whereas the Tyr-biased Sfh5^{H173Y} variant stabilizes less-reactive ferryl/tyrosyl intermediates with slower kinetics. Engineering the distal pocket further demonstrates that a properly positioned His^{191} promotes efficient peroxide activation, O–O bond cleavage, and ferryl-radical formation, while His^{221} is comparatively ineffective and favors hydroperoxo-like intermediates. In parallel, Tyr^{222} functions as a redox-active radical sink that redistributes oxidizing equivalents and modulates catalytic turnover. Together, these results identify Sfh5 as a ligand-switchable heme scaffold bridging peroxidase- and catalase-like chemistry and show how subtle changes in proximal ligation, distal proton transfer, and second-sphere redox buffering can redirect ferryl reactivity and catalytic function.

SWRM 2026 SW95

Characterization of perliplasmic FtrB, a novel ferrous oxidase with a cupredoxin like fold expressed by *Brucella* spp.

***Sambuddha Banerjee**, sambuddhabon@gmail.com. Texas A&M San Antonio, San Antonio, Texas, United States*

FtrB is one of the components of the four-component iron transport system, FtrABCD, expressed by Gram negative Brucella abortus under iron starvation. Unlike other bacterial iron uptake systems, this four-component system does not rely on ATP derived energy for ligand translocation. Rather, based on phylogenetic and structural modeling data it was predicted that periplasmic FtrB oxidizes Fe^{2+} to Fe^{3+} and the free energy derived from that is used by the membrane permease to translocate the ligand. In this work we show that wild-type FtrB binds Cu^{2+} and Fe^{2+} with μM affinities and the Cu^{2+} bound wild-type FtrB can oxidise Fe^{2+} under slightly acidic condition. X-ray crystal structure of wild-type FtrB identifies a cupredoxin like fold, however, instead of the typical Type-1 copper binding residues, FtrB show a conserved Asp and a His residues, implicated with Cu^{2+} coordination. Although the crystal structure do not show Cu^{2+} bound to the protein, taking all data together we propose a novel Cu^{2+} coordination site in cupredoxin like proteins which can also act as a ferrous oxidase.

SWRM 2026 SW96

Metal–ligand cooperative electroreduction of N_2O by molecular copper complexes

***Seif Eid**, seid@smu.edu, Saikat Mishra, Pokhraj Ghosh. Chemistry, Southern Methodist University, Dallas, Texas, United States*

Nitrous oxide (N_2O) is a potent greenhouse gas and a major contributor to stratospheric ozone depletion, making its conversion to environmentally benign N_2 an important area of research. However, this poses a significant challenge, as N_2O is kinetically inert and its activation is hindered by a substantial kinetic barrier. In nature, this transformation is carried out by nitrous oxide reductase (N_2OR), a copper-containing enzyme composed of two distinct copper centers: the CuA site, which facilitates electron transfer, and the CuZ site, a

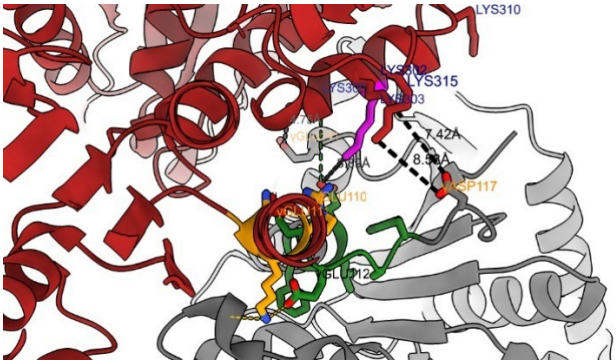
(m4S-Cu4) unit containing a copper cluster responsible for N_2O binding and reduction. Inspired by this biological system, we explore in this project the synthesis of three dicopper complexes supported by deceptively simple, neutral, tridentate pyridine–amine ligands (RL; R = Me, iPr, tBu). The resulting $(RL)_2Cu_2$ complexes were comprehensively characterized by single-crystal X-ray crystallography, NMR spectroscopy, mass spectrometry, and FTIR spectroscopy. These complexes provide a well-defined platform for investigating copper-mediated electrochemical reduction of nitrous oxide (N_2O) to N_2 and H_2O. Cyclic voltammetry reveals that the concentration of the proton source strongly influences the electrochemical deoxygenation of N_2O. Control experiments using the corresponding Zn(II) analogue further establish the essential role of copper in the reaction. Complementary theoretical calculations and spectroscopic studies, together with evidence for metal–ligand cooperativity, support a copper-mediated pathway for the reduction of N_2O to N_2.

SWRM 2026 SW97

Mapping the electrostatic interface of the *Azotobacter vinelandii* MoFe protein for light-driven, bio-hybrid nitrogen reduction

***Marguba Kamrun**, margubakamrun28@gmail.com, Florence Mus, John W. Peters. Chemistry and Biochemistry, The University of Oklahoma, Norman, Oklahoma, United States*

The Haber–Bosch process consumes roughly 1% of global energy and generates 1.4% of global CO_2 emissions. Nitrogenase performs the same N_2-to-ammonia conversion at ambient temperature and pressure, using ATP and its obligate electron donor, the Fe protein. Replacing the Fe protein with 3-mercaptopropionate-capped CdS quantum dots (QDs) drives this chemistry with photons instead of ATP, offering a route to solar-driven ammonia synthesis. QD binding is electrostatic and size-dependent, and proposed to occur at two positively charged, lysine-rich surface patches on the MoFe protein: one adjacent to the P-cluster and one near FeMo-cofactor. However, these sites have not been directly tested. Here, we investigate these putative binding sites using site-directed mutagenesis combined with structural analysis. Lysine residues in both patches of *Azotobacter vinelandii* MoFe protein were substituted with glutamate, singly and in combination. Variants were recovered by rescuing a Δ*nifDK* strain and screened for diazotrophic growth, yielding three distinct phenotypic classes: wild-type growth, measurable growth defects, and failure to rescue.
To interpret these phenotypes, we modeled each mutated residue against the Fe protein across crystallographically characterized docking geometries. The P-cluster patch displays a graded interface with closest approaches ranging from 3.9 to 8.2 Å; βK303 forms a salt bridge with an Fe protein glutamate and alone retains contact across geometries, identifying it as a candidate conformational pivot. Conversely, the neighboring K400 patch forms four hydrogen bonds where this patch forms none, showing distinct binding modes. Because QDs bind through charge rather than directional contacts, the electrostatic patch is the stronger candidate photosensitizer site.
Current work pairs these defined MoFe variants with synthesized 3.4–4.3 nm CdS QDs to establish a platform where photosensitizer binding and catalysis can be varied independently.



Two MoFeP surface patches grip one acidic Fe protein loop. βK303 salt-bridges γGlu110 at 3.9 Å; the β399–401 patch hydrogen bonds to γGlu111/γGlu112 DG1, PDB 2AFH.

SWRM 2026 SW98

Investigating structure-activity relationships of photoactive metallodrugs as antimicrobials

Gurleen Kaur*, gxk7129@mavs.uta.edu, Alisher Talgatov, Dalton Lucas, Broderick Nelson, Ge Shi, Brayden Stackhouse, Chelsea Kimberlin, Kim Luu, Abbas Vali, Colin Cameron, Sherri A. McFarland. Chemistry and Biochemistry, The University of Texas at Arlington, Arlington, Texas, United States*

Despite ongoing efforts to develop novel antibiotics, there is continued and rapid emergence of antimicrobial resistance. Conventional antimicrobials work by blocking steps in a metabolic pathway that are crucial for the survival of pathogens. Over time bacteria can evolve to mount resistance against these mechanisms, rendering the antibiotics ineffective. Therefore, it is advantageous to have complementary approaches in our arsenal against antibiotic resistant bacteria. Photodynamic inactivation (PDI) is an alternative therapeutic strategy for tackling bacterial infections by exploiting light-molecule interactions. PDI utilizes an otherwise nontoxic drug, called a photosensitizer (PS), which can be activated with light in the presence of oxygen to become a powerful antibacterial agent. The premise behind PDI is that PS activation with a certain wavelength of light creates an excited triplet state of the PS that can then sensitize primarily cytotoxic singlet oxygen but also other reactive molecular species (RMS). The immediate burst of relatively nonspecific RMS offers a way to treat bacteria that have already developed resistance to traditional antibiotics. Our research centers on developing new photosensitizer metallodrugs through systematic structural modifications to elucidate structure–activity relationships, with the goal of designing effective lead compounds. In my presentation, I will highlight the significance of these structural modifications and their impact on alternate modes of cytotoxicity against various bacterial strains.

SWRM 2026 SW99

Investigating activity of photoactive metallodrugs as antimicrobial therapeutic agents

Chelsea Kimberlin*, cpk4326@mavs.uta.edu, Alisher Talgatov, Gurleen Kaur, Ge Shi, Brayden Stackhouse, Kim Luu, Broderick Nelson, Dalton Lucas, Abbas Vali, Colin Cameron, Sherri A. McFarland. Chemistry and Biochemistry, The University of Texas at Arlington, Arlington, Texas, United States*

Conventional antimicrobials exert their effects through inhibition at a given step of a vital metabolic pathway. Unfortunately, this creates an artifical selection pressure which favors attaining antimicrobial resistance. One strategy for tackling the issue is photodynamic inactivation (PDI), which utilizes a photosensitizer (PS), light, and oxygen to destroy unwanted pathogens. Illumination of the PS at a given wavelength of light results in activation, as excited electrons populate an excited triplet state. From this state, the PS can then sensitize cytotoxic singlet oxygen and other reactive molecular species (RMS), which damage and destroy the bacterial cell, thus overcoming antimicrobial resistance. Metal complexes are emerging as powerful PS candidates: their purity, their activation by longer wavelengths,and their longer triplet excited lifetimes are among many advantages. We will highlight metallodrug PSs that can inactivate/inhibit the growth of bacteria upon light activation.

SWRM 2026 SW100

Chirality-guided design of pH-responsive self-healing peptide hydrogels

Umesha Subhani Kumbalathara Arachchige Dona*, ukumbal@rockets.utoledo.edu, Olga Makhlynets. Chemistry and Biochemistry, Baylor University, Waco, Texas, United States*

Peptide hydrogels are attractive biomaterials for antimicrobial therapy, tissue engineering, and controlled drug delivery because of their biocompatibility, tunable self-assembly, and stimuli-responsive behavior. We previously developed the L-enantiomeric 11-amino-acid peptide (F11), which exhibits potent antibacterial activity and forms a robust, self-healing hydrogel under mildly basic conditions. In this work, we examine how peptide chirality and sequence modification affect molecular self-assembly and hydrogel formation. The corresponding D-enantiomer (D-F11) was synthesized by solid-phase peptide synthesis and characterized to evaluate its pH-responsive self-assembly and gelation behavior. In addition, histidine at the ninth position was substituted with glutamic acid to examine the effect of this sequence modification on hydrogel formation. Preliminary results demonstrate that D-F11 retains pH-responsive self-assembly and hydrogel-forming behavior. Additionally, the E9 sequence also undergoes hydrogelation, suggesting that a small modification in peptide sequence can either maintain or modify the molecular interactions. Furthermore, mixing the L- and D-enantiomers in water results in spontaneous gel formation, revealing a distinct co-assembly behavior that may arise from intermolecular chiral interactions between the two stereoisomers. A comparative study of the L-F11, D-F11, D-E9, L-E9, and L/D mixtures provides a platform for understanding the relationship between peptide stereochemistry, sequence, self-assembly, and hydrogel mechanics. These findings highlight the potential of chirality-directed assemblies for proteolytic-stable, stimuli-responsive biomaterials. Future studies will characterize the structural basis of L/D co-assembly and evaluate the resulting hydrogels for proteolytic stability, antimicrobial activity, and controlled therapeutic delivery.

SWRM 2026 SW101

Minimizing H_2O_2 driven oxidative stress in immortalized human keratinocytes using a manganese catalase mimic

Slade Lee*[2], s.lee11@tcu.edu, Nora Del Bosque[2], Grant Elam[1], Giridhar Akkaraju[3], Timothy J. Hubin[1], Kayla N. Green[2]. (1) Chemistry, Southwestern Oklahoma State University, Weatherford, Oklahoma, United States(2) Chemistry, Texas Christian University College of Science & Engineering, Fort Worth,*

Texas, United States(3) Biology, Texas Christian University College of Science & Engineering, Fort Worth, Texas, United States

Hydrogen peroxide is a major intermediate involved in the generation of oxidative stress in the human body. A growing number of diseases have been found to have unregulated oxidative stress as an etiological contributor, yet interventions for this imbalance have not been developed. Catalase, a bioprotective enzyme, disproportionates hydrogen peroxide into water and oxygen as a means to regulate oxidative stress. As such, one current approach to minimizing the effects of this oxidative stress is the use of biomimetic compounds, such as manganese-based complexes. The current gold standard for this line of work is EUK-134, a manganese-salen complex which mimics catalase activity. While EUK-134 does show effective cytoprotective effects against hydrogen peroxide, it is limited in its longevity. The Green Group, in conjunction with collaborators at Southwestern Oklahoma State University, have sought to design similar catalase mimics to increase this longevity. By utilizing tetraazamacrocylic scaffolds to provide more rigid manganese complexes, a more stable framework can be achieved.. Here we present the results of biological assays utilizing immortalized human keratinocytes (HaCaT cells) to show the cytoprotective effects of both MnL and industry standard EUK-134. One (MnL) in particular showed strong cell viability across a range of hydrogen peroxide concentrations, compared to EUK-134. This improved cell viability demonstrates that MnL is effective as a cytoprotective catalase mimic, showcasing the potential for development of future macrocyclic manganese-based catalase mimetics.

SWRM 2026 SW102

Comparison of the bioelectrochemical activity of *Methylobacterium extorquens* AM1 grown with La^{3+} and Ca^{2+}

***Chengyang Li**, lic5989@uwec.edu, Krysti L. Knoche Gupta. Chemistry and Biochemistry, University of Wisconsin-Eau Claire, Eau Claire, Wisconsin, United States*

This study compares the bioelectrochemical activity of *Methylobacterium extorquens* AM1 grown in separate media containing La^{3+} or Ca^{2+}. Recent studies have demonstrated that some enzymes in bacteria isolated from lanthanide-rich areas use lanthanides as metal cofactors in place of more common metals like calcium and that these lanthanide enzymes have enhanced catalytic properties. The bioelectrochemical activities of these bacteria have not previously been compared. Nafion modified with tetrabutylammonium bromide (TBAB) is used to immobilize the bacteria on the electrode surface. Cyclic voltammetry is used in Tris-HCl buffer at pH 9 to evaluate the bioelectrochemical activity of methanol oxidation to formaldehyde at different methanol concentrations. Several mediators are also being investigated to identify a suitable mediator for this system. Current results show that the reduction peak increases with increasing methanol concentration for both La^{3+} grown and Ca^{2+}grown *M. extorquens.* If La^{3+} grown *M. extorquens* has higher bioelectrochemical activity than Ca^{2+} grown *M. extorquens*, this could contribute to the development of improved biofuel cells and sensors.

SWRM 2026 SW103

Transmembrane Cu(I) P-type ATPases transport Pt(II)-drugs as electrogenic uniporters

*Madujika A. Horadigala Gamage[1], **Nadeesha Tharangani Liyana Withanage**[1], lxn220033@utdallas.edu, Alessandra Barbanente[2], Yalini H. Wijesundara[1], Jeremiah J. Gassensmith[1], Fabio Arnesano[2], Giovanni Natile[2], Gabriele Meloni[1]. (1) Department of Chemistry and Biochemistry, The University of Texas at Dallas, Richardson, Texas, United States(2) Department of Chemistry, Universita degli Studi di Bari Aldo Moro, Bari, Apulia, Italy*

Cu(I) P-type ATPases are essential transmembrane proteins that regulate cellular copper homeostasis by actively exporting Cu(I) ions across cellular membranes against their electrochemical gradients, thereby functioning as primary-active ion pumps. Overexpression of Cu(I) pumps in tumor cells is associated with pre-target drug resistance to Pt(II)-based chemotherapy, suggesting that they may also facilitate the vesicular sequestration and/or cellular efflux of Pt(II)-complexes. However, the ability of Cu(I) P-type ATPases to translocate Pt(II)-drugs, their selectivity towards Pt(II)-complexes, and the Pt(II)-cargo translocation mechanism remain elusive due to the complexity of monitoring in-vitro turnover Pt(II)-translocation events with purified pumps in membrane-mimetic systems.
In this study, we developed supramolecular mercaptosuccinic acid-capped CdTe core-type quantum dot-encapsulated proteoliposomes (MSA-CdTe QD PLs) to investigate the translocation of Pt(II)-complexes by Cu(I) P-type ATPases in real-time. Since Cu(I) P-type ATPases couple ATP hydrolysis to substrate transport, Pt(II)-complex-stimulated ATPase activity was benchmarked with the real-time translocation of Pt(II)-complexes to validate the developed MSA-CdTe QD PLs platform. Furthermore, by incorporating pyranine and oxonol VI fluorescent probes into the proteoliposome lumen, which are responsive to pH and membrane potential, respectively, we confirmed that Cu(I)-pumps function as primary-active electrogenic Pt(II)-drug uniporters. Additionally, the activity towards Pt(II)-complexes with cis-configuration (such as cisplatin and carboplatin) compared to trans-Pt(II)-complexes (such as transplatin) revealed a characteristic stereoselectivity of Cu(I)-pumps. This work also validates the transmembrane sulfur-based translocation pathway for Pt(II)-complexes by investigating an inactive mutant lacking key conserved cysteine and methionine residues at the transmembrane translocation pathway. Overall, this work unravels the selectivity of Cu(I) P-type ATPases towards Pt(II)-complexes, their translocation mechanism, and establishes the MSA-CdTe QD-encapsulated proteoliposome platform as a versatile tool to study Pt(II) transport across lipid bilayers in other transporter classes.

SWRM 2026 SW104

Synthesis and characterization of light-triggered metal complexes for cancer treatment

***Dalton Lucas**, dsl7696@mavs.uta.edu. Chemistry & Biochemistry, University of Texas at Arlington Research Institute, Fort Worth, Texas, United States*

Photodynamic therapy (PDT) is a clinically approved, minimally invasive treatment modality that uses light activation of a photosensitizer (PS) in the presence of oxygen to generate reactive oxygen species (ROS). These ROS selectively destroy tumor cells and vasculature while sparing healthy tissue and can also stimulate antitumor immune responses. PDT can be used as a standalone treatment or in combination with conventional therapies, particularly when resistance limits their efficacy. In recent years, transition metal complexes, especially those derived from ruthenium (Ru), have garnered significant attention as next-generation PSs due to their tunable photophysical and redox properties. Our lead compound, TLD1433—a Ru(II) tris-diimine complex bearing an imidazo-phenanthroline-terthienyl moiety—has advanced to phase II clinical trials for the treatment of non-muscle invasive bladder cancer. Building on this framework, we have developed a new class of Ru(II) polypyridyl complexes featuring oligothiophene substituents. Here, we systematically examine how varying the number of thienyl groups influences the chemical stability, photophysical characteristics,

and biological activity of these complexes to identify structure–function relationships relevant to improved PDT agents.

SWRM 2026 SW105

Neuroplastics: Learning from real-world plastic particles to uncover the bioaccumulated plastics in the human brain

Alexis Maranan[2,1]*, ironptrp@gmail.com. (1) Science, Carlsbad High School, Carlsbad, New Mexico, United States(2) Pharmacy, University of New Mexico, Albuquerque, New Mexico, United States*

This study aims to examine the physicochemical characteristics of real-world plastic particles generated from environmentally weathered ocean plastics using spectroscopy and microscopy. The overall goal of this research is to define real-world nanoplastics that bioaccumulate in the environment and in the human brain

SWRM 2026 SW106

Ligand-dependent nitroxyl generation from dinitrosyl iron complexes

Esther O. Mosebolatan[1]*, emosebolatan@smu.edu, Aruzhan Abdikaiym*[2]*, Saikat Mishra*[1]*, Chandradeep Ghosh*[3]*, Krish Pudu*[1]*, Marek Freindorf*[1]*, Jeffery Bertke*[4]*, Brad Pierce*[2]*, Paul A. Lindahl*[3]*, Pokhraj Ghosh*[1]*. (1) Chemistry, Southern Methodist University Dedman College of Humanities and Sciences, Dallas, Texas, United States(2) Chemistry, University of Alabama at Birmingham Health System, Birmingham, Alabama, United States(3) Chemistry, Texas A&M University System, College Station, Texas, United States(4) Chemistry, Georgetown University, Washington DC, District of Columbia, United States*

Nitric oxide (NO) is an important signaling molecule involved in diverse physiological processes, while its reduction to nitroxyl (HNO) and N_2O is relevant to NO metabolism. Dinitrosyl iron complexes (DNICs) are recognized as biological NO-storage motifs, but their strongly delocalized $Fe(NO)_2$ electronic structure generally suppresses NO-centered reduction and N-N coupling. We hypothesized that a redox-active formazanate ligand could accommodate an additional electron and perturb this electronic structure to enable HNO formation.
A formazanate ligand containing a nitrile substituent, $[Me_2fNNCN]^-$, or $[L]^-$, was deprotonated to [L]Na, and cyclic voltammetry shows reversible oxidation at -0.30 V and irreversible reduction at -2.68 V vs. $Fc^{+/0}$. Using [L]Na, $[LFe(NO)_2]^0$ (**1**), assigned as $\{Fe(NO)_2\}^9$, was prepared by oxidation of $[Fe(CO)_3NO]^{1-}$ with two equivalents of $[NO]BF_4$. Treatment of the $\{Fe(NO)_2\}^9$ species with a derivative of cobaltocene results in reduction to $[LFe(NO)_2]^{1-}$ (**2**), $\{Fe(NO)_2\}^{10}$. Their ν(NO) bands shift from 1795 and 1735 cm^{-1} (1) to 1692 and 1649 cm^{-1} (2). ^{15}NO labeling gives ν(^{15}NO) = 1760 and 1702 cm^{-1} (1) and 1656 and 1614 cm^{-1} (2). Complexes 1 and 2 undergo reversible $1e^-$ interconversion. X-ray analysis of 2 shows a pseudo-tetrahedral Fe center (tau 4 = 0.16), Fe-N(NO) = 1.659 and 1.642 A, and Fe-N-O angles of 169.8 and 168.4 degrees. Complex 2 is diamagnetic, whereas EPR of 1 gives S = 1/2 and g = 2.010, 2.032, and 2.053, with ^{14}N hyperfine coupling and isotope-dependent splitting.
Reduction of 2 with KC_8 affords $[LFe(NO)_2]^{2-}$ (**3**), formally $\{LFe(NO)_2\}^{11}$, with ~25% conversion in THF and >75% in toluene. Its ν(NO) bands are 1669 and 1620 cm^{-1}, respectively; ^{15}NO labeling gives 1637 and 1591 cm^{-1}. EPR shows S = 1/2 (g = 2.039, 2.039, 2.016) with no significant ^{15}N isotope

shift, indicating ligand-centered spin density. DFT calculations support a $[L^{2-\cdot}]\{Fe(NO)_2\}^{10}$ description and show enhanced Fe-NO covalency. Protonation of 3 produces N_2O ($\nu(^{14}N_2O)$ = 2224 cm^{-1}; $\nu(^{15}N_2O)$ = 2154 cm^{-1}) with an estimated 20% yield. PPh_3 trapping provides $O{=}PPh_3$ (^{31}P = 26.1 ppm) and $HN{=}PPh_3$ (^{31}P = 21.04 ppm; ^1JPN = 61 Hz), directly supporting HNO formation. DFT predicts HNO-bound intermediate formation (deltaG = -14.4 kcal mol^{-1}), HNO release (deltaG = -31.5 kcal mol^{-1}), and conversion of HNO to N_2O (deltaG = -44 kcal mol^{-1}). Mössbauer spectroscopy is ongoing to further confirm the oxidation state of iron in the DNICs.

SWRM 2026 SW107 - Withdrawn

SWRM 2026 SW108

Design and evaluation of photoactive metallodrugs for cancer therapy

***Broderick Nelson**, nelsonbroderick17@gmail.com, Alisher Talgatov, Dalton Lucas, Gurleen Kaur, Ge Shi, Brayden Stackhouse, Kim Luu, Abbas Vali, Colin Cameron, Sherri A. McFarland. Chemistry, University of Texas at Arlington Research Institute, Arlington, Texas, United States*

Photodynamic therapy (PDT) is an alternative cancer treatment that offers high spatial selectivity through the use of light activation. PDT employs a light-activated drug, or photosensitizer (PS), which in the presence of molecular oxygen generates reactive molecular species (RMS) that induce localized cell death. Clinically approved PSs are typically organic tetrapyrroles that mediate cytotoxicity via singlet oxygen and other reactive oxygen species (ROS). Transition metal complexes have emerged as promising alternatives due to their tunable excited-state properties and diverse photochemical mechanisms. Our own ruthenium(II)-based complex, TLD1433 (Ruvidar®), is currently in Phase II clinical trials for non–muscle-invasive bladder cancer (NMIBC). In this work, we describe the design, synthesis, and characterization of new metal-based complexes structurally analogous to TLD1433 that display potent phototoxicity upon light irradiation. Systematic modification of these complexes enables fine-tuning of their photophysical and photobiological properties, offering insights into the structure–activity relationships governing photoactivated cancer therapeutics.

SWRM 2026 SW109

Persulfide-driven oxygen-atom transfer from copper-bound nitrate towards nitric oxide formation

***Esther O. Olatunji**, starola25@gmail.com, Anagha Kuruvayil, Pokhraj Ghosh. Chemistry, Southern Methodist University, Dallas, Texas, United States*

Nitrogen and sulfur redox chemistry intersect in biological systems through reactions involving nitrogen oxides and reactive sulfur species. Nitrate is reduced to nitrite by nitrate-reducing bacteria in the mouth, followed by nitrite reduction to nitric oxide (NO), an important vasodilator. Hydrogen sulfide has been shown to reduce nitrite to NO through an oxygen-atom transfer (OAT) pathway. Sulfur exhibits redox flexibility (-2 to +6), with species such as hydrogen sulfide and thiols showing antioxidant properties. Their reactions with oxidants can involve OAT, providing a pathway for sulfur species to mitigate oxidative stress. Hydrogen sulfide reacts with oxidized thiols, including disulfides

and sulfenic acids, to generate persulfides, whose reactivity is influenced by their S-S bond. At physiological pH, they are present as the anionic form, and the terminal sulfur is highly nucleophilic. This reactivity allows them to participate in reactions with electrophiles and oxidants, making them useful in sulfur-mediated redox chemistry. Here, I investigate whether this reactivity can promote OAT from metal-bound nitrate to drive nitrate reduction to NO. To investigate this, a tridentate pyridine-diimine ligand was synthesized and coordinated to Cu(I) using tetrakis(acetonitrile)copper(I) hexafluorophosphate to give the Cu(I) complex. Reaction with silver nitrate generated the Cu(II)-nitrate complex, characterized by X-ray diffraction, IR, EPR, UV-Vis, and ESI-MS. The complex was then treated with *tert*-butyl persulfide generated in situ, resulting in *tert*-butyl thiosulfonate and NO, which was trapped using cobalt(II) tetramethoxyphenylporphyrin, giving a 38% yield of NO. IR spectroscopy supported NO binding with a band at 1679 cm^{-1}, assigned to v(N-O). The formation of *tert*-butyl thiosulfonate was confirmed by ESI-MS at *m/z* 153. Together, these results support OAT from copper-bound nitrate by the persulfide, producing NO and an oxygenated sulfur product. Future work will optimize NO yield, investigate the reaction mechanism, and use computational studies to support the proposed OAT pathway.

SWRM 2026 SW110

Cu- and Ni-based transition metal catalysts for efficient electrocatalytic CO_2 reduction

***Snehil Patel**, snehilp306@gmail.com, Anagha Kuruvayil, Saikat Mishra, Pokhraj Ghosh. Chemistry, Southern Methodist University, Dallas, Texas, United States*

One of the main causes of the greenhouse effect, global warming, climate change, ocean acidification, and related downstream environmental disruptions is the rising amount of CO2 in the atmosphere. To decrease the adverse effects of CO2 on the environment and advance a circular carbon economy, techniques for its reduction and use must be developed. Using renewable electricity, electrocatalytic CO2 reduction (CO2RR) provides a sustainable method of turning CO2 into fuels and value-added products. By lowering reliance on expensive and scarce precious metals, using earth-abundant transition metals like Cu and Ni as electrocatalysts can further improve the process's sustainability and economic viability. Transition metal catalysts are promising candidates for effective CO2 reduction to value-
added chemicals. This project focuses on electrocatalytic CO2 reduction using Cu and Ni complexes supported by versatile pyridinedicarboxamidate ligands, which can stabilize metals in higher oxidation states. Our design of molecular electrocatalysts is inspired by the active site of the NiFeCODH enzyme, in which the reduced Ni-CO2 intermediate is stabilized by strategically positioned lysine and protonated histidine residues. Using the aminoindole residues in the secondary coordination sphere of the ligand system, our aim is to understand the effect of hydrogen bonding in the stabilization of intermediates and overall electrocatalytic CO2 reduction. We have synthesised metal(II) complexes, [7-indLNi]− and [7-indLCu]− that incorporate 7-indole-based hydrogen-bond donors in the secondary coordination sphere. The complexes [7-indLNi]NBu4 and [7-indLCu]NBu4, were further characterised by X-ray diffraction in the solid state. Electrochemical studies reveal the proton-assisted CO2 activation. Current investigations are going on to analyze the CO2 reduction products and the efficiency of the catalyst.

SWRM 2026 SW111

Assembly and characterization of human Ag(I)- and Au(I)-metallothionein metal-thiolate clusters: Comparative investigation of MT-2 and MT-3 isoforms

***Nazer Hossain Qasimi**, n.h.qasimi1992@gmail.com. Chemistry and Biochemistry, The University of Texas at Dallas School of Natural Sciences and Mathematics, Richardson, Texas, United States*

Human metallothioneins (MTs) are small (6-7 kDa) cysteine-rich metal-binding proteins central to zinc homeostasis and detoxification of a variety of xenobiotic metals. While MT-2 and MT-3 share 20 conserved metal-binding cysteines, isoform-specific non-coordinating residues modulate their functional metal selectivity bias. This study investigates the interaction of the soft monovalent metals Ag(I) and Au(I) with MT-2 and the brain-specific MT-3 isoform, characterizing their metal-binding mechanisms, cluster structures, and reaction kinetics in a comparative framework.
Electronic absorption and circular dichroism (CD) spectroscopies were applied to monitor the progressive formation of silver- and gold-thiolate clusters in Zn7MTs, confirming metal-driven displacement of Zn(II) from both isoforms. Low-temperature (77 K) luminescence spectroscopy revealed that Ag(I) binding proceeds via a highly cooperative mechanism, with titration data identifying distinct break points suggesting stepwise, domain-specific cluster assembly in both isoforms. Parallel characterization of Au(I) binding also revealed characteristic isoform-distinct cluster structures and assembly profiles. To complement these equilibrium thermodynamic observations, stopped-flow spectroscopy was employed to resolve the kinetic profiles of the metal substitution reactions. A marked isoform-dependent kinetic bias was observed for Ag(I), with MT-3 exhibiting significantly faster Zn(II) displacement and metal binding rates compared to MT-2. Conversely, Au(I) substitution kinetics revealed the opposite trend, with MT-2 reacting faster than MT-3, thus representing a reversal of isoform-specific kinetic bias relative to Ag(I). These findings demonstrate that the kinetic selectivity between MT isoforms is governed by an interplay between the coordination chemistry of the incoming metal and isoform-specific protein determinants, including the distinct chemical properties of Ag(I) and Au(I) and the non-coordinating residues unique to each MT isoform.

SWRM 2026 SW112

Synthesis and characterization of nickel(II) and manganese(III) complexes as phosphoester hydrolase mimics

***Lorena Reyes**, lorenaalydiaa@gmail.com, Briaunna Zamarripa, Hadi D Arman, Ghezai T. Musie. Chemistry, The University of Texas at San Antonio College of Sciences, San Antonio, Texas, United States*

Phosphoester bonds are remarkably resistant to spontaneous hydrolysis, a property that is essential in biological systems but problematic when these bonds are present in persistent organophosphate pesticide and pollutants, including chlorpyrifos. Metalloenzymes such as alkaline phosphatase overcome this stability by using metal centers in nitrogen and oxygen coordination environments to activate water and promote phosphoester bond cleavage under mild conditions. Inspired by these systems, we are investigating water-soluble nickel and manganese complexes supported by the amine and carboxylate-rich ligand N,N′-bis[2-carboxybenzomethyl]-N,N′-bis[carboxymethyl]-1,3-diaminopropan-2-ol (H_5ccdp). Using the same ligand framework, we synthesized and fully characterized a mononuclear nickel(II) complex [Ni(Hccdp)(OH_2)$_2$], a dinuclear nickel(II) complex [Ni_2(ccdp)($NCCH_3$)(OH_2)], and a tetranuclear manganese(III) complex [Mn_4(ccdp)$_2$(μ-OH)$_2$(μ-OAc)$_2$]. The hydrolytic activity of these complexes towards 4-nitrophenyl phosphate (pNPP) and bis(4-nitrophenyl) phosphate (BNPP) as model phosphoester substrates is being investigated in aqueous buffer solution. Preliminary studies at pH 8 and different temperatures show that the observed rate

increases as the pNPP concentration increases. These results establish a trend among structurally related nickel(II) and manganese(III) complexes that can be used to directly examine how metal identity, coordination environment, and nuclearity affect the rate of phosphoester hydrolysis in water.

SWRM 2026 SW113

Life cycle of chemotherapy drugs in our environment

John-David Rodriguez*, johndavid.rodriguez@go.tarleton.edu, Rajani Srinivasan, Parvathi Nair, Arthur A. Low, Anne Egelston. Chemistry, Geosciences, And Physics, Tarleton State University, Stephenville, Texas, United States*

The increasing prevalence of cancer treatment drugs in the environment raises concerns about their impact on non-target organisms, particularly invertebrates. This study investigates the absorption of various cancer treatment drugs into invertebrate tissues by exposing them to controlled concentrations of these pharmaceuticals. The first phase of the research involves systematically monitoring the uptake of the drugs within selected invertebrate species, employing analytical techniques to quantify drug concentrations in their tissues. The results will help elucidate potential bioaccumulation and toxicity risks associated with environmental exposure to these compounds. The second phase aims to address the environmental persistence of cancer drugs by evaluating the efficacy of biopolymers in removing them from the aquatic environment. Various biopolymer materials are tested for their ability to bind and sequester the drugs, thereby preventing their absorption by invertebrates. The implications of this research extend to developing strategies for mitigating the ecological risks posed by pharmaceutical contaminants, enhancing our understanding of drug-environment interactions, and informing future regulations on cancer treatment drug disposal. This study underscores the importance of interdisciplinary approaches in evaluating the environmental fate of pharmaceuticals and safeguarding aquatic ecosystems.

SWRM 2026 SW114

NO-H2S crosstalk at the zinc centre: Isolation and reactivity of zinc-perthionitrite complex

Yasmina Said*, ysaid@smu.edu, Anagha Kuruvayil, Pokhraj Ghosh. Southern Methodist University, Dallas, Texas, United States*

Both nitric oxide (NO) and hydrogen sulfide (H2S) are crucial gasotransmitters that support physiological processes like vasodilation, immunological response, and neurotransmission, while being well-known poisons at greater concentrations. The potential participation of many cross-talk intermediates, including thionitrous acid (HSNO) and perthionitrous acid (HSSNO), is raised by the chemical reactivity profiles of NO (either as reductant or oxidant) and H2S (as reductant). HSNO is most likely present in the anionic thionitrite (SNO) form under physiological conditions (pKa = 3.5). Similar to HSNO, perthionitrous acid (HSSNO) is mostly found as anionic perthionitrite (SSNO-) at physiological pH (pKa=0.2) and is likewise hypothesized in H2S/NO crosstalk. The coordination chemistry of SNO-/SSNO- with biologically relevant metal centres is complex and not well understood. This project is exploring the reactivity of perthionitrite and thionitrite at a biologically relevant redox- inactive zinc centre. Here we report the synthesis and crystallographic characterisation of a zinc-bound perthionitrite complex. With the use of an electronically and sterically tunable tridentate pyridinediimine as ligand platform, we have synthesised zinc perchlorate complex.

Reaction of the pyridinediimine Zinc perchlorate complexes with Na(15-C-5)SSNO at -40 °C, we were able to isolate the perthionitrite-bound zinc complexes. We characterised the zinc perthionitrite complexes by SC- XRD, UV-vis, and FTIR spectroscopies. Future reactivity studies will analyse the conversion of Zn-SSNO to Zn-SNO using phosphine at low temperature under UV-vis conditions. We will also examine the reactivity and signalling output of isolated Zn-SSNO complexes in reactions with biologically relevant acids, thiols, and nucleophiles.

SWRM 2026 SW115

Photobiological applications of light-activated metallodrugs

***Alisher Talgatov**, alisher.sct97@gmail.com, Dalton Lucas, Broderick Nelson, Ge Shi, Gurleen Kaur, Brayden Stackhouse, Kim Luu, Chelsea Kimberlin, Abbas Vali, Colin Cameron, Sherri A. McFarland. Chemistry and Biochemistry, The University of Texas at Arlington, Arlington, Texas, United States*

Photodynamic therapy (PDT) is a selective cancer treatment strategy that combines a nontoxic prodrug -known as a photosensitizer (PS)- with light and molecular oxygen to generate reactive molecular species (RMS) that induce localized cell death. Clinically approved PSs are typically organic tetrapyrroles (e.g.: Photofrin, the only FDA-approved PS for cancer therapy), which mediate their effects primarily through singlet oxygen ($^1O_2$) and other reactive oxygen species (ROS). Our research focuses on developing next-generation metallodrug PSs that leverage unique excited-state configurations and alternate modes of action for photocytotoxicity. One such compound, TLD1433 (Ruvidar®), a Ru(II) oligothienyl polypyridyl complex designed and synthesized in our laboratory, is currently in Phase 2 clinical trials (ClinicalTrials.gov identifier: NCT03945162) for photodynamic treatment of non-muscle invasive bladder cancer (NMIBC). In this work, we present a new class of Ru-based PSs structurally related to TLD1433 and demonstrate their potent light-driven cytotoxicity. These complexes expand the design space for metal-based PDT agents, offering tunable photophysical properties and potentially distinct modes of biological action. Beyond their therapeutic applications, these complexes provide a unique opportunity to probe fundamental photochemical and photobiological processes—offering insight into alternative modes of cellular damage and energy transfer that may be harnessed in other light-driven biomedical or materials applications.

SWRM 2026 SW116

Computational analysis of nitric oxide dioxygenase biomimicry with tetra-aza macrocycles

***Caden-Jack Walls**[1], wallscaden@gmail.com, Kayla N. Green[1], Benjamin G. Janesko[1], Pokhraj Ghosh[2]. (1) Chemistry & Biochemistry, Texas Christian University College of Science & Engineering, Fort Worth, Texas, United States(2) Chemistry & Biochemistry, Southern Methodist University Dedman College of Humanities and Sciences, Dallas, Texas, United States*

Nitric oxide (NO) is a gaseous, free-radical and serves as a 2◦ messenger with a half-life of 3-5 seconds. Nitric oxide can be expressed in response to invading microbial species, cardiac vasodilation, or neuronal signaling. Overexpression of the cytoprotective NO can lead to high concentrations of cytotoxic peroxynitrite ($OONO^-$), causing nitroxidative stress. Biology neutralizes toxic concentrations of this species using Nitric Oxide Dioxygenase (NOD), whose activity we hypothesize can be mimicked using water-soluble, non-heme macrocycles to convert NO to NO_3^-. This potential biomimetic activity was explored using Density Functional Theory (uM11/LANL2DZ) as

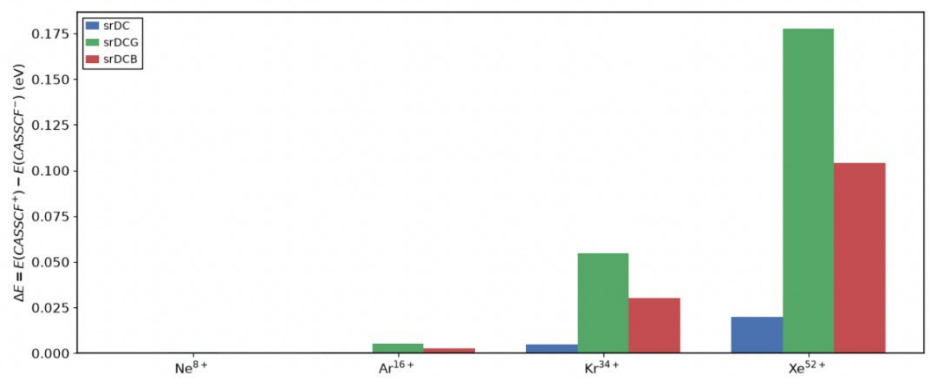
well as Conformer-Rotamer Ensemble Sampling Tool (CREST) on three Fe^{II}-centered tetra-aza macrocycles (cyclen, cyclam, and pyclen). The results to date suggest that the overall catalysis is exergonic and cis/trans geometry of the free reactive coordination sites may play a large role in the stability of key intermediates. Transition state modeling was also carried out to better understand the overall mechanism of the catalysis. Further experiments will be performed with reactivity studies to confirm these computational observations, as well as changes to the structures of the macrocycles to improve the free energies of each step in the reaction pathway.

SWRM 2026 SW117

Converging electron correlation for scalar-relativistic 4-component CASSCF

***Emmy Morrissey**, ejhenshaw@miners.utep.edu, Chad E. Hoyer. Chemistry, The University of Texas at El Paso, El Paso, Texas, United States*

Lanthanides and actinides play critical roles in applications including energy production, catalysis, and medicine. Computational modeling of these systems remains challenging because partially occupied *f*-orbitals give rise to numerous low-lying states and significant static correlation. Multi-reference methods, such as complete active space self-consistent field (CASSCF), are therefore essential for accurately describing near-degenerate states. In addition, relativistic effects become increasingly important for heavier elements and must therefore be incorporated. Relativistic CASSCF calculations permit orbital rotations between positive- and negative-energy states, increasing computational cost. However, the extent to which these rotations contribute to the recovery of electron correlation remains unclear. To assess their importance, relativistic CASSCF calculations employing several scalar-relativistic Hamiltonians were performed on closed-shell ions, alkaline-earth atoms, and the actinide complex UO_2^{2+}. These systems were used to probe core-electron correlation, valence-electron correlation, and actinide chemistry, respectively. Results show that the contribution of negative-energy orbital rotations to core-electron correlation increases with atomic number, while valence-electron correlation is largely unaffected. These findings suggest that restricting orbital rotations to the positive-energy manifold may therefore reduce computational cost while maintaining accuracy in valence-electron correlation treatments.



Effect of Negative-Energy Orbital Rotations on Core-Electron Correlation Energy

SWRM 2026 SW118

Accelerating mechanistic discovery in Pd-catalyzed transformations using MLIP-driven automated workflows

***Dev Dodiya**, devdodiya27@gmail.com, Kyohei Yamada, Vladimir Gevorgyan, Alistair Sterling. Department of Chemistry and Biochemistry, The University of Texas at Dallas, Richardson, Texas, United States*

The discovery of catalytic reaction mechanisms is often constrained by the high computational cost of quantum chemical calculations and the manual effort required for reaction pathway exploration. Here, we present an automated workflow that combines machine-learned interatomic potentials (MLIPs) with quantum mechanical (QM) refinement for reaction exploration through ChemRefine to accelerate mechanistic studies in organometallic catalysis. This approach enables efficient exploration of complex reaction landscapes while automating the execution and management of computational workflows. The utility of this workflow is tested on two Pd-catalyzed asymmetric transformations. In both cases, MLIPs are employed to rapidly sample the potential energy surface and identify candidate intermediates and transition states, providing a computationally efficient alternative to extensive direct QM searches. The resulting structures are subsequently refined and validated using higher-level quantum chemical calculations to ensure reliable energetic characterization. In the first example, our mechanistic analysis uncovers a pair of competing cationic and neutral pathways that control enantioselectivity in a Pd-catalyzed allylic C–H amination reaction. In the second example, we successfully reproduce experimental regio- and enantioselectivity for a Pd-catalyzed radical cyclization, suggesting a “memory of chirality” hypothesis. By integrating fast MLIP-based exploration with QM refinement, our workflow significantly reduces the computational cost of mechanistic investigations while maintaining reliable energetic predictions. The use of MLIPs as a rapid screening tool makes the exploration of numerous mechanisms in large catalytic systems with hundreds of atoms computationally feasible. These results demonstrate the potential of MLIP-enabled high-throughput computational workflows to support scalable reaction discovery and accelerate mechanistic investigations in catalysis.

SWRM 2026 SW119

Understanding SiO_2 etching using HF(aq) via first-principles molecular dynamics

***Stacie R. Moreno**[2,1], morenostacie81@gmail.com, Kriti Alam[2], Prajay Patel[1,2], Hsin-Yu Ko[2]. (1) Chemistry, University of Dallas, Irving, Texas, United States(2) Chemistry, University of North Texas, Denton, Texas, United States*

Despite decades of research on etching mechanisms, understanding the behavior of aqueous hydrofluoric acid (HF(aq)) as an etchant remains critical for advanced semiconductor manufacturing. Using *Ab-Initio* Molecular Dynamics (AIMD), this study aims to model explicit condensed-phase systems associated with HF-based SiO_2 etching processes to obtain a mechanistic understanding at quantum-level accuracy. We begin by probing the concentration effects on reactive proton-transfer events that connect HF with other relevant ionic forms (e.g., F^- and HF_2^-). The ideas are also extended towards understanding the impact of the microelectronic dielectric surface, SiO_2 on the dissociation equilibrium of HF. The results in this study demonstrate the importance of an explicit account of the condensed-phase environments in understanding, modeling, and ultimately controlling the complex interplay of reactive processes at this important microelectronic interface.

SWRM 2026 SW120

Investigating the effects of mutation on the dissociation kinetics of barnase-barstar using atomistic simulations in implicit solvent

Cecilia Fojut[1,2]*, cfojut@udallas.edu, Dipesh Shrestha*[1]*, Prajay Patel*[2,1]*, Omar Valsson*[1]*. (1) Chemistry, University of North Texas, Denton, Texas, United States(2) Chemistry, University of Dallas, Irving, Texas, United States*

Protein-protein interactions facilitate many biochemical processes in our bodies. When these interactions become disrupted by mutations or irregularities, our bodies can fall prey to diseases like cancer. Understanding the unbinding mechanisms of protein-protein interactions is vital to our understanding of causes and cures for many diseases. Although not all mutations in a protein complex result in disease, many do affect the unbinding kinetics of protein-protein interactions. Studying unbinding kinetics is crucial to drug research and development because it helps determine how safe and effective a drug will be when applied to a protein system. Atomistic simulations can effectively study protein-protein systems and their dissociation dynamics, but advanced sampling methods are usually necessary to observe unbinding because protein-protein dissociation is a rare event. One such advanced sampling method is infrequent metadynamics, which has been widely used for protein-ligand unbinding. The Barnase-Barstar complex is a prototypical protein-protein complex that is very strongly bound by salt bridges and hydrogen bonding, leading to a unbinding time of around 2.4 to 75 hours for the wild-type. However, a single mutation at the interface of Barnase-Barstar complex decreases the unbinding time from about 75 hours to 1 second. Previous results from the Valsson Research Group have shown that atomistic simulations in explicit solvent using infrequent metadynamics can accurately capture both absolute and relative unbinding kinetics of Barnase-Barstar wild-type and different mutants. In this work, we investigate whether atomistic simulations with implicit solvent can yield unbinding kinetics as accurate as explicit-solvent simulations. We perform infrequent metadynamics simulations on Barnase-Barstar pseudo wild-type and its mutant using implicit solvent. While further investigation is needed, our results indicate that implicit solvent model does not accurately capture unbinding kinetics, as they do not reproduce either the absolute rates or the relative difference in unbinding kinetics between the pseudo wild-type and its mutant. In addition, the unbinding pathways do not seem to align with behavior in explicit-solvent simulations. Further research is underway to verify these results and understand the reason for the inaccuracy in the implicit-solvent simulations.

SWRM 2026 SW121

DFT guided optimization of a general aziridine synthesis

Priyanka Maharana*, maharanapriyanka1002@gmail.com, Sukumar Pradhan, Alex Saucedo, Hannah Cardenas Avila, Alistair Sterling, Connor P. Delaney. Department of Chemistry and Biochemistry, The University of Texas at Dallas, Richardson, Texas, United States*

The aziridine ring is both a stereochemically defined and reactive synthetic handle and a common motif in natural products and medicines. The classical Blum-Ittah synthesis offers a stereospecific means to convert stereodefined epoxides into N–H aziridines. The sequence involves addition of azide to the epoxide, then combination of the resulting 1,2-azido alcohol with triphenylphosphine to form the aziridine. Given the synthetic utility of the reaction, the mechanism of the critical cyclization step has been the subject of persistent debate within the literature. This lack of mechanistic clarity has complicated efforts to rationally optimize the transformation. Herein, we demonstrate

comprehensive modeling of the various mechanisms proposed in the literature using density functional theory (DFT). To streamline these computational studies, we utilized ChemRefine to automate the conformer sampling and optimization for all DFT calculations. Our DFT calculations support a previously unconsidered concerted chain mechanism, rather than those proposed in the literature. Guided directly by these computational insights, we developed a new set of mild, highly efficient reaction conditions that successfully address previous synthetic challenges associated with the cyclization step, providing general access to N–H aziridines.

SWRM 2026 SW122

Unraveling the importance of angular momentum symmetries in phaseless AFQMC trial wavefunctions for atoms and diatomics

Jackson Maxwell[1], *jwmaxwell1@crimson.ua.edu, Don Danilov*[1], *James Shee*[1,2]*. (1) Chemistry, Rice University, Houston, Texas, United States(2) Physics and Astronomy, Rice University, Houston, Texas, United States*

Phaseless auxiliary-field quantum Monte Carlo (ph-AFQMC) is a stochastic electronic structure method that can achieve excellent accuracy for many strongly correlated systems with polynomial-cost scaling with system size. Due to importance sampling and the phaseless constraint, the choice of trial wavefunction can greatly impact the performance of ph-AFQMC. This work investigates the importance of preserving angular momentum symmetries in the trial wavefunctions used to predict ground-state properties of heteronuclear transition metal diatomics (spanning Σ, Π, Δ, and Φ ground states) and f-block atoms. Trial wavefunctions that are eigenfunctions of LZ are generated by diagonalizing the LZ operator within the space of state-averaged complete active space self-consistent field (SA-CASSCF) solutions, and the resulting ph-AFQMC energies are compared against those obtained from state-specific and unpurified SA-CASSCF trials along with unrestricted mean-field trials; Near-exact ASCI+PT2 total energies and bond dissociation energies are used as benchmark values. f-block atoms are treated with a scalar-relativistic X2C Hamiltonian, and first, second, and third ionization potentials are compared with both CCSD(T) and experimental values.

SWRM 2026 SW123

Generation of polarized Hamiltonians on classical computers for simulating open quantum systems with NISQ devices

Abeda Sultana Shamma[1,2], *axs220282@utdallas.edu, Sasanka Dowarah*[2], *Yazdan Maghsoud*[3,1], *Gerardo A. Cisneros*[2,1], *Michael Kolodrubetz*[2]*. (1) Department of Chemistry and Biochemistry, The University of Texas at Dallas, Richardson, Texas, United States(2) Department of Physics, The University of Texas at Dallas, Richardson, Texas, United States(3) School of Chemistry and Biochemistry, Georgia Institute of Technology, Atlanta, Georgia, United States*

This work presents an investigation of molecular electronic transport in OPE-SMe (oligophenylethynylene-sulfurmethyl) systems, focusing on the fundamental challenge of determining how chemical environments and solvent interactions affect charge transport at the molecular scale. This mechanism remains incompletely understood despite experimental observations showing that solvent polarity can modulate single-molecule conductance by nearly an order of magnitude. A hybrid classical/quantum computing workflow was developed in which polarizable QM/MM simulations,

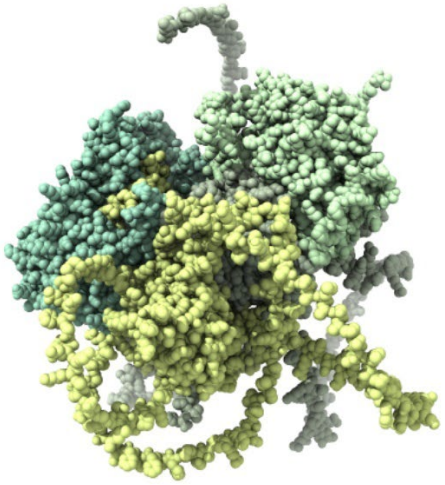
implemented through LICHEM by integrating Gaussian 16 and PySCF with the TINKER molecular dynamics engine and the AMOEBA polarizable force field, generate physically realistic molecular Hamiltonians that incorporate environmental polarization effects from tetrahydrofuran (THF) solvent. These Hamiltonians are converted into second-quantized form following active-space selection using the 6-31+G(d,p) basis set and mapped onto quantum circuits for steady-state charge-transport simulations on a noisy intermediate-scale quantum (NISQ) device. The simulations are performed using classical emulators as well as IBM quantum processors. An additional component of this framework is the integration of NVIDIA GPU acceleration into the PySCF pipeline, enabling larger active-space and higher-accuracy Hamiltonian calculations at substantially reduced computational cost. This capability provides a foundation for planned integration with NVIDIA CUDA-Q and CUDA-QX frameworks to extend the workflow toward increasingly complex molecular electronic-transport systems.

SWRM 2026 SW124

Molecular dynamics simulations of BRAF kinase mutant complexes reveal variant effects and activation mechanisms

Daniel Pearson[1], *daniellouispearson@gmail.com, Abeda Shamma*[1], *Gerardo A. Cisneros*[2,1]. *(1) Chemistry and Biochemistry, The University of Texas at Dallas School of Natural Sciences and Mathematics, Richardson, Texas, United States(2) Physics, The University of Texas at Dallas School of Natural Sciences and Mathematics, Richardson, Texas, United States*

RAF proteins are serine/threonine kinases within the MAPK signaling pathway that regulate cell growth and division. Among them, BRAF is often mutated in cancer, and its kinase activity is associated with specific conformational states and dimerization behavior. There are three classes of BRAF missense mutations that result in distinct signaling pathways through different mechanistic routes, necessitating a framework to explain how sequence variation alters kinase regulation. In this work, we use Molecular Dynamics (MD) simulations with the AMBER ff14SB force field to investigate how oncogenic mutations affect structural and dynamical features in BRAF activation. Specifically, BRAF monomers, BRAF-BRAF homodimers, and BRAF-CRAF heterodimers are simulated to characterize mutation-dependent effects on stability, flexibility, correlated motions, and domain interactions in the kinase region. Each type of assembly is simulated with three independent PTM 500 ns replicates; a complementary set of 200 ns replicates of the non-phosphorylated PTM state is performed by A. \ Shamma to help understand the contribution of phosphorylation to kinase activation across all mutation classes. Our goal is to determine whether computational methods can distinguish the known classes of BRAF mutations based on their structural and dynamical properties. We include representative mutations from each established class: V600E (Class 1, RAS-independent active monomers), G464E (Class 2, constitutively active dimers), and D594H (Class 3, kinase-impaired, RAS-dependent). Additional mutations with less well-defined behavior, including G469A, G469E, and R384G, are analyzed to test whether these signatures can be used to classify variants of unknown mechanism. For each system, an extensive comparative analysis set is performed, ultimately providing a detailed picture of how each mutation class affects BRAF structural dynamics and allosteric communication.



BRAF-CRAF-MEK1 Complex with 14-3-3

SWRM 2026 SW125

Adaptive regularization of density fitting for MP2 and molecular density projection

***Jose Marc Madriaga**, josemmadriaga@gmail.com, Gerardo A. Cisneros. Physics, The University of Texas at Dallas, Richardson, Texas, United States*

Density fitting (DF) is widely used to reduce the computational and storage cost of correlated electronic-structure methods, but inversion of the Coulomb fitting metric can become numerically unstable in the presence of small eigenvalues and near-linear dependencies. We present an adaptive approach that combines the Tikhonov Regularization (TR) with Discrete Picard Condition (DPC) to stabilize the DF metric in second-order M{\o}ller--Plesset perturbation theory (MP2). Rather than relying on a fixed eigenvalue cutoff, the effective truncation of the auxiliary space is determined from the behavior of the discrete Picard spectrum using either a two-line fit to the L-curve or local sharp-corner criteria. The accuracy and computational performance of the resulting protocols were evaluated relative to conventional DF-MP2 for the S22 benchmark set and a hydrogen-atom-transfer reaction involved in AlkB-mediated DNA repair. The three-point sharp-corner protocols provide the best overall agreement with conventional DF-MP2, with SC1-3 showing the most consistent behavior across basis sets, intermolecular systems, and reaction structures. For the S22 dimers, the alternative protocols also exhibit more favorable fitted scaling than conventional DF, with the greatest computational advantage observed for large and diffuse auxiliary spaces. The sensitivity of the regularization to auxiliary-basis size and diffuseness was further examined using the isolated S22 monomers. Increasing the flexibility of the auxiliary representation generally improves the sharp-corner protocols, whereas substantial compression leads to larger and less systematic errors. The two-line protocol is comparatively more robust under these reduced auxiliary spaces. These results also provide insight into the transferability of TR-DPC to density-projection approaches such as the Gaussian Electrostatic Model, where high-level molecular densities are represented using compact auxiliary Gaussian bases. Overall, the results demonstrate that adaptive regularization of the Coulomb metric can provide a balance between numerical stability, accuracy, and computational efficiency across different electronic-structure applications.

SWRM 2026 SW126

Quantifying strong correlation with AFQMC

***Saisrinivas Gudivada**, saigudiva@gmail.com, Brad Ganoe, James Shee. Chemistry, Rice University, Houston, Texas, United States*

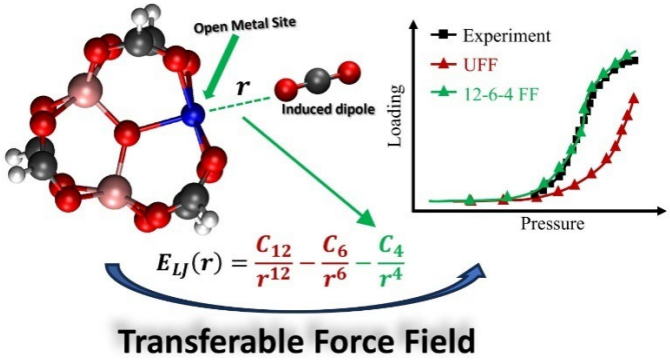
Strong correlation is challenging to describe with most approximate quantum chemical models, including single-reference methods such as Density Functional Theory (DFT), low-order perturbation and coupled cluster theories. Meanwhile, exact methods such as Full CI (FCI) are only feasible for very small systems (generally less than 18 electrons). We aim to shed light on how effectively auxiliary-field quantum Monte Carlo (AFQMC) describes correlated electronic systems, given its low-polynomial scaling with system size and its demonstrated ability to capture strong correlation when using suitable trial wavefunctions such as symmetry-broken mean-field states. We show how AFQMC can qualitatively and qualitatively resemble results from FCI and CC in a set of small molecules with challenging bond dissociation coordinates and motivate applications to larger systems.

SWRM 2026 SW127

Transferable force field for simulating adsorption in metal-organic frameworks with open metal sites based on the 12-6-4 Lennard-Jones potential

***Meng Du**, mengdu.chem@gmail.com. Chemistry Department, Southern Methodist University, Dallas, Texas, United States*

Metal–organic frameworks (MOFs) containing coordinatively unsaturated open metal sites (OMSs) exhibit strong host–guest interactions, making them promising sorbents for low-concentration gas adsorption applications such as direct air capture and atmospheric water harvesting. However, accurately describing host–guest interactions involving OMSs remains challenging for classical force fields (FFs) based on the 12–6 Lennard–Jones (LJ) potential, which does not explicitly account for guest polarization induced by positively charged OMSs. Here, we introduce a 12–6–4 LJ force field that incorporates charge–induced dipole interactions and is parameterized against a diverse set of host–guest potential energy surfaces (PESs) obtained from density functional theory (DFT). The resulting FF, trained on a generic tri-metallic cluster, performs well in both host–guest binding energetics and gas adsorption isotherms across different OMS-containing MOFs, including the MOF-74 series and Cu-BTC. These results demonstrate the strong transferability of our approach and its potential to improve the accuracy and robustness of high-throughput MOF discovery workflows, particularly for gas adsorption and separation across large and chemically diverse MOF databases.



SWRM 2026 SW128

Robust approximation to rank-reduced CCSD(T)$_\Lambda$

***Daniel Devore**, ddevorecollege1@gmail.com, Devin Matthews. Chemistry, Southern Methodist University Dedman College of Humanities and Sciences, Dallas, Texas, United States*

CCSD(T), often regarded as the gold standard of quantum chemistry, performs exceptionally well for molecular structures near equilibrium. However, for bond-breaking processes and nonequilibrium structures, CCSD(T) can produce energies substantially below the full configuration interaction (FCI) limit. CCSD(T)$_\Lambda$ was introduced as a minimal correction that retains the same O(N^7) scaling by incorporating the left-hand Λ eigenvector. In this work, we employ non-antisymmetrized Goldstone diagrams to simplify the implementation of closed-shell rank-reduced coupled cluster theory with single, double, and perturbative triple excitations and left hand Λ amplitudes (RR-CCSD(T)$_\Lambda$). The Singular Value Decomposition (SVD) is applied through the Higher-Order Orthogonal Iteration (HOOI) algorithm to reduce the dimensionality of the triple excitation tensor, t^{abc}_{ijk} , lowering the overall scaling of CCSD(T) from O(N^7) to O(N^6). Three general approaches are considered for approximating the CCSD(T)$_\Lambda$ energy within the rank-reduced framework: 1) compressing the Λ_3 amplitudes and contracting them with the uncompressed Z_3 /T_3 amplitudes; 2) compressing the Z_3/T_3 amplitudes and contracting them with the uncompressed Λ_3 amplitudes; and 3) compressing both Λ_3 and Z_3/T_3 amplitudes before performing their contraction. We introduce these three approaches and assess their accuracy relative to canonical CCSD(T)$_\Lambda$. Finally, we demonstrate how the three approaches can be combined to provide a robust and computationally efficient approximation to RR-CCSD(T)$_\Lambda$.

SWRM 2026 SW129

Locally-optimal construction of pair and hybrid pair grids in LS-THC-MP2

***Afifa Yousaf**, ayousaf@smu.edu, Devin Matthews. Chemistry, Southern Methodist University, Dallas, Texas, United States*

The computational scaling advantages of Tensor Hyper-Contraction (THC) in post-Hartree–Fock methods depend strongly on how the underlying grid is pruned, making grid quality a key bottleneck for the broader adoption of THC. An efficient grid rests on two aspects: (1) the comprehensive representation of the grid, and (2) the algorithm used to select its points. Our previous work has shown that a new type of grid point, pairs of grid points, is critical for a better representation of the correlation between electrons. In addition, we proposed a new grid-pruning algorithm that selects points according to their individual contributions to the total energy, rather than relying on the conventional Cholesky decomposition approach. In this work, we integrate these two methods into a unified scheme and investigate the spatial distribution of the most energetically important pair points, as well as the locally-optimal convergence of the MP2 energy in hybrid single/pair point bases. Tested across several molecular systems, three correlated wavefunction methods, and four basis sets, this scheme yields faster and more consistent convergence of both the Coulomb and exchange energies. These results highlight a promising direction for the continued development of THC methodology.

SWRM 2026 SW130

Non-Markovian dynamics of exciton-polaritons

***Rajanya Sarkar**, rajanyasarkar67.rs@gmail.com. Chemistry, Texas A&M University, College Station, Texas, United States*

Recent experiments demonstrate that exciton-polaritons, i.e. hybrid light-matter quasiparticles, can sustain coherent quantum propagation across mesoscopic length scales, even at room temperature. However simulating such mesoscale dynamical phenomena is a challenging task. To resolve this issue we develop a non-Markovian master equation approach which is combined with a custom coarse graining scheme. Using this approach we simulate exciton-polariton transport at room temperature and show that phonons renormalizes group velocity which is similar to what has been observed in recent experiments. Finally we combine our approach with on-the-fly DFTB/TD-DFTB simulations and make predictions that are experimentally relevant.

SWRM 2026 SW131

Microscopic theory of spin-orbit interactions of light

***Michael Fowler**, michaelfowler135@gmail.com, Saeed Rahmanian Koshkaki, Arkajit Mandal. Chemistry, Texas A&M University, College Station, Texas, United States*

We investigate how phonon-induced decoherence plays a role in the spin-polarized transport of spin-orbit coupled light. To provide microscopic insights, we adapt a light-matter Hamiltonian beyond the long-wavelength approximation and perform quantum dynamics using a mixed quantum-classical approach. Within this approach, the phonon degrees of freedom are evolved using Hamilton's equations of motion, while spin-orbit coupled photons are treated quantum mechanically. Using this approach, we investigate the dynamics of spin-polarized transport near the diabolical point, for which extensive experimental results are readily available. We provide insight into how phonon-induced dynamical disorder leads to the decoherence of photonic spin dynamics and how this ultimately impacts spin-polarized transport. We also analyze how such phonon-induced disorder also breaks photonic spin-momentum locking. Overall, our results provide crucial microscopic material design principles to control and manipulate photonic spin-polarized transport in both coherent and incoherent regimes.

SWRM 2026 SW132

***In-situ* grown metal organic framework UTSA-16 on $Ti_3C_2T_x$ MXene improves electrochemical seawater splitting**

***Eugenie Marie Pranada**[1], emapranada@tamu.edu, Desiree Young[2], Bright Ngozichukwu[3], Ray Ozdemir[2], Abdoulaye Djire[3,1]. (1) Department of Materials Science and Engineering, Texas A&M University, College Station, Texas, United States(2) framergy, Inc., College Station, Texas, United States(3) Artie McFerrin Department of Chemical Engineering, Texas A&M University, College Station, Texas, United States*

Direct seawater electrolysis offers a compelling pathway toward sustainable hydrogen production by eliminating the need for energy-intensive desalination; however, its practical implementation remains limited by sluggish kinetics, competing side reactions, and electrode instability in ion-rich

environments. In this work, we report the in-situ growth of the metal–organic framework UTSA-16 on $Ti_3C_2T_X$ MXene, forming a hybrid electrocatalyst that integrates ion-regulating functionality with a conductive two-dimensional scaffold. Structural characterization by X-ray diffraction (XRD), scanning electron microscopy coupled with energy-dispersive spectroscopy (SEM–EDS), and X-ray photoelectron spectroscopy (XPS) confirms the successful formation of the UTSA-16@ $Ti_3C_2T_X$ composite and the preservation of the MXene framework following MOF growth. The resulting heterostructure exhibits improved interfacial integration and surface functionality relative to the pristine components, suggesting effective coupling between the MOF layer and MXene substrate. Electrocatalytic performance was evaluated for both direct seawater and alkaline water splitting. In commercial seawater, the composite achieves a hydrogen evolution reaction (HER) overpotential of 0.474 V at 10 mA cm^{-2}, outperforming the individual UTSA-16 and $Ti_3C_2T_X$ materials under identical conditions, and demonstrates stable operation over 18 h. For the oxygen evolution reaction (OER) in alkaline seawater (KOH + seawater), an overpotential of 0.384 V at 10 mA cm^{-2} is obtained. In 1 M KOH, the composite exhibits significantly enhanced HER activity, requiring an overpotential of 0.180 V, while OER proceeds at 0.461 V, with both reactions maintaining stability over 18 h. The improved HER performance is attributed to the synergistic coupling of the conductive MXene substrate with the ion-interacting MOF layer, which facilitates charge transfer while modulating the local ionic environment. For OER, the composite exhibits comparable activity to its pristine counterparts while maintaining low overpotentials in chloride-containing electrolytes, indicating electrochemical compatibility under oxidative conditions. These findings highlight the role of electrode–substrate interactions in governing performance and demonstrate that MOF/MXene composites can serve as multifunctional platforms for seawater electrolysis.

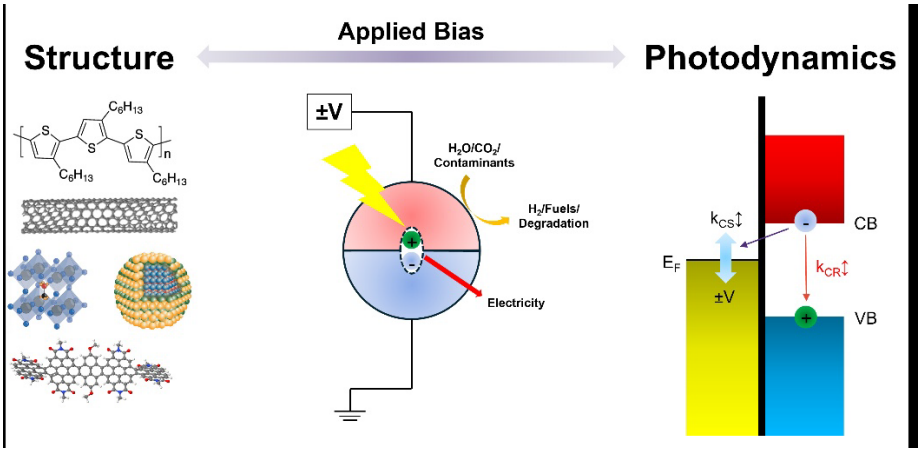
SWRM 2026 SW133

Spectroelectrochemical understanding of the electronic nature of mixed-dimensional excitonic systems

***Hyun Suk Kang**, hkang@tarleton.edu, Christopher Marble. Department of Chemistry, Geosciences, and Physics, Tarleton State University, Stephenville, Texas, United States*

Optoelectronic heterointerfaces with mixed dimensionality, integrating zero-, one-, and two-dimensional (0D, 1D, 2D) excitonic semiconductors, have emerged as a powerful platform for tailoring photodynamics through controlled exciton confinement and interfacial engineering. However, they often suffer from poorly designed interfaces with unwanted recombination channels through traps and energy-level misalignments, hindering photoinduced charge generation and undermining device performance and operational stability.
Previous studies on photoinduced charge separation dynamics in optoelectronic heterojunctions involving 1D semiconducting single-walled carbon nanotubes (s-SWCNTs) and organic electron-accepting materials have shown efficient charge separation and long-lived charge carriers that persist for more than 1.5 μs. However, some heterojunctions show inconsistent interfacial photodynamic properties, such as charge separation rate and yield, with Marcus Theory, which relates band energetics to photoinduced charge separation rates. We hypothesize that different interfacial molecular interactions create discrepancies between interfacial and bulk energetics, such as band offsets and interfacial trap states, which critically contribute to this inconsistency. To resolve this, using spectroelectrochemistry (SEC), we will systematically study donor/acceptor optoelectronic heterojunctions between s-SWCNTs and other low-dimensional semiconductors, such as quantum dots (QDs, 0D), transition metal dichalcogenides (TMDCs, 2D), and 2D metal halide perovskites (MHPs, pseudo-2D), as our model systems. SEC is well established for photodynamic characterization under applied bias and can reveal hidden electronic characteristics of excitonic

systems, including accurate interfacial band offsets via steady-state SEC and possible trap-mediated photodynamics via time-resolved SEC.
New fundamental models will be developed to understand the complex interplay among chemical structures, interfacial coupling, and photoinduced charge separation dynamics, disentangling the intertwined structure-property relationships that govern photodynamics in mixed-dimensional optoelectronic systems.



SWRM 2026 SW134

High purity titanium nitride MXene using repetition synthesis for lithium energy storage

Laura Hoagland[1], *lahoags@yahoo.com, Rabea Kahkahni*[1], *Abdoulaye Djire*[1,2], *Mark Barteau*[1,3]. *(1) Artie McFerrin Department of Chemical Engineering, Texas A&M University System, College Station, Texas, United States(2) Department of Materials Science and Engineering, Texas A&M University System, College Station, Texas, United States(3) Department of Chemistry, Texas A&M University System, College Station, Texas, United States*

MXenes are a family of 2D materials that show great promise in material science and electrochemistry. Nitride MXenes have been less explored due to their more difficult synthesis requirements. However, their predicted electronic conductivity and high surface-area-to-volume make nitride MXenes worthwhile for energy storage research. In this work, a novel repetition approach is used to produce high purity $Ti_4N_3T_x$. To remove aluminum from the precursor Ti_4AlN_3 phase, a eutectic mixture of fluoride salts is combined with the MAX phase and heated to 550°C under argon gas. Then the argon gas is turned off an air is allowed to diffuse into the tube for one hour before the outlets are closed. This oxygen addition is required for the etching to finalize. Once cooled, the molten salt treated sample is washed with acid washed and dried in a vacuum oven. This process is repeated a second time which results in full removal of the aluminum. The sample is then treated with tetramethylammonium hydroxide (TMAOH) which delaminated the MXene's layers and removes a separate oxide phase that forms during etching. Once the suspension has been centrifuged and neutralized, the mixture is left untouched overnight, which separates the MXene from the oxide phase. This produces high purity $Ti_4N_3T_x$ that can be used in electrocatalysis and energy storage. Elemental analysis such as Energy-dispersive X-ray spectroscopy (EDS) and X-ray photoelectron spectroscopy (XPS) shows the removal of aluminum and the presence of nitrogen, while secondary electron microscopy (SEM) proves the formation of accordion-like structures and the removal of the oxide phase. X-ray Diffraction (XRD) indicated the material's crystallinity as well as its high purity, showing no residual Ti_4AlN_3 or oxide peak. The energy storage capability of the material is tested by using the MXene as an electrode in a half-cell against lithium foil.

SWRM 2026 SW135

Metal clusters with well-defined nuclearity for CO_2-assisted propane dehydrogenation

***Elmul Jamal**, elmuljamal@my.unt.edu, Linxiao Chen. Chemistry, University of North Texas, Denton, Texas, United States*

Propylene is an important feedstock for the chemical industry. With the shale-gas boom, propane dehydrogenation (PDH) became an important route for propylene production, which requires high temperatures and often suffers from catalyst deactivation. CO_2-assisted PDH (CO_2-PDH) has become more interest as an alternative approach because CO_2 can be used as a mild oxidant to drive thermodynamics at lower temperatures and alleviate deactivation. Meanwhile, the activity and selectivity of supported metal catalysts depend strongly on the nuclearity of the metal sites, which is difficult to control precisely. In this work, we aim to retain well-defined Rh nuclearity in organometallic complexes on a heterogeneous catalyst by using dispersed In_2O_3 on SiO_2 as anchoring sites for Rh. In_2O_3 was chosen for not only retaining metal nuclearity, but also its ability to assist in CO_2 activation. In_2O_3/SiO_2 supports with 2, 5 and 10 wt% In_2O_3 loadings were prepared, followed by the addition of various wt% of Rh, and their performance was studied for CO_2-PDH. Adding monomeric Rh to the In_2O_3/SiO_2 support significantly improved both the reaction rate and propylene selectivity compared with Rh/SiO_2 and In_2O_3/SiO_2 alone. Among the catalysts studied, 0.02 wt% Rh–2 wt% In_2O_3/SiO_2 showed the best performance, reaching approximately 98% propylene selectivity at 550 °C, with substantially lower apparent activation energy than Rh/SiO_2 and In_2O_3/SiO_2 alone. Increasing the Rh loading to 0.05 wt% did not further improve the catalytic performance, with more severe side reaction, propane cracking, indicating the importance of precisely controlling Rh nuclearity. Kinetic measurements also showed that the reaction rate was strongly influenced by propane partial pressure but changed very little with CO2 partial pressure under the conditions studied. Overall, these results show that combining monomeric Rh with dispersed In_2O_3 can significantly improve the activity and selectivity for CO_2-PDH and highlight the importance of controlling Rh nuclearity in the design of these catalysts.

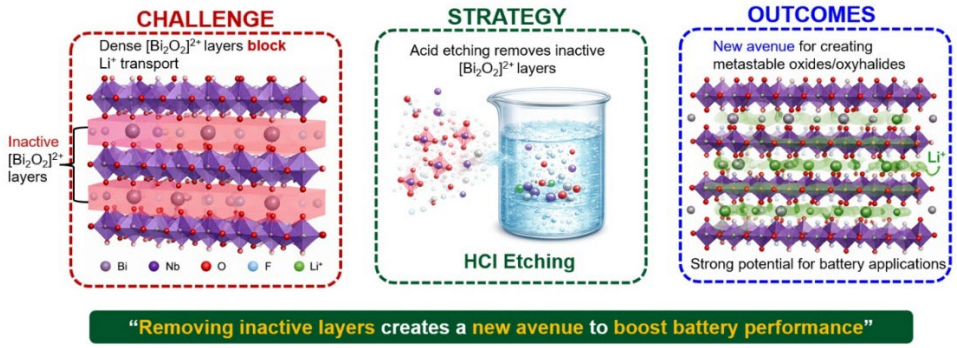
SWRM 2026 SW136

Selective etching strategy for unlocking ion transport in Aurivillius phases

***Nhu Quynh Nguyen**, nhuquynh.nguyen@unt.edu, Ruocun Wang. Materials Science and Engineering, University of North Texas, Denton, Texas, United States*

The discovery of next-generation battery materials is increasingly constrained by the limited structural space accessible through conventional synthesis. Selective etching offers an alternative route to generating new structural frameworks that are difficult to access via conventional synthetic approaches. Here, we extend this concept to layered Aurivillius oxyfluorides, whose electrochemically inactive fluorite-like $[Bi_2O_2]^{2+}$ layers occupy a significant fraction of the crystal structure. We hypothesize that selectively removing these layers can generate a more open framework with increased ion-accessible space. Using Bi_2NbO_5F as a model, we systematically investigated acidic etching by varying the HCl concentration and etching time. X-ray diffraction (XRD) revealed the formation of a new crystalline phase distinct from the precursor, while X-ray photoelectron spectroscopy (XPS) confirmed local chemical reconstruction. Energy-dispersive X-ray spectroscopy (EDS) mapping and spectrum analysis further demonstrated substantial depletion of Bi species while

largely preserving the overall particle morphology. To evaluate the functionality of the etched material, it was investigated as a lithium-ion battery anode, delivering an initial charge capacity of 165.49 mAh g^{-1} over 0.1 – 3.0 V versus Li/Li^+. The material exhibited reversible charge storage at rates up to 20 C (1C = 150 mAh g^{-1}). These findings establish selective acidic etching as a promising strategy for engineering the Aurivillius phases toward next-generation energy storage materials.



SWRM 2026 SW137

Correlating different silver nanoparticle sizes and synthetic routes with CO_2-to-CO selectivity

Soundarzo Tasnim[1]*, stasni1@lsu.edu, Jhonattan David D. Manosalvas Mora*[1]*, Md Yeasin Kabir*[2]*, Md Sohag Hossain*[2]*, Ignace K Agbadan*[1]*, Monsuru O. Dauda*[1]*, Cigdem Atalay-Oral*[1]*, John C. Flake*[1]*, Qingbo Zhang*[1]*, Vicki L. Colvin*[1]*. (1) Cain Department of Chemical Engineering, Louisiana State University, Baton Rouge, Louisiana, United States(2) Department of Chemistry, Louisiana State University, Baton Rouge, Louisiana, United States*

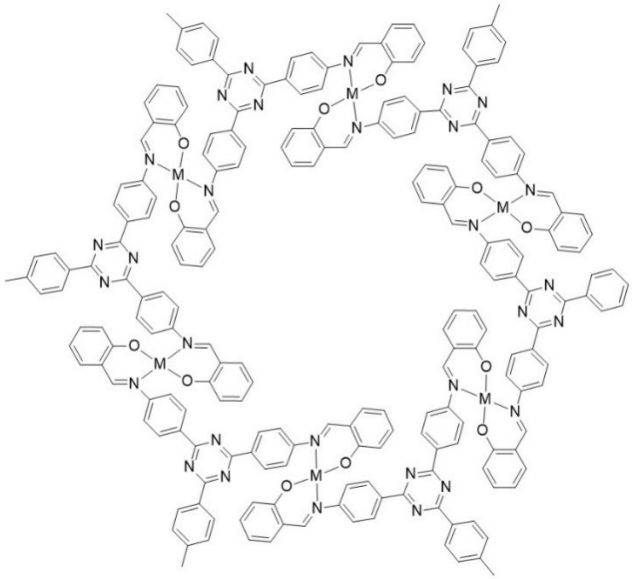
Electrochemical carbon dioxide reduction reaction (CO_2RR) is a promising approach for producing carbon-based chemicals using renewable electricity. However, highly selective catalysts that operate at relevant current densities are still needed. Silver is an attractive CO_2RR catalyst because of its intrinsic selectivity toward carbon monoxide, but the effects of nanoparticle size, morphology, and synthesis-derived surface chemistry remain incompletely understood. Here, we developed a colloidal silver nanoparticle (Ag NP) library using multiple synthetic routes to vary particle size and surface ligand environments. Transmission electron microscopy (TEM) confirmed Ag NP populations spanning approximately 2 to10 nm, including samples with mean diameters of 2.1 ± 0.3, 3.9 ± 0.5, 5.8 ± 0.6, 9.4 ± 1.2, and 9.8 ± 1.2 nm. High-resolution TEM showed multiple twinned domains, indicating twin boundaries and associated lattice strain in our Ag NPs. The Ag NP library was evaluated for CO_2RR at current densities of 100–250 mA/cm^2 in membrane electrode assembly (MEA) cells. It was found that 5.8 ± 0.6 nm Ag NPs achieved a maximum CO faradaic efficiency (FE) of 83% at 150 mA/cm^2, while the 3.9 ± 0.5 nm sample reached 75% CO FE at 200 mA/cm^2. In comparison, the approximately 2 nm nanoparticles showed substantially lower CO selectivity and greater hydrogen evolution. These results identify an optimal Ag NPs size regime for CO_2-to-CO conversion at commercially relevant current densities in MEA cells.

SWRM 2026 SW138

Synthesis and performance of multimetallic Schiff base MOFs in hybrid supercapacitors

***Connor Naseiro**, connornaseiro@gmail.com, Kenneth J. Balkus. Chemistry and Biochemistry, The University of Texas at Dallas, Richardson, Texas, United States*

Supercapacitors are promising energy storage solutions that can help meet the increasing energy demands of AI and EV infrastructure while reducing our dependence on lithium. Hybrid supercapacitors combine the high power density and cycle stability of electrical double layer capacitors (EDLCs) with the high energy density of pseudocapacitors (PCs), creating a better overall capacitor. In past research, MOFs have been used as precursors for the transition metal and transition metal oxide nanoparticles needed for the pseudocapacitive fraction of a hybrid supercapacitor. The Schiff base MOF (SOF) shown in image 1 can also be used for this purpose, however, its Schiff base ligand structure allows it to coordinate with a variety of metals and even multiple metals at once. By using the SOF as a precursor for multiple transition metal nanoparticles within a single hybrid supercapacitor electrode, the electrode becomes redox active at multiple potentials, resulting in a redox cascade that improves energy density. The SOF is synthesized through a Schiff base reaction between the transition metal acetate and salicylaldehyde, with the resulting ligand being linked together with 1,3,5-tris(4-aminophenyl)triazine (TAPT). The SOF is then carbonized by heating to 1000°C under nitrogen. This produces a black powder, which is a mixture of transition metal nanoparticles and carbon. This mixture is characterized using Raman spectroscopy (to determine the graphitic content of the carbon) and XRD (to confirm the presence of metals and find particle size using the Scherrer equation). To form the supercapacitor, the black powder is combined with a binder to form a paste, which is then assembled into a coin cell. Its electrical performance is then characterized by using cyclic voltammetry, galvanostatic charge-discharge, impedance spectroscopy, and a cycle stability test.



Structure of the titular MOF, M = transition metal

SWRM 2026 SW139

Thermal and morphological control of α-CuV_2O_6 photoanodes toward enhanced photoelectrochemical water oxidation

***Mohammad Arham Shamim**, mxs9154@mavs.uta.edu, Abhishek Rawat, Rajeshwar Krishnan. Department of Chemistry and Biochemistry, The University of Texas at Arlington, Arlington, Texas, United States*

Microstructural engineering offers an effective approach to improve semiconductor photoelectrodes without altering their intrinsic electronic structure. Here, phase-pure α-CuV_2O_6 photoanodes were mechanically and thermally tuned to establish relationships among particle size, film morphology, interfacial charge-transfer kinetics, and photoelectrochemical (PEC) water oxidation performance. Mechanical grinding reduced the average particle size from micrometer to submicrometer dimensions while preserving the triclinic crystal structure and optical band gap (~1.8-1.9 eV), enabling the formation of uniform, high-coverage photoelectrode films. Systematic variation of spray-coating cycles and post-deposition annealing temperature identified 60 spray cycles and 450 °C as optimal fabrication conditions. The resulting microstructure provided improved film densification and maximized electrochemically active surface area, promoting carrier utilization while suppressing interfacial recombination. The optimized α-CuV_2O_6 photoanode achieved a photocurrent density of 1.70 mA cm^{-2} at 1.80 V vs RHE, representing the highest experimentally reported photocurrent for α-CuV_2O_6 photoelectrodes to date. Transient photocurrent analysis further indicated that the performance enhancement originated predominantly from reduced surface recombination rather than changes in optical absorption. These results demonstrate how morphology-driven kinetic control can unlock the latent PEC activity of copper vanadate photoanodes and provide a scalable strategy for improving metal-oxide photoelectrodes for solar water oxidation.

SWRM 2026 SW140

Lattice-matched RuO_2-TiO_2 interfaces enable highly active Ru/rutile-TiO_2 catalysts for NH_3 decomposition

***Aswathi Rajeevan V V**, aswathirajeevanvannantevalappil@my.unt.edu, Linxiao Chen. Chemistry, University of North Texas, Denton, Texas, United States*

Hydrogen (H_2) is a promising clean energy carrier for advancing the transition toward sustainable energy systems. However, its storage and transportation as a flammable, high-volume gas cause significant challenges. To avoid this, one can use ammonia (NH_3) as a promising liquid hydrogen carrier with existing infrastructure for safe transportation. NH_3 decomposition at the point of use provides an effective route for on-site H_2 production without direct carbon emissions. The practical implementation of this approach, however, requires catalysts capable of maintaining high activity during extended operation.
In this study, we use a flow reactor coupled with gas chromatography to examine ruthenium (Ru)-based catalysts, particularly epitaxially grown Ru/rutile-TiO_2, for NH_3 decomposition. Our previous study demonstrated that disintegrating epitaxial rutile-RuO2 thin films on rutile-TiO_2 creates sintering-resistant metallic Ru particles of coverage-independent size and shape, with extreme proximity. Here, we found that Ru/rutile-TiO2 catalysts with higher Ru loadings provide significantly higher NH3 decomposition rates. The rates surpass the current benchmark, Ru/MgO, and diminish to negligible, when the TiO2 support phase is switched to anatase, and thus the epitaxy and particle proximity are lost. The high efficacy of Ru/rutile-TiO2 is thus attributed to the particle proximity effects leading to facile N-H activation, as supported by detailed kinetic analysis. Although Ru/rutile-TiO_2 exhibits greater resistance to sintering than Ru/anatase-TiO_2 and Ru/MgO, it undergoes gradual deactivation during NH_3 decomposition, due to structural evolution of the Ru particles during the reaction shown by

operando characterization. This work provides a framework for designing active and stable catalysts through an epitaxial-growth approach. This approach may advance the development of durable catalytic systems for on-demand H2 production from NH_3, supporting ammonia as a practical hydrogen storage and transportation medium. Broadly, our approach provides a general strategy for the facile activation of chemical bonds.

SWRM 2026 SW141

Growing carbon on yttrium doped ceria (CeO_2) nanorods for hybrid supercapacitor application

S M ANYET ULLAH SHOHAG*, anyetullah@gmail.com, Kenneth J. Balkus Jr., **Asher Grills**, Asher.Grills@UTDallas.edu. Chemistry and Biochemistry, The University of Texas at Dallas School of Natural Sciences and Mathematics, Richardson, Texas, United States*

Supercapacitors are a prospective candidate for the technological gap created by increased power consumption and the low power density of traditional batteries like li-ion, which are falling behind the growing demand for electricity. Hybrid supercapacitors have vastly higher power density than traditional batteries with similar energy density, which is still being rapidly improved. Yttrium doped Cerium(IV) oxide (CeO_2) is a promising electrode material for hybrid supercapacitors because its reversible Ce^{4+}/Ce^{3+} redox reactions, oxygen-vacancy-rich structure and, high chemical stability. Growing conductive carbon on it enables enhanced pseudo capacitance, improved cycling stability, and higher energy density. Cerium and Yttrium salts and Sodium Hydroxide precursors were used via hydrothermal process as shown in figure 1 to synthesize Y doped CeO_2 nanorods. Characterization was done by X-ray diffraction which ensures the crystal structure and the particle size was found to be ~20.06 nm using Scherrer's Equation. The conductive carbon was grown on the Y doped CeO_2 ($C@Y_XCe_{1-X}O_2$) using an acetylene-steam method as shown in figure 2. Thermogravimetric Analysis was done to determine the 26.21% carbon deposition on $Y_XCe_{1-X}O_2$ before washing. 1M HCl and DI water was used for washing and drying at 90 °C. Raman Spectroscopy was used to determine the type of carbon grown on the top of $Y_XCe_{1-X}O_2$. Along with a binder like PTFE and $C@ Y_XCe_{1-X}O_2$ was used to prepare the working electrode of a coin cell. Cyclic voltammetry was used to determine the redox activity of the electrodes and galvanic charge discharge to calculate the energy density and power density. Scanning electron microscopy (SEM), and high-resolution transmission electron microscopy (HRTEM) will be done for characterization.

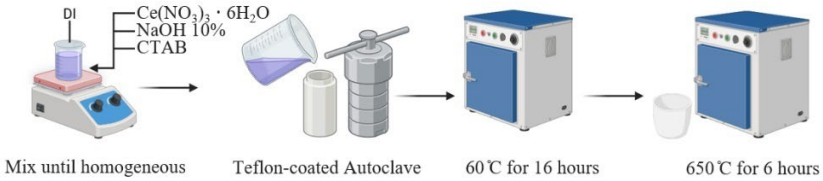


Figure 1: Synthesize Y doped CeO_2 nanorods via hydrothermal process.

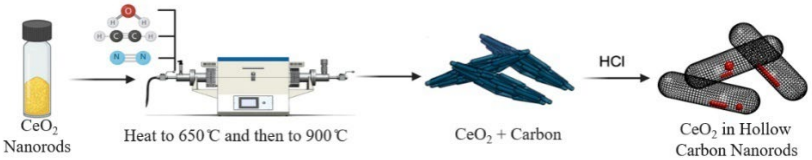


Figure 2: Growing Carbon on the $Y_XCe_{1-X}O_2$

SWRM 2026 SW142

Tuning surface and oxidative charge through interlayer anions for enhanced OER kinetics

***Abhirami V. Krishnan**, avkrishnan@miners.utep.edu, Sreeprasad Sreenivasan. The University of Texas at El Paso College of Science, El Paso, Texas, United States*

The oxygen evolution reaction (OER) involves dynamic charge accumulation and oxidation of transition-metal centers before and during catalytic turnover, making the electrochemical charge state of a catalyst an important factor governing its activity. Here, we investigate NiFe layered double hydroxides (NiFe-LDHs) containing different interlayer anions to understand how the interlayer environment regulates charge accumulation and OER kinetics. Two charge contributions are considered: surface charge, associated with electrochemical charging at the catalyst–electrolyte interface, and oxidative charge, associated with potential-induced oxidation and redox-state evolution of the catalyst. Incorporation of different interlayer anions modifies the local electrostatic and electronic environment of the positively charged LDH layers, thereby influencing surface charging and the accessibility of oxidized metal states under OER conditions. Electrochemical measurements are used to resolve these charge contributions as a function of applied potential and establish their relationship with OER current density. Particular emphasis is placed on determining how changes in surface charge induced by interlayer chemistry affect the accumulation of oxidative charge and, consequently, the catalytic OER rate. The relationship between accumulated oxidative charge and OER current is further compared with conventional potential-dependent Tafel analysis, providing insight into whether differences in apparent OER kinetics originate from changes in catalyst charging, catalytic turnover, or their coupling. By directly connecting interlayer anion chemistry, surface charge, oxidative charge, and OER rate, this study provides a charge-based framework for understanding OER kinetics in NiFe-LDHs and demonstrates the importance of interlayer charge regulation in controlling the electrochemical state and catalytic response of layered electrocatalysts.

SWRM 2026 SW143

Synthesis, characterization, and testing of heteropolyacid-based carbide catalysts for chemical plastic recycling

***Nadiira K. Hassan**[1], nadiirakhadar006@gmail.com, Paige Schreckengost[2], Arpita Vengadessane[1], Linxiao Chen[1]. (1) Chemistry, University of North Texas, Denton, Texas, United States(2) Chemistry and Biochemistry, Angelo State University, San Angelo, Texas, United States*

The accumulation of polyolefin waste highlights the need for effective catalytic processes to convert discarded plastics into value added hydrocarbons. Hydrocracking is a promising chemical-recycling route requiring bifunctional catalysts with balanced hydrogenation and acid functionalities for controlled C–C bond cleavage. This work investigates Heteropolyacid (HPA) as an alternative precursor to WO3 for preparing multifunctional tungsten carbide catalysts. We hypothesize that phosphorus- and oxygen-containing surface species retained after carburization modify catalyst acidity and enhance polypropylene (PP) hydrocracking.
Paired WO3 and HPA derived catalysts were synthesized under flowing CH4 and H2 at temperatures of 400, 590, 750, and 950 °C. The resulting eight materials were screened in a high-pressure reactor (1.0 g PP model feed) under hydrogen atmosphere. Catalytic performance depended on both precursor identity and carburization temperature. The WO3 derived catalyst carburized at 590°C achieved the highest overall PP conversion of 24.8%, whereas the optimal HPA-derived catalyst required 750 °C. Carburization at 950 °C severely suppressed HPA activity.
Ongoing XRD, XPS, BET surface area, particle-size, and temperature-programmed desorption (TPD) acidity measurements will determine whether retained phosphorus species provide beneficial acid

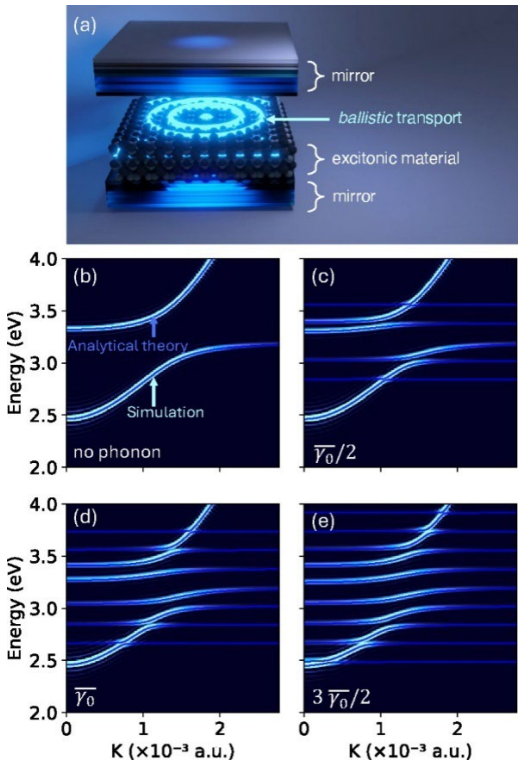
sites or inhibit activity. Establishing these structure-performance relationships will guide the design of optimized carbide catalysts for polyolefin upcycling.

SWRM 2026 SW144

Microscopic theory of polaron-polariton dispersion and propagation

Logan P. Blackham*, lblackha@tamu.edu, Arshath Manjalingal, Saeed Koshkaki, Arkajit Mandal.*
Chemistry, Texas A&M University System, College Station, Texas, United States

We introduce a phonon field picture to tackle the complex interactions between excitons, photons, and phonons, providing microscopic and physical insights into complex light-matter systems. Our approach recovers the exciton-polariton band structure in the presence of strong phonon interactions, which we refer to as the polaron-polariton dispersion. Within our approach, we treat the phononic bath quasi-classically and show that under classical path approximation, the phonon interactions to the polaritons can be reduced to an effective field interacting with exciton-polaritons. We use the Floquet formalism to quantize this phonon field and obtain an analytical expression for the polaron-polariton bands. These bands also provide insights into the renormalization of exciton-polariton group velocity observed in recent experiments. We find that our theory also provides an explanation for the relatively long-lived coherent nature of exciton-polaritons, even for states with high excitonic character.

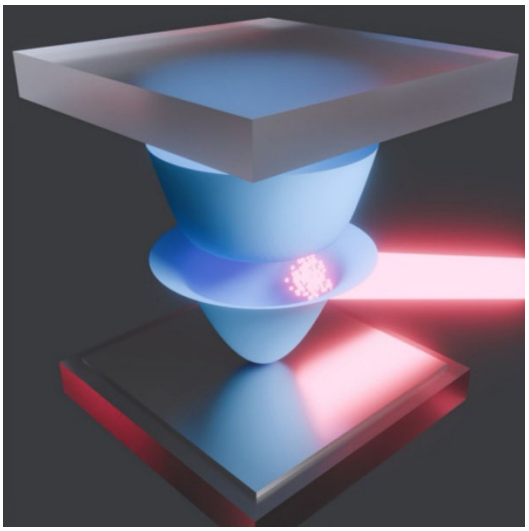


SWRM 2026 SW145

Many-body quantum dynamics of exciton-polaritons

***Pritha Ghosh**, pritha2000@tamu.edu, Arshath Manjalingal, Saeed Koshkaki, Rajanya Sarkar, Sachith P. Wickramasinghe, Arkajit Mandal. Chemistry, Texas A&M University, College Station, Texas, United States*

We develop a mixed-quantum classical mean-field many-body approach that enables us to simulate the exciton-polariton dynamics in Fabry-Perot cavities, so that we go beyond the single-excitation subspace. We do this by combining the multitrajectory mean-field Ehrenfest approach, which treats phonon degrees of freedom classically, along with a mean-field description, equivalent to the Gross-Pitaevskii approach, that describes the many-body nature of the exciton-photon subsystem. Using this approach, we simulate the exciton-polariton dynamics, including its transport, phonon-induced Fröhlich scattering, and decoherence. We demonstrate that these properties are non-linearly modulated by the strength of the driving field due to the intrinsic non-linear exciton-exciton interaction term. Finally, we extend this approach to incorporate many-body correlations that go beyond the mean-field Gross-Pitaevskii description.



SWRM 2026 SW146

Engineering functional gelatin networks through thiol–ene chemistry for tunable 3D biomaterials

*Sara Swank, **Melanie Ecker**, melanie.ecker@unt.edu. Biomedical Engineering, University of North Texas, Denton, Texas, United States*

Functional hydrogels derived from naturally occurring polymers offer an attractive route toward biomimetic materials that combine the biological activity of extracellular matrix components with the chemical tunability of synthetic polymer networks. However, conventional photocrosslinked gelatin hydrogels frequently rely on chain-growth polymerization, which can produce heterogeneous network structures and limit independent control over material properties. Here, we investigate Gel-AGE, a chemically modified gelatin platform designed to exploit thiol–ene click chemistry for the formation of tunable, three-dimensional hydrogel networks. Gel-AGE incorporates pendant alkene functionalities into the gelatin backbone that can react with multifunctional thiol crosslinkers through light-mediated thiol–ene polymerization. The step-growth nature of this reaction provides a versatile approach for controlling network formation through crosslinker structure, functionality, concentration, and thiol-to-ene stoichiometry. Current work focuses on establishing relationships between hydrogel formulation, network architecture, and resulting physicochemical properties, including gelation behavior, swelling,

degradation, and mechanical performance. These studies aim to determine how molecular-level changes in network design translate into macroscopic material properties relevant to biomedical applications. As a model application, Gel-AGE hydrogels are being developed as three-dimensional extracellular matrix mimics for articular cartilage and osteoarthritis research. Ongoing studies are evaluating how hydrogel network composition and mechanical properties influence chondrocyte viability, phenotype, extracellular matrix production, and responses to inflammatory stimulation. Ultimately, the platform will be evaluated for its ability to reproduce key features of healthy and osteoarthritic cartilage and support therapeutic screening. This work explores thiol–ene chemistry as a modular strategy for transforming a biologically derived macromolecule into a functional polymer network with controllable properties. Establishing relationships among chemical formulation, network structure, material properties, and biological response may enable Gel-AGE hydrogels to serve as adaptable biomaterials for tissue engineering, disease modeling, and regenerative medicine.

SWRM 2026 SW147

Discovery and optimization of dynamic covalent polymer formulations using 3D printing

Ronald Smaldone*, ronsmaldone@gmail.com. Chemistry and Biochemistry, The University of Texas at Dallas, Richardson, Texas, United States*

3D printing is primarily considered to be a manufacturing tool, converting polymeric materials and precursors into objects based on a computer model. However, given the ability of a 3D printer to produce many types of different designs, using a range of different materials, they are also beneficial for materials discovery. Our group aims to use digital light projection photoprinting (DLP) to study the effects of form factor and processing conditions on the properties of polymeric materials with dynamic covalent and supramolecular linkages. Dynamic covalent chemical bonds, which can undergo exchange under thermodynamic control, can be used to create self-healable polymers that are compatible with 3D printers and resin formulations. Previously, we have found that dynamic covalent bonds are beneficial for use in thermoset polymer printing as their reconfigurable bonds can improve recyclability as well as reduce internal strain through thermal treatment after printing. Many 3D printed materials lack the strength of conventionally processed polymers and will fail prematurely during use, so the optimization of composition and processing parameters are critically important to improving the quality of 3D printed parts. This talk will discuss methods to use 3D printing as a discovery tool for new thermoset materials and their properties.

SWRM 2026 SW148 - Withdrawn

SWRM 2026 SW149

Coordination-enabled processing of chitosan into moldable, mechanically robust functional materials

Balasubramanian Rukmanikrishnan*, Balasubramanian_RUKM@baylor.edu, Ning Zhang. Mechanical Engineering, Baylor University, Waco, Texas, United States*

The inability to melt-process many naturally derived polymers remains a major barrier to transforming abundant biopolymers into high-value, shape-defined materials and devices. Chitosan is particularly challenging because its highly crystalline structure and dense intermolecular hydrogen-bonding network severely restrict chain mobility, limiting conventional processing primarily to acidic dissolution, hydrogel formation, and solvent-cast films. Here, we introduce a ZnCl2-enabled coordination-processing strategy that unlocks the processability of chitosan, transforming the normally rigid biopolymer into a homogeneous, moldable state within approximately 20 min at only 70 degrees C. Zn2+ coordination is proposed to disrupt native hydrogen-bonded crystalline packing and increase chain mobility, creating a transient processable network that can be readily molded and extruded in the hot state. Upon cooling and solidification, the material forms rigid, mechanically robust three-dimensional objects with stable, well-defined geometries. This rapid, low-temperature process eliminates the need for conventional acidic dissolution and drying-mediated shape formation while enabling direct fabrication of dense chitosan-rich structures. Importantly, the coordination-enabled matrix also permits homogeneous incorporation of nanomaterials, providing a route to simultaneously engineer mechanical and functional properties. These findings establish metal-ion coordination as a powerful strategy for overcoming the intrinsic processing limitations of strongly hydrogen-bonded biopolymers and transforming chitosan from a difficult-to-process biomaterial into a versatile platform for shape-defined functional materials. The approach opens opportunities for advanced applications including bioelectronic and iontronic devices, patient-specific biomedical structures, transient electronics, energy-storage components, and additively manufactured functional biocomposites.

SWRM 2026 SW150

Maleimide–enediyne-functionalized poly(ε-caprolactone) micelles for DNA-cleaving anticancer nanotherapy

***Mihaela C. Stefan**, mihaela@utdallas.edu. Department of Chemistry and Biochemistry, University of Texas at Dallas, Richardson, Texas, United States*

Natural enediynes, exemplified by calicheamicin, possess remarkable DNA-cleaving activity through the generation of highly reactive radicals following Bergman cyclization. However, the clinical translation of synthetic enediyne systems is hindered by poor aqueous solubility, limited stability, and nonspecific cytotoxicity. Here, we report a polymeric nanotherapeutic platform in which maleimide–enediyne motifs are covalently integrated into poly(ε-caprolactone) (PCL) block copolymers through post-polymerization functionalization. The resulting amphiphilic polymers spontaneously self-assemble into spherical micelles with an average diameter of approximately 120 nm and a critical micelle concentration of 9.1×10^{-4} mg mL^{-1}. Micellar assembly significantly improves the aqueous compatibility of the hydrophobic enediyne functionality while providing a versatile platform for the incorporation of hydrophobic chemotherapeutics, including doxorubicin. Electron paramagnetic resonance spectroscopy provides evidence for radical generation and Bergman cyclization under physiologically relevant conditions, supporting the proposed DNA-cleavage mechanism. The functionalized polymers exhibit pronounced DNA-cleaving activity in vitro and induce cytotoxicity in MDA-MB-231 breast cancer cells. These findings demonstrate that covalently integrating reactive enediyne motifs within biodegradable PCL-based nanostructures can combine intrinsic DNA damage with nanoscale drug-delivery functionality. The resulting maleimide–enediyne micelles therefore represent a promising strategy for the development of multifunctional nanotherapeutics for cancer treatment.

SWRM 2026 SW151

Directed self-assembly of chiral liquid crystals into biomimetic Bouligand structures in thin film for functional material design

***Xiao Li**, xiao.li@unt.edu. Materials Science & Engineering, University of North Texas, Denton, Texas, United States*

Chiral nematic or cholesteric phases in liquid crystals (LCs) exhibit asymmetrical packing of molecules, resulting in a finite twist angle between adjacent molecules, and long-range chiral ordering similar to helical superstructures in DNA. The chiral properties of LCs (from nano to micrometers) are widely used in display technologies, electro-optics, and sensors. However, exploiting the full potential of such beneficial chiral structures to adapt to diverse engineering conditions, e.g., temperature, stress, and chemical environments, needs to overcome the inherently weak mechanistic nature of LCs. The Bouligand structure, renowned for its helicoidal arrangement and enhanced mechanical properties, has attracted significant research interest for its ability to impart enhanced strength to intrinsically soft materials. Biomimetic approaches have centered on fibrous structures in bulk materials, but translating this architecture into thin-film regime for miniaturized-wearable devices with programmable functions remains challenging. Here, we direct the self-assembly of cholesteric liquid crystals (CLCs) into hierarchical helical structures using chemically patterned surfaces. Alternating surface anchoring regions align uniform lying-down helices at the nanoscale, guiding a secondary microscale helical structure exhibiting both left- and right-handed twists. This mimetic Bouligand structure in CLCs enables optical modulation under applied field and strain with enhanced mechanical response.

SWRM 2026 SW152

How backbone chirality and charge segmentation influence solution phase separation in polypeptoids and polypeptides

***Donghui Zhang**, dhzhang@lsu.edu. Chemistry, Louisiana State University, Baton Rouge, Louisiana, United States*

Electrostatic interactions between oppositely charged polyelectrolytes and polyampholytes can drive macroscopic phase separation in aqueous solution, producing distinct complexation morphologies through liquid-liquid or liquid-solid phase separation. Understanding how molecular features of these charged polymers can be tuned to control solution phase behavior is of fundamental interest. Moreover, coacervate phases formed by liquid-liquid phase separation are especially promising for applications such as drug encapsulation, bioadhesion, and underwater coatings. Previous studies of oligomeric peptide complexation have shown that backbone chirality influences the stability and morphology of the resulting phases. Here, we synthesize longer-chain synthetic polypeptides and polypeptoids by controlled ring-opening polymerization and investigate how backbone chirality, specifically homochirality, mixed chirality, and achirality, affects solution phase behavior and complexation morphology. We further examine complexation with nucleic acids, revealing that nucleic acid structure and polyelectrolyte backbone chirality together modulate the resulting complex morphologies and their stability in salted solution. In addition, we show that charge segmentation patterns strongly influence liquid-liquid phase separation in polypeptoid multiblock copolymers, leading to distinct pH windows for coacervate formation and varying salt resistance.

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Multifunctional nanoparticle–essential oil topical gels for synergistic antibacterial activity, hemostasis, and accelerated wound healing

Blessing A. Aderibigbe*, blessingaderibigbe@gmail.com. Chemistry, Geosciences, and Physcics, Tarleton State University, Stephenville, Texas, United States*

Developing multifunctional wound dressings that can prevent infection, promote tissue regeneration, and facilitate rapid hemostasis is critical for effective wound management. In this study, topical wound gels based on carboxymethyl cellulose (CMC) and sodium alginate (SA) were loaded with essential oils and metallic nanoparticles. The combination of selected essential oils and metallic nanoparticles was performed to induce synergistic antibacterial activity while maintaining a favourable environment for wound healing. The prepared gels were characterized to determine their physicochemical properties, including homogeneity, pH, viscosity, spreadability, and storage stability. Biological performance was evaluated through cytocompatibility, in vitro scratch wound-healing, antibacterial, and blood-clotting assays. Both CMC and SA gels exhibited excellent cytocompatibility, maintaining cell viability in the range of 75–100% against HaCaT cell lines, indicating their suitability for topical biomedical applications. In vitro scratch assays demonstrated outstanding wound-closure efficiencies of 99-100%, reflecting enhanced cellular migration and proliferation. The incorporation of essential oil and metallic nanoparticles resulted in strong antibacterial activity against wound pathogens, suggesting effective inhibition of microbial growth and potential reduction of wound infection. In addition, the gels displayed good blood-clotting capability, indicating their ability to promote rapid hemostasis during the early phase of wound repair. The combined physicochemical and biological results demonstrate the efficacy of essential oil and nanoparticles in wound healing.

SWRM 2026 SW154

Decoding chemical communication: Structural insights and gating mechanisms of pheromone-binding proteins

Smita Mohanty*, smita.mohanty@okstate.edu. Chemistry, Oklahoma State University, Stillwater, Oklahoma, United States*

Insects possess an extraordinarily sophisticated olfactory apparatus, enabling males to detect and track female-secreted pheromones across distances exceeding three miles. Central to this hypersensitive system are pheromone-binding proteins (PBPs), highly soluble carriers operating within the antennal sensillar lymph. PBPs encapsulate hydrophobic pheromone ligands, safely escorting them through the aqueous extracellular matrix to the olfactory receptor neurons (ORNs). This transport cycle relies on an elegant, pH-dependent molecular switch where ligands are tightly bound at physiological pH but rapidly ejected upon reaching the acidic microenvironment near the ORN, triggering an immediate neuroelectrical response. In the giant silk moth *Antheraea polyphemus*, this structural transition is driven by two distinct biological gates—a histidine pair (His70/His95) flanking one side of the binding pocket and a flexible C-terminal tail acting as a remote molecular plug. Intriguingly, while the PBP of the highly invasive Asian corn borer *Ostrinia furnacalis* shares over 50% sequence homology with that of *A. polyphemus*, its biological gating regions feature key residue substitutions that alter binding dynamics. This presentation will elucidate the comparative structure-function relationships, microsecond dynamics, and mechanistic evolutionary adaptations defining these critical chemical communication targets. This research was supported by the National Science Foundation Award CHEM 1807722 and CHEM 2402694 to Smita Mohanty.

SWRM 2026 SW155

Solution conformational changes in P_{1B}-type ATPase copper binding and Post-Albers cycle states

***Yaamini Subramanian**, yaaminisubramanian@gmail.com, Medhansh Kashyap, Gabriele Meloni, Sheena D'Arcy. Chemistry, The University of Texas at Dallas, Richardson, Texas, United States*

Copper is an essential trace element acting as a catalytic cofactor in several cuproenzymes and is central to critical cell signaling and biochemical pathways. However, its ability to redox cycle at physiological redox potentials can lead to the production of free radicals and reactive oxygen species via Fenton and Haber-Weiss reactions, which are highly toxic to cells. P_{1B}-type ATPases, also known as Cu(I)-pumps (named CopAs in prokaryotes), are transmembrane copper exporters which, in all branches of life, play a key role in regulating cellular copper concentrations to prevent copper toxicity. The CopA pumps feature a multi- domain topology including three catalytic cytosolic domains (involved in ATP hydrolysis and auto- phosphorylation), a transmembrane core, and zero to multiple soluble metal binding domains (MBD). Together, these structural elements enable the transfer of Cu(I) ions from the intracellular to the extracellular environment through the catalytic Post-Albers cycle. Studies on Cu(I)-pumps have provided information about the topological framework by which CopAs perform their function. However, the structural and functional roles of the individual domains during the catalytic cycle remain elusive. In particular, the dynamic communication between the metal-binding domains (MBDs), catalytic cytosolic domains, actuator domain, and transmembrane domain is not fully understood, including how these domain-specific conformational changes are coupled to copper binding, ATP hydrolysis, phosphorylation, and copper transfer.
To address this gap, we employed HDX-MS to study the conformational dynamics associated with copper binding in the model Cu(I) pump from *Escherichia coli* (*Ec*CopA). We characterized CopA under distinct catalytic states in the presence and absence of copper. Comparison of deuterium uptake profiles revealed that conformational changes are highly localized rather than distributed uniformly throughout the protein. Copper binding primarily perturbed the soluble metal-binding domains, whereas nucleotide binding produced changes within the catalytic N and P domains, and formation of the E2P-like state was associated predominantly with changes in the actuator(A) domain. Interestingly, the ground state and E2P state revealed similar HDX profiles, suggesting that these states share a similar overall conformational changes while preserving localized differences associated with catalytic progress.

SWRM 2026 SW156

Mechanistic and structural characterization of wild-type and active-site variants of F_{420}-dependent sugar-6-phosphate dehydrogenase from *Cryptosporangium arvum*

***Lakshitha Madalagama**[1], lcm9339@mavs.uta.edu, Alaa Aziz[1], Ana Ledesma[1], Md Sabid Ahamed[1], Ghader Bashiri[2], Kayunta L. Johnson-Winters[1]. (1) Chemistry and Biochemistry, The University of Texas at Arlington, Arlington, Texas, United States(2) School of Biological Sciences, The University of Auckland, Auckland, Auckland, New Zealand*

F_{420}-dependent glucose-6-phosphate dehydrogenase (FGD) catalyzes the oxidation of glucose-6-phosphate (G6P) to 6-phosphogluconolactone (6PG) using cofactor F_{420}. Phylogenetic analyses have identified a subclass of FGDs, termed F_{420}-dependent sugar-6-phosphate dehydrogenases (FSDs),

which exhibit an activity towards fructose-6-phosphate (F6P), mannose-6-phosphate (M6P), and additional sugar-phosphates. FGD from *Cryptosporangium arvum* (*Cryar*-FGD) retains conserved catalytic residues found in the *Mycobacterial* FGD yet exhibits isomerase activity unlike the *Mycobacterial* enzyme. Here, we kinetically characterize *wtCryar*-FGD and variants using enzyme kinetics, chemical inactivation, mutagenesis and crystallography. Our previous work yielded dissociation constants (K_d) less than 100 mM for all three substrates with an $^{F420}K_d$ = 0.9 ± 0.8 μM. Steady-state kinetic analyses showed the highest catalytic efficiency toward G6P and an $^{app}k_{cat}$ of 6.4 ± 0.2 s^{-1}, compared with 1.4 ± 0.1 s^{-1} for F6P and 0.32 ± 0.02 s^{-1} for M6P. Pre steady-state analyses indicated that hydride transfer is not rate-limiting, and no detectable catalytic intermediates. NMR studies revealed isomerization of F6P to G6P, suggesting that *Cryar*-FGD possesses coupled dehydrogenase and isomerase activities. Temperature-dependent experiments yielded ΔH_{ion} = 6.3 ± 0.7 kcal mol^{-1}, consistent with participation of an acidic imidazole during catalysis. Chemical inactivation using diethylpyrocarbonate displayed monophasic kinetics, with an inactivation efficiency (k_{inact}/K_I) of 25 ± 10 M^{-1} s^{-1} consistent with a deprotonated histidine. Furthermore, fluorescence binding studies of the H38A and E107A variants showed substantially weaker substrate binding, with K_d values of 377 ± 60 μM and 92 ± 11 μM, respectively, indicating that those residues might be important in G6P binding. Ongoing kinetic characterization of E11A, E11Q, H38A, H38Q, E107A, and E107Q variants, together with X-ray crystallographic studies, will further define the roles of these conserved active-site residues in substrate recognition and catalysis. These studies will provide a mechanistic framework for understanding substrate promiscuity and functional divergence within the FGD/FSD family.

SWRM 2026 SW157

Energy transmission in ATP synthase

***Yunxiang Li**, yli7@twu.edu. Texas Woman's University, Denton, Texas, United States*

ATP synthase plays a critical role in aerobic respiration by converting the energy stored in the proton-motive force across the membrane into the chemical energy of ATP. ATP synthase consists of rotor and stator subcomplexes and functions analogously to a hydroelectric generator. As protons flow down their electrochemical gradient through the membrane-embedded F_o portion, their movement drives rotation of the c-ring and central γ subunit. This rotational energy is transmitted to the catalytic F_1 portion, where conformational changes in the β subunits drive ATP synthesis.
Efficient energy transmission in ATP synthase depends on specific interactions between the rotor and stator complexes. In this study, we examined two γ-subunit loops ($γ^{85}$GLCGG^{89} and $γ^{176}$NTMS^{179}) that may mediate interactions with the stator subunits. Through mutational analyses and biochemical assays, we found that deletion of the glycine-rich G loop (GLCGG) completely abolished aerobic respiration, whereas replacement of the G loop with five alanine residues resulted in approximately 20% of the growth yield observed for the wild type in 8 mM succinate medium. In contrast, deletion or alanine substitution of the NTMS motif had little effect on ATP synthase function.
Together with previous studies of the γC87 and βDELSEED mutations, these findings suggest that residues within the G loop are critical for energy transmission in ATP synthase. The G loop may interact with neighboring regions of the α, β, γ, and ε subunits to facilitate efficient transmission of rotational energy to the catalytic F_1 sector. Further site-directed mutagenesis of individual residues within this interaction cluster, combined with structural analyses, will help elucidate the molecular mechanism of energy transmission in ATP synthase.

SWRM 2026 SW158

Targeting factor XIIa: A step towards safer anticoagulant therapy

Jabila Mary[1]*, jabila@unt.edu, Jade C. Foka*[2]*, Anika Godavarti*[3]*, Shakila M. Silva*[1]*, Rami Al-Horani*[4]*, Daniel Afosah*[1]*. (1) Chemistry, University of North Texas, Denton, Texas, United States(2) Biochemistry and Chemistry, Southwestern University, Georgetown, Texas, United States(3) Texas Academy of Mathematics and Science, Denton, Texas, United States(4) Division of Basic Pharmaceutical Sciences, Xavier University of Louisiana, New Orleans, Louisiana, United States*

Vascular disorders remain a leading cause of mortality worldwide, with pathological thrombosis contributing substantially to disease complications. Although current anticoagulants are effective, their use is constrained by bleeding risk, underscoring the need for safer strategies. Factor XIIa (FXIIa), an initiator of the intrinsic coagulation pathway, is a promising target because its inhibition may reduce pathological thrombosis while preserving normal hemostasis. This study aimed to identify a selective FXIIa inhibitor with anticoagulant potential.
A panel of glycosidic compounds was screened against FXIIa, FXIa, FXa, thrombin, and plasmin using chromogenic substrate assays. Potency and selectivity were determined by IC50, and Michaelis-Menten kinetic analysis defined the inhibition mechanism. Plasma coagulation effects were evaluated using activated partial thromboplastin time (aPTT), prothrombin time (PT), kinetic clotting assays (kPTT and kPT). Whole blood coagulation effects were assessed by thromboelastography (TEG). In vivo safety was assessed in zebrafish larvae by monitoring survival for 96 hours.
Among the compounds screened, CJF-08 was identified as a selective FXIIa inhibitor, with an IC50 of 39.2 ± 3.5 μM and minimal activity against the other serine proteases tested. Kinetic analysis demonstrated competitive inhibition, with increased Km and no significant change in Vmax. CJF-08 significantly and dose-dependently prolonged aPTT without affecting PT; 135 μM was sufficient to double aPTT. Consistent with selective intrinsic-pathway inhibition, CJF-08 delayed clot formation in kPTT assays while producing minimal effects in kPT assays. TEG further showed increased R-time and K-time, with decreased α-angle and maximum amplitude, indicating delayed clot initiation and reduced clot strength. In zebrafish larvae, survival analysis showed that 50 μM was well tolerated, supporting its use as a safe concentration for subsequent in vivo studies.
Collectively, these findings identify CJF-08 as a selective, competitive FXIIa inhibitor that preferentially targets the intrinsic pathway. CJF-08 represents a promising lead for development of next-generation anticoagulants with potentially improved safety profiles.

SWRM 2026 SW159

Functional dynamics of water in New Delhi metallo-β-lactamase catalysis

Palanisamy Kandhan[1]*, palanisathish333@gmail.com, Chuanye Xiong*[1]*, Timothy Palzkill*[3]*, Peng Tao*[2]*. (1) Chemistry, Southern Methodist University, Dallas, Texas, United States(3) Biochemistry and Molecular Pharmacology, Baylor College of Medicine, Houston, Texas, United States*

Water plays a central role in antibiotic hydrolysis by New Delhi metallo-β-lactamases (NDMs), major contributors to β-lactam antibiotic resistance. NDM-catalyzed hydrolysis involves nucleophilic attack on the β-lactam ring, C–N bond cleavage, and formation of an anionic nitrogen intermediate that must subsequently be protonated by a water molecule recruited from bulk solvent. Despite extensive characterization of the NDM catalytic mechanism, how this protonating water reaches the active site remains poorly understood. Here, we use molecular dynamics simulations to investigate water dynamics across the hydrolysis cycle of the NDM-1–cefiderocol complex. By characterizing the apo,

substrate-bound, intermediate, and product states, we identify state-dependent changes in solvent-access pathways and active-site conformations. In the enzyme–intermediate state, coordinated rearrangements of NDM-1 and cefiderocol facilitate water entry and coordination to Zn2, positioning the water molecule to protonate the anionic nitrogen generated upon β-lactam ring cleavage. Concurrently, conformational changes restrict an alternative solvent-access pathway associated with Zn1. Together, these results reveal a state-dependent mechanism of water recruitment in which coupled protein and substrate dynamics regulate solvent access to the binuclear zinc center. Our findings link conformational dynamics, water recruitment, and protonation during NDM catalysis, providing mechanistic insight into NDM function and highlighting features of the active-site water network that could inform metallo-β-lactamase inhibitor design.

SWRM 2026 SW160

Metal ion substrate discrimination principles in transmembrane nickel-cobalt transporters (NiCoTs): Understanding and engineering cargo selectivity in NiCoT permeases

*Jayoh Hernandez, **Sean Alec Lois Sunga**, seanalecbsunga@gmail.com, Paul Micus, Gabriele Meloni. Chemistry & Biochemistry, The University of Texas at Dallas School of Natural Sciences and Mathematics, Richardson, Texas, United States*

The transmembrane Nickel-Cobalt transporter (NiCoT) protein family was identified as a primary system evolved for cellular acquisition of Ni(II) and non-corrinoid Co(II) in prokaryotic pathogens. The family is proposed to feature three subclasses based on the transport selectivity towards Ni(II) *vs.* Co(II), with Class I exclusively transporting Ni(II), while the other two classes being promiscuous but with preferred substrates – Ni(II) for Class II, and Co(II) for Class III. The first putative Class I transporter, NixA from *Helicobacter pylori*, was recently characterized using a novel *in vitro* proteoliposome platform as a strictly selective electrogenic, non-promiscuous Ni(II) uniporter. Contrarily, no molecular characterization of the transport properties for the other two NiCoT classes is currently available. In this study, we characterized representative Class II (NicT from *Mycobacterium tuberculosis*) and Class III (NisA from *Staphylococcus aureus*) NiCoTs. By exploiting our developed proteoliposome platform that allows to monitor in real-time substrate transport using fluorescent sensors encapsulated in the proteoliposome lumen, we established the cargo selectivity and transport properties of both NicT and NisA, validating for the first time the NiCoTs' proposed classification. As established for NixA, NicT and NisA also transport both metal substrates as electrogenic uniporters, demonstrating a preserved transport mechanism in the entire NiCoT family. With the gained information we designed mutations to understand the substrate selectivity bias in NiCoTs. We identified a single mutation in NisA translocation pathway (A74C) which dramatically enhanced Ni(II) transport and abolished Co(II) selectivity, transforming a Class II NiCoT into a Class I-like counterpart. Since this mutation illustrates the importance of this residue in the discrimination of substrates, we extended this approach to Class III NiCoTs by mutating the corresponding NicT residue (A86C). Transport assays confirmed that A86C NicT behaved as a Class I-like protein. Additional residues (T230, C263, M215) in NicT also contributed to changes in selectivity towards Ni(II) *vs.* Co(II) upon mutation to the corresponding NixA residues. This work demonstrates that each NiCoT class can be successfully rationally engineered into another, thereby unraveling principles of metal ion substrates discrimination in the entire protein family.

SWRM 2026 SW161

Structural and biophysical characterization of OfurPBP3, a pheromone-binding protein from the Asian corn borer

***Pratikshya Paudel**, pratikshya.paudel@okstate.edu, Smita Mohanty. Chemistry, Oklahoma State University, Stillwater, Oklahoma, United States*

The Asian corn borer (ACB), *Ostrinia furnacalis* (Lepidoptera: Crambidae) is a polyphagous agricultural pest of many crops, widely distributed across Asia, Australia, and Oceania. The current approach for controlling ACB infestation primarily relies on pesticides. Nevertheless, the adverse outcomes from pesticide use cannot be disregarded, including issues such as environmental pollution, risks to human well-being, the emergence of pest resistance, and the possibility of secondary pest outbreaks. Thus, there is an urgent need for controlling this invasive pest in an environmentally friendly and species-specific manner. The mating process in the moth, *Ostrinia furnacalis* is facilitated through the sex pheromones emitted by the females and detected by the males. Pheromone Binding Proteins (PBPs), present in male moth antennae bind and transport the hydrophobic pheromones to the olfactory receptors initiating olfaction. *Ostrinia furnacalis* Pheromone Binding Protein 3 (OfurPBP3) is preferentially expressed in male moth antennae. A detailed structural characterization and mechanistic study of the OfurPBP3 is needed to design the pheromone mimetic for effective pest management. The cloning, expression of the recombinant OfurPBP3 in *E. coli*, refolding from the inclusion bodies (IBs), and the characterization of the protein by fluorescence spectroscopy, circular dichroism, small-angle X-ray scattering (SAXS), and high-resolution solution NMR will be presented.

SWRM 2026 SW162

Exploring the role of the secondary coordination sphere in Ni CO_2RR

***Shrivignesh Senthil Kumar**, shrivigneshs1999@gmail.com, Alison R. Fout. Chemistry, Texas A&M University, College Station, Texas, United States*

The conversion of carbon dioxide into value-added chemicals via electrocatalytic CO_2 reduction (CO_2RR) is a key target for sustainable energy chemistry. While cationic nickel complexes like $[Ni(cyclam)]^{2+}$ are widely recognized for their high selectivity toward carbon monoxide over hydrogen evolution, neutral nickel electrocatalysts and those featuring dedicated secondary coordination spheres remain relatively rare. Recently, hydrogen-bonding interactions in the secondary sphere have proven effective in tuning reactivity and product selectivity across transition metal catalysts. In this work, we present the synthesis and electrocatalytic CO_2RR evaluation of two new neutral nickel complexes featuring pyrrole–imine ligands. A dipodal ligand lacking a secondary coordination sphere on Ni serves as a control system. To investigate the role of pendant hydrogen-bonding donors, a novel macrocyclic ligand incorporating a dangling N–H group was synthesized and metalated with nickel. A comparative study of their electrochemical behavior, reactivity, and product selectivity highlights the structural impact of the secondary coordination sphere on stabilizing reaction intermediates and directing pathway selectivity during CO_2 reduction.

SWRM 2026 SW163

Nitrate reduction by thiols at Ni(II) site

***Ayoola Ayodele**, asayodele@smu.edu, Saikat Mishra, Pokhraj Ghosh. Chemistry, Southern Methodist University, Dallas, Texas, United States*

Nitrate (NO_3^-) is an essential component of the global nitrogen cycle and a major environmental contaminant from agricultural and industrial activities. In biological systems, nitrate and nitrite (NO_2^-) serve as reservoirs for nitric oxide (NO), a key signaling molecule in physiological processes. Nitrate is thermodynamically stable and kinetically inert to reduction, making its conversion to NO challenging. Low-valent sulfur species, particularly thiols (RSH), are ubiquitous biological reductants, yet their role in reducing nitrogen oxoanions at biogenic Ni(II)-sites remains poorly understood.
To explore thiol-mediated nitrate reduction at Ni(II) sites, we developed a pyridine–amine ligand (L) featuring a pendant thioether donor. This ligand supports both nickel(II)-nitrate, $[L_2Ni(\kappa^2\text{-}O_2NO)]ClO_4$, and nickel(II)-nitrite, $[L_2Ni(\kappa^2\text{-}O_2N)]ClO_4$, within the same ligand framework, and both exhibit distorted octahedral geometries. Reactivity studies with thiols of varying pK_a and steric profiles (RSH; where R = adamantyl, phenyl, trityl, etc.) reveal reduction of nickel nitrate to NO, which was trapped using tetrakis(4-methoxyphenyl)porphine cobalt(II) and quantified by ^1H NMR spectroscopy.
Mechanistic investigations support consecutive oxygen-atom transfer (OAT) from coordinated nitrate and nitrite to thiols, generating sulfenic acids (RSOH). These transient species were trapped with dimedone and characterized by ESI-MS, providing experimental support for OAT. Diphenyl disulfide (PhSSPh) was also isolated from reactions of nickel(II)-nitrate and nickel(II)-nitrite with thiophenol and characterized by single-crystal X-ray diffraction, providing evidence for thiol oxidation. To probe the subsequent reduction step, independently synthesized nickel(II)-nitrite was reacted with a thiol, yielding a Ni-nitrosyl species $[L_2NiNO]^+$ supported by FTIR ($\nu(NO)$ = 1777 cm^{-1}) and UV-vis spectroscopy (λ_{max} = 474 nm). This unstable Ni-nitrosyl species transforms into a bimetallic Ni-nitrosyl product $[LNi^{II}(SPh)_3Ni(NO)]$, which is crystallographically characterized. These results support stepwise nitrate reduction and indicate that nickel-bound nitrite is a competent precursor for nitrosyl formation. This work offers molecular insight into the interplay between thiol oxidation and nitrogen oxoanion reduction at a biogenic Ni(II) site.

SWRM 2026 SW164

Organo-p-block element oxides as synthetic ZnX_2 transporters

***Soumadipta Biswas**, soumadipta@tamu.edu, Francois P. Gabbai. Chemistry, Texas A&M University System, College Station, Texas, United States*

In this presentation, I will discuss our ongoing efforts to use organo-p-block element oxides to transport ZnX_2 across phospholipid bilayers. Solid-state structural analysis reveals that these oxides coordinate ZnX_2 to form the corresponding 2:1 tetrahedral complexes. When deployed in a newly developed Mg-G assay to monitor Zn^{2+} transport, we observed that the activity of the heavier organo-p-block element oxides exceeded that of their lighter congeners. The transport activity could be modulated by systematically modifying the organic substituents on the scaffolds. The activity of the heavier scaffolds could be traced back to their enhanced Lewis basicity of the oxide terminus and the greater lipophilicity down the series. These results demonstrate that simple organo-p-block element oxides frameworks can mediate ZnX_2 transport by exploiting the strong oxophilicity of Zn^{2+} center and the overall augmented membrane-inserting capability of the resulting complexes.

SWRM 2026 SW165

Investigating the impact of metal identity in complexes supported by an adaptable ligand framework on electrochemical oxygen reduction

***Fiona Roche**, froche24@tamu.edu. Texas A&M University, College Station, Texas, United States*

The $2H^+/2e^-$ electrochemical reduction of oxygen (O_2) to hydrogen peroxide is an attractive method for the generation of an essential oxidant. First-row transition metal complexes decorated with secondary coordination spheres employed in the oxygen reduction reaction (ORR) allow for tunable reactivity and enhanced product selectivity. Further modulation of reactivity is achieved through the identity of the metal center. For example, the oxygen activation reactivity of a series of Mn, Fe, and Co complexes in a tetradentate monoanionic ligand framework ($BNPAPh_2O^-$), 2-(bis((6-(neopentylamino)pyridin-2-yl)methyl)amino)phenolate varies dramatically across the series, highlighting the impact of metal identity on both primary and secondary coordination spheres, and hence the reactivity of the complex.
A previously reported non-heme iron complex ,$[N(afa^{Cy})_3Fe]OTf_2$, $N(afa^{Cy})_3$ =tris(5-cyclohexylamine azafulvene-2-methyl)amine, facilitated selective chemical oxygen reduction to hydrogen peroxide (H_2O_2= 97 %) though electrochemical selectivity studies are not yet explored. The high selectivity is proposed to arise from involvement of the secondary coordination sphere in proton transfer steps preceding product release. A previously Mn analogue is capable of oxygen activation, though reduction remains unexplored. In this work, we investigate the outcomes of metal identity in a series of $[N[(afa^{Cy})_3M]X_2$ where M= Mn, Fe, Co, and Cu complexes employed in electrochemical ORR.

SWRM 2026 SW166

Optimizing the phototherapy effects of metallodrug photosensitizers for cancer treatment

***Ge Shi**, ge.shi2@uta.edu. University of Texas at Arlington Research Institute, Arlington, Texas, United States*

Cancer remains a global health challenge, and tumor hypoxia could hinder effective treatment. Low oxygen levels disrupt drug uptake and function while driving adaptive cellular responses that promote therapeutic resistance. In photodynamic therapy (PDT), light activation of photosensitizers (PSs) in the presence of oxygen generates singlet oxygen and other reactive oxygen species (ROS) that selectively damage tumor cells with minimal dark toxicity. PDT has emerged as a promising treatment modality, supported by an increasing number of successful clinical trials. However, its reliance on molecular oxygen renders PDT particularly vulnerable to hypoxic tumor microenvironments. Building on our development of transition metal complexes as next-generation PSs with alternate mechanisms of action, we will present proof-of-concept strategies for achieving light-induced cytotoxicity under both normoxic and hypoxic conditions. One of our lead compounds, TLD1433, is currently in Phase 2 clinical trials (NCT03945162) for the PDT treatment of bladder cancer. We further explore optimization of PDT efficacy by modulating key light parameters and evaluating potential induction of anti-tumor immune responses. While hypoxia-tolerant photocytotoxicity remains relatively uncommon, uncovering such activity provides valuable insight into alternative photochemical pathways and may inform the design of new light-responsive therapeutics with broader biomedical applications. Even if hypoxia is not clinically limiting, elucidating oxygen-independent photoreactivity provides mechanistic insights that extend to photocatalysis, photoredox chemistry, and energy-conversion systems.

SWRM 2026 SW167

Unveiling SNO^{1-}, $SSNO^{1-}$, and HONO intermediates in H2S-mediated nitrite reduction at zinc

***SAIKAT MISHRA**, contact.smishra@gmail.com, Anagha Kuruvayil, Esther Olatunji, Pokhraj Ghosh. CHEMISTRY, Southern Methodist University, Dallas, Texas, United States*

H_2S is now well recognized as a gasotransmitter and contributes significantly as a reductant in microbial denitrification and as a modulator of NO signaling pathways. The activity of the metalloenzyme cytochrome c Oxidase (C*c*O) is regulated by the concentration of H_2S present in the system, which is crucial in human respiration. At low concentrations of H_2S, it can reduce the ferric heme a_3, yielding HS radical, increasing oxygen consumption and thereby enhancing respiration. In addition to that, H_2S in the presence of O_2 can broadly persulfidate the zinc finger proteins, and $His_3Zn(II)$ site in carbonic anhydrase (CA) can produce NO gas through nitrite hydratase activity. Herein, we have prepared zinc octahedral complex, $[L_2Zn](ClO_4)_2$ (1), supported by *2-(methylthio)-N-(1-(pyridin-2-yl)ethyl)aniline* (L), which affords the nitrite complex $[L_2Zn(ONO)]$ (ClO_4) (2), upon treatment with excess sodium nitrite in methanol. Complex 2 reacts with H_2S at -35^0C to provide zinc aqua complex $[L_2Zn(H_2O)_2](ClO_4)_2$ (3), NO, N_2O, and sulfane sulfur via the intermediacy of $[L_2Zn$-$SNO](ClO_4)$ (4), $[L_2ZnSSNO](ClO_4)$ (5), HNO (nitroxyl), and HONO (nitrous acid). The mechanism of reduction of 2 with H_2S is governed by the amount of H_2S used. Stoichiometric addition of H_2S (1-2 equivalents) produces NO (48%) and N_2O (21%) via a proton-assisted nucleophilic attack mechanism, while excess addition causes NO (80%) as the major signaling output via an acid-base exchange mechanism. Interestingly, we have successfully established, using low-temperature UV-Vis and ^{15}N NMR techniques, that nitrite reduction by a less-equivalent amount of H_2S proceeds via the zinc-thionitrite and zinc-perthionitrite intermediates, which closely resemble the spectral features of the independently prepared 4 and 5 complexes. The HNO is verified by trapping with PPh_3, yielding O=PPh3 and HN=PPh3, as evidenced by ^{31}P NMR and ESI-MS. However, in the presence of excess H_2S (5 eqv), nitrite reduction generates HONO, detected by UV-Vis and 15N NMR, which is responsible for the production of NO as the major product. Additionally, under basic conditions (pKa > 11), a thiohydroxide-bound zinc–nitrite intermediate, [LZn(ONO)(SH)], can be isolated as a solid and is stable to nitrite reduction. These findings provide significant mechanistic details of nitrite reduction by H_2S and illustrate the often-overlooked role of nitrite in various signaling pathways.

SWRM 2026 SW168

Electrochemical and spectroelectrochemical behavior of $[Ru(tpy)(tpy\text{-}nT)]^{2+}$ as a function of thiophene chain length

***Abbas Vali**, abbas.vali@uta.edu, Houston Cole, Alisher Talgatov, Elamparuthi Ramasamy, Dalton Lucas, Brayden Stackhouse, Gurleen Kaur, Ge Shi, Colin Cameron, Sherri A. McFarland. The University of Texas at Arlington, Arlington, Texas, United States*

Photodynamic therapy (PDT) uses a nontoxic photosensitizer (PS) and light to destroy cancerous cells. Our laboratory has a longstanding interest in the development of metal complex photosensitizers for PDT. We have been particularly focused on metal oligothiophene complexes, with our Ru-based TLD1433 having advanced to Phase 2 clinical trials for treating bladder cancer with PDT. Our approach involves tuning the orbital energy levels of metal complexes to drive the desired excited state photosensitization and photochemical reactions. This is accomplished through rational manipulation of the coligand identities and their substituents. To better understand the exceptional PDT activity of TLD1433 and related analogs, and possibly increasing the PDT activity of TLD1433, we are now investigating the effect of metal and coligand identity on the excited state dynamics of metal complex photosensitizers. As part of this effort, we are undertaking a systematic

study of the electrochemical and spectroelectrochemical properties of these metal oligothiophene complexes. This study addresses the effect of increasing number of thiophene rings on electrochemical and spectroelectrochemical properties of $[Ru(tpy)(tpy\text{-}nT)]^{2+}$ family, where, tpy is 2,2':6',2''-Terpyridine and nT is the number of thiophenes (n=0 to 4).

SWRM 2026 SW169

Catalytic reduction of carbon dioxide with a bimetallic Mn(I) complex of a pyridine-based polyamine macrocycle: Applications in renewable energy

Md Mhahabubur Rhaman[1]*, mdmhahabubur.rhaman@enmu.edu, Matilda Kaabo*[1]*, Mathew Ogbe*[1]*, Manual Quiroz*[2]*, Nobuyuki Yamamoto*[3]*, Eric S. Wiedner*[2]*. (1) Physical Sciences, Eastern New Mexico University, Portales, New Mexico, United States(2) Catalysis Science, Pacific Northwest National Laboratory, Richland, Washington, United States(3) Department of Chemistry and Biochemistry, The University of Oklahoma, Norman, Oklahoma, United States*

Many catalysts featuring diverse metals and ligands have been reported for the hydrogenation of CO_2 to produce high-energy-density chemicals, such as formic acid and methanol. However, their kinetics, efficiency, solvent compatibility, stability, and cost must still be suitable for large-scale, economical energy processes. New approaches and detailed mechanistic studies of catalysis are needed, using economical, readily available, and environmentally friendly chemicals. In this research, phosphene-free, a pyridine-based polyamine macrocycle, was synthesized from commercially available compounds and converted to a bimetallic Mn(I) complex by reaction with $[Mn(CO)_5]Br$ in refluxing methanol. Two single-crystal structures of the complex reveal that each ligand contains two Mn(I) with an octahedral coordination sphere, where three carbonyl and three amines coordinate Mn(I). The ability of this complex to catalytically hydrogenate CO_2 was studied using the organic base DBU (1,8-diazabicyclo[5.4.0]undec-7-ene) at 500 psi and a 3:1 H_2/CO_2 ratio at 80 °C in acetonitrile in a batch reactor. The catalyst reduced CO_2 to formic acid with a turnover number (TON) of 107. Without a base, the complex didn't show catalysis, suggesting a key role of DBU in activating the complex for catalysis. Acknowledgment: This work was primarily supported by Eastern New Mexico University internal grant PIRR3 for ligand and catalyst **synthesis** and U.S. Department of Energy, Office of Science, Office of Workforce Development for Teachers and Scientists (WDTS) under the Visiting Faculty Program (VFP) for catalytic studies. MK and MOO acknowledge the Sponsor Project at Eastern New Mexico University for providing the graduate assistant positions. Additional support for the catalytic studies was provided by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Chemical Sciences, Geosciences, and Biosciences Division, Catalysis Science program, FWP 47319 (MQ and ESW). Support for the acquisition of the Bruker D8 Quest diffractometer from the NSF MRI program (CHE-1726630) is gratefully acknowledged.

SWRM 2026 SW170

***Ostrinia furnacalis* pheromone-binding protein 2: Role of Arg70 in ligand release**

sanjana gautam*, sanjana.gautam@okstate.edu. Chemistry, Oklahoma State University The College of Arts and Sciences, Stillwater, Oklahoma, United States*

Olfaction is the sense of smell by which organisms detect chemical signals in the environment. In moths, males rely on olfaction to detect female sex pheromones and locate mates. Pheromone

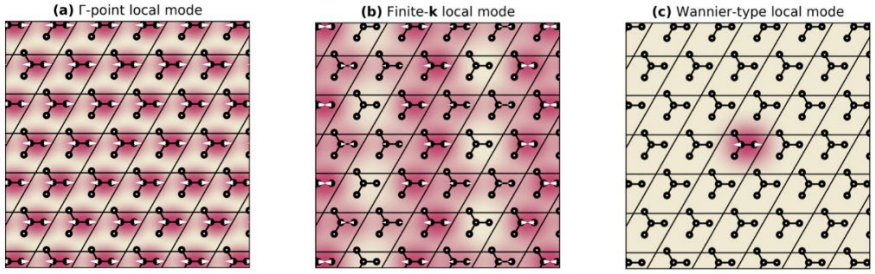
binding proteins (PBPs) in the male antennae mediates the transport of hydrophobic pheromones through the aqueous sensillar lymph to olfactory receptor neurons.
The Asian corn borer, *Ostrinia furnacalis* (Ofur), is a major agricultural pest responsible for significant crop damage and is difficult to control due to insecticide resistance. Consequently, understanding the molecular basis of pheromone binding and release may facilitate the development of environmentally sustainable alternatives to insecticides. OfurPBP2, a key olfactory protein, contains two regulatory features a histidine-arginine gate and a C-terminal gate that controls ligand binding and release. Unlike other common lepidopteran PBPs, which possess a conserved His70–His95 histidine gate, OfurPBP2 contains an Arg70 residue in place of His70. Structural studies suggest that Arg70 forms a novel Arg70–His88 gate that replaces the classical histidine gate. Whether the Arg70-His88 gate play any role in regulating the pH-dependent pheromone binding and release is not known. Furthermore, it has also been reported that OfurPBP2 may release ligand through a molten globule like state rather than the canonical pH-dependent conformational switch observed in other lepidopteran PBPs.
To investigate the functional role of Arg70, an R70A mutant was generated, expressed in *Escherichia coli* using both IPTG induction as well as autoinduction media. While IPTG induction produced inclusion bodies requiring refolding, autoinduction yielded soluble recombinant protein. Both the refolded and soluble proteins were purified using anion-exchange chromatography and size-exclusion chromatography. Circular-dichroism, fluorescence spectroscopy, and nuclear magnetic resonance spectroscopy will be used to characterize the effect of mutation on protein function. These studies will provide mechanistic insight into OfurPBP2 function and would support the development of environmentally sustainable strategies to limit use of insecticides.

SWRM 2026 SW171

From numbers to insight: A chemical interpretation of phonon band structures

***Elfi Kraka**, ekraka@gmail.com. Southern Methodist University, Dallas, Texas, United States*

Charles Coulson challenged quantum chemists to "give us insight, not numbers", while Frank Neese has argued that modern quantum chemistry should provide both "insight and numbers"; a challenge in particular relevant for lattice vibrations in crystalline solids. A phonon is a quantized lattice vibration that, unlike a molecular vibration, propagates through a crystal as a wave characterized by a wavevector **k**, giving rise to phonon dispersion relations throughout the Brillouin zone.
We present a unified local vibrational framework that connects chemical bonding in real space with phonon dispersion in reciprocal space. At the Γ-point (**k** = 0), where all unit cells vibrate in phase, the crystal behaves like a giant molecule, allowing molecular Local Vibrational Mode Analysis (LMA) and Composition of Normal Modes (CNM) to provide comprehensive bonding analyses. [1] At finite wavevectors, the relative phases between neighboring unit cells reveal how local chemical bonding evolves across reciprocal space and governs lattice vibrations. Wavevector-resolved LMA and CNM follow the evolution of bond stretching, angle bending, and torsional character along phonon branches throughout the Brillouin zone. [2] Wannier-type LMA transforms the reciprocal-space description into localized real-space vibrational modes, providing bond strengths that are encoded in the complete phonon dispersion. [3] Applications to polymeric chains, perovskites, diamond, and magnesium iodate under pressure [4] demonstrate how wavevector-resolved and Wannier-type LMA provide complementary views of lattice dynamics in periodic materials. Together, they link crystal structure, phonon dispersion, and chemical bonding, offering a unified framework that provides the chemical insight envisioned by Coulson and Neese while offering an intuitive basis for understanding and tuning structure-property relationships in functional materials.



(a) Γ-point and (b) finite-wavevector and (c) the Wannier-type local modes

SWRM 2026 SW172

Benzene in the excited state: A playground for photochemical transformations

***Judy Wu**, judyicwu@gmail.com. University of Houston, Houston, Texas, United States*

Benzene, in the excited state, is a remarkably reactive chemical motif. The year 2025 marks the 200-year anniversary of Faraday's discovery of benzene, and in this talk I will explore how its excited-state behavior offers a unique platform for photochemical transformations. The talk begins with a quick introduction to Baird's rule, the reversal of the Hückel electron-counting rule for aromaticity and antiaromaticity in the lowest ππ* states of annulenes. I will then highlight computational explorations from our group over the past decade on how relief of excited-state antiaromaticity in benzene derivatives and heteroarenes can drive diverse photochemical transformations, including proton transfer, electron transfer, π-bond activation, tunable Lewis interactions, and photo-HF elimination.

SWRM 2026 SW173

Pauli exclusion, electron (de)localization, and the origin of the transition state barrier in the H_2 + $H^\bullet$ hydrogen atom transfer reaction

***Shehan H. Fernando**, m.shehan111@gmail.com, Alistair Sterling. Department of Chemistry and Biochemistry, The University of Texas at Dallas, Richardson, Texas, United States*

The decrease in electronic energy that accompanies chemical bond formation can be interpreted through its energy components, namely the electronic kinetic energy (T) and potential energy (V) of the system. While debate about the interpretation of changes in T and V during chemical bond formation is ongoing, recent work by Head-Gordon and co-workers demonstrates the utility of analyzing electron (de)localization through the electronic kinetic energy term. In comparison with the rich variety of theoretical studies on chemical bonding, studies on chemical reactivity have typically been limited to orbital or energy decomposition analyses. Here, we take inspiration from Head-Gordon's kinetic energy analysis by using an "energy composition analysis" approach to investigate the origin of the transition state barrier in the hydrogen atom transfer reaction of the H_2 + $H^\bullet$ ($^2[H_3]$) system. Using non-optimized natural orbitals (NONOs) we isolate the effect of Pauli exclusion on kinetic energy changes during the reaction. Our results demonstrate that Pauli exclusion is the primary cause of the transition state barrier, since it is responsible for both the initial energy increase and geometric distortion—each of which is a hallmark associated with transition states. Overall, this

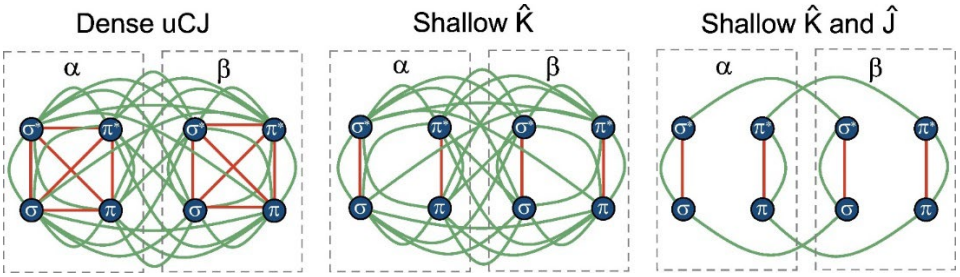
study emphasizes the importance of electronic kinetic energy as a physically meaningful descriptor that has the potential to explain the underlying physics of chemical reactions.

SWRM 2026 SW174

Chemically informed pruning of unitary cluster Jastrow ansätze using localized orbitals

Aradhika Paul[1]*, aradhika.paul-1@ou.edu, Nikolay V. Tkachenko*[2]*. (1) Department of Physics and Astrophysics, The University of Oklahoma, Norman, Oklahoma, United States(2) Department of Chemistry and Biochemistry, The University of Oklahoma, Norman, Oklahoma, United States*

Near term quantum simulations of molecular systems require compact ansätze that can describe important electron correlation while reducing circuit resources. We propose a chemically informed approach to constructing and pruning unitary cluster Jastrow (uCJ) ansätze using localized bonding and antibonding orbitals. Adaptive natural density partitioning is used to identify chemically meaningful bonding elements, which are then used to construct an orthonormal active orbital basis with corresponding antibonding orbitals. In this localized basis, orbital rotation and Jastrow operators can be restricted to chemically relevant orbital pairs and further pruned using orbital quantum mutual information from approximate correlated calculations. As a proof of principle, we apply this approach to C2H4 using real, imaginary, and generalized uCJ ansätze with progressively pruned connectivity. The generalized uCJ ansatz restores 97.9% of the correlation energy in the dense case, 95.1% with restricted orbital rotations, and 78.8% when both orbital-rotation and Jastrow couplings are pruned. These restrictions reduce the CNOT count by 37.5% and 68.75%, respectively, relative to dense uCJ. The most-pruned circuit requires 40 CNOT gates, compared with 753 CNOT gates for a single-Trotter-step UCCSD ansatz for the same active space. These results demonstrate that chemically localized orbitals can enable compact, chemically interpretable uCJ ansätze for near-term quantum simulations.



Schematic representation of the uCJ ansatz for C2H4, with the K and J operators represented as connectivity graphs. Nodes represent localized spin orbitals, red lines denote K connections, and green curves denote J connections.

SWRM 2026 SW175

Assessing the stability of metal-organic frameworks with local vibrational mode theory

Sophia Trejo*, sophiaflores1201@gmail.com, Juliana J. Antonio, Elfi Kraka, Haoyuan Chen. Chemistry, Southern Methodist University, Dallas, Texas, United States*

The stability of metal-organic frameworks (MOFs) is crucial for their industrial applications, with metal-linker coordination bonds often representing the weakest structural points. We assessed the strength of these bonds in representative MOF series (UiO-66, MOF-5, and ZIFs) using local vibrational mode theory, which transforms delocalized normal modes into local vibrational modes and associated local mode force constants that reflect bond strength. The bond strengths obtained from local force constants were in good agreement with the experimental stability data, which in some cases was not reflected by the electron density at the bond critical points. Linker functionalization was also investigated, with *ortho*-NH_2 substitutions found to weaken adjacent coordination bonds through intramolecular hydrogen bonding. These findings establish a readily computable quantum-mechanical metric for evaluating bond strengths in MOFs, paving the way for improved evaluation and prediction of MOF stability. Current efforts are expanding this approach to periodic models of MOF-5 to investigate whether the extended lattice environment yields meaningful differences in bond strengths compared with cluster models, potentially capturing structural effects that are more representative of MOFs under realistic conditions.

SWRM 2026 SW176

Machine learning prediction of gas solubility in deep eutectic solvents using electrostatic potential-derived descriptors

***Sahar Heidari**, sahar.heidari@utdallas.edu, yuvraj danget, garima Gupta, Karishma Pilla, Hedieh Torabifard. The University of Texas at Dallas School of Natural Sciences and Mathematics, Richardson, Texas, United States*

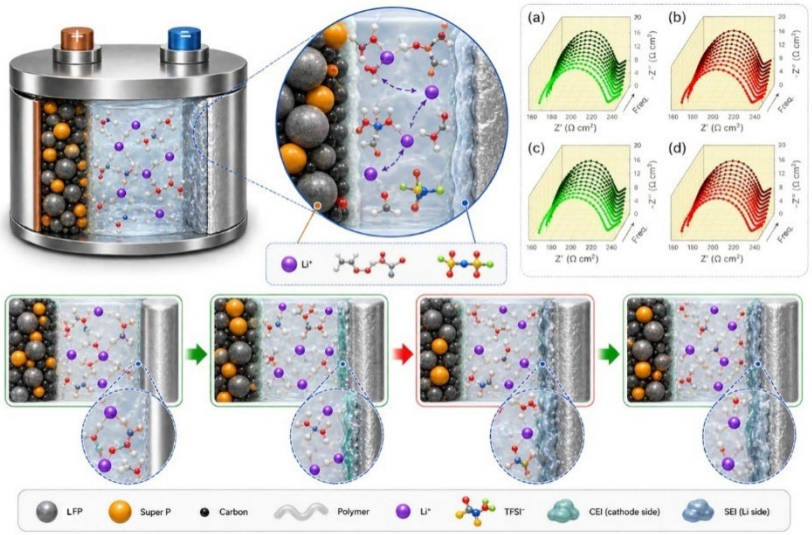
Deep eutectic solvents (DESs) offer a highly tunable platform for gas capture and separation, but the large number of possible hydrogen-bond acceptor (HBA) and hydrogen-bond donor (HBD) combinations makes experimental screening inefficient. In this work, we combine quantum-chemical molecular descriptors with machine learning to predict the solubility of six environmentally and industrially important gases, CO_2, CH_4, SO_2, H_2S, NO, and NO_2, in DESs. Experimental solubility data collected from the literature were integrated with solvent composition, temperature, pressure, and electrostatic potential (ESP)-derived descriptors calculated separately for the HBA and HBD components. The ESP distributions were converted into numerical descriptors that characterize the surface electrostatic environments relevant to solvent-gas interactions. A series of linear and nonlinear regression models were evaluated using repeated train/test splitting and cross-validation to examine both predictive performance and robustness. XGBoost provided the strongest overall performance among the tested models. SHapley Additive exPlanations analysis identified the relative contributions of thermodynamic conditions and ESP-derived descriptors of the HBA and HBD components to the model predictions, highlighting the importance of molecular electrostatic characteristics in predicting gas solubility in DESs. The trained models were incorporated into a web-based tool that enables rapid evaluation of HBA/HBD combinations and operating conditions and can extend predictions to new DES systems using ESP descriptors generated from user-provided quantum-chemical calculations. This integrated quantum chemistry-machine learning approach provides an efficient strategy for screening DESs and guiding the design of task-specific solvents for gas capture and separation.

SWRM 2026 SW177

***Operando* EIS for probing interfacial evolution in lithium metal batteries**

*Lamartine Meda[1,2], **Tariq Bashir**[1,2], tbashir@xula.edu. (1) Department of Chemistry, Xavier University of Louisiana, New Orleans, Louisiana, United States(2) Energy Storage Research Alliance, Argonne National Laboratory, Lemont, Illinois, United States*

Lithium metal batteries (LMBs) represent a path to next-generation high-energy-density energy storage, but their practical development is hampered by complex interfacial processes such as continuous solid electrolyte interphase (SEI) evolution, non-uniform lithium plating/stripping, and increasing interfacial polarization. The application of galvanostatic electrochemical impedance spectroscopy (GEIS) offers a robust method for studying these dynamic phenomena in real electrochemical environments. This talk examines the utilization of operando EIS to monitor the changes in bulk, interfacial, and charge-transfer resistances in lithium metal batteries relative to state of charge, cycle count, and operational parameters. Impedance responses that change with voltage and time are associated with the dynamics of lithium plating and stripping, as well as interfacial modifications, enabling the distinction between changes in cell resistance due to reversible electrochemical processes and irreversible degradation. Equivalent-circuit analysis and the clarification of characteristic impedance properties associated with mass-transport limitations, interfacial charge transfer, and composite solid polymer electrolyte resistance are given considerable attention. By combining operando EIS with electrochemical cycling, we demonstrate that the evolution of impedance may provide early signals of interfacial instability and performance degradation before apparent capacity loss. These results illustrate the efficacy of operando EIS as a diagnostic instrument for understanding interfacial stability and reaction kinetics in lithium metal batteries, as well as for guiding the advancement of more resilient high-energy battery systems.



SWRM 2026 SW178 - Withdrawn

SWRM 2026 SW179

Electrode surface modification with conductive carbon support for enhanced porphyrin electrocatalyzed oxygen reduction reaction

***Justin Ratliff**, justinratliff@my.unt.edu, Alankar Kafle, Thomas R. Cundari, Francis D'Souza. Chemistry, University of North Texas, Denton, Texas, United States*

As the global energy landscape shifts away from traditional fossil fuels towards cleaner and more sustainable technologies, fuel cells are emerging as a viable replacement with efficient and low-emission energy conversion. In proton/anion exchange membrane fuel cells, the oxygen reduction reaction (ORR) functions as the essential chemical sink at the fuel cell cathode, where diatomic oxygen accepts electrons from the hydrogen oxidation reaction (HOR) taking place at the anode to complete the circuit. However, the sluggish kinetics of the oxygen reduction reaction limits the overall efficiency of the cell. Current technologies rely heavily on expensive and less abundant noble metal-based electrocatalysts, particularly Pt/C. Thus, developing efficient, earth-abundant alternatives to noble-metal catalysts capable of enhanced kinetics with the 4-electron oxygen reduction reaction pathway is essential. This study explores a hybrid (homogeneous/heterogeneous) catalytic strategy by pairing a tetrachloro salt of [tetrakis(N-methylpyridyl)porphyrinato]cobalt, $[Co(TMPyP)]Cl_4$ suspended in the electrolyte with four distinct, commercially available carbon supports: Acetylene Black, Black Pearls 2000, Ketjenblack EC-600JD, and Vulcan XC-72. The glassy carbon surface modified with different carbon supports was employed for systematic evaluation of how the physical properties of the support impact the activity of the solution-phase molecular catalyst. Electrochemical studies, including cyclic voltammetry, rotating ring disk electrode (RRDE), and electrochemical impedance spectroscopy (EIS) measurements, revealed significant differences in ORR performance across the supports. This work provides critical insights into tailoring carbon microenvironments for optimized molecular catalysis, directly addressing modern challenges in sustainable energy conversion.

SWRM 2026 SW180

One-step synthesis of highly active and conductive transition metal nitride for oxygen evolution in alkaline anion exchange membrane electrolysis

Scott Folkman[1], *scott.folkman1.618@gmail.com, Ilario Gelmetti*[3], *Stefano Giancola*[2], *Felipe Andrés Garcés-Pineda*[3], *Maria Chiara Spadaro*[4,5], *Andrés Camilo Muñoz*[1], *Tharaka Wickramasinghe*[1], *Jordi Arbiol*[5], *Jose Ramon Galan-Mascaros*[2,3,6]. *(1) New Mexico State University College of Arts and Sciences, Las Cruces, New Mexico, United States(2) Orchestra Scientific, Tarragona, Spain(3) Institut Catala d'Investigacio Quimica, Tarragona, CT, Spain(4) Universita degli Studi di Catania, Catania, Sicily, Italy(5) Institut Catala de Nanociencia i Nanotecnologia, Barcelona, CT, Spain(6) Institucio Catalana de Recerca i Estudis Avancats, Barcelona, CT, Spain*

Transition metal nitrides (TMNs) offer a promising alternative to conventional metal oxides for alkaline oxygen electrocatalysis because they combine high electrical conductivity with tunable composition and surface chemistry. We developed a one-step route for synthesizing cobalt, nickel, iron, and mixed-metal TMNs directly from metal salts containing volatile anions. This approach provides quantitative conversion to nitride products without the purification steps required in many conventional multistep syntheses. The resulting materials exhibit porous, sponge-like morphologies and compositions that can be readily varied across mono-, bi-, and trimetallic systems.
The electrocatalytic activity of these materials was evaluated for the oxygen evolution reaction (OER) in alkaline media. Trimetallic TMNs displayed the highest activity, with $Co_{57}Ni_{14}Fe_{29}N_x$ outperforming benchmark IrO_x and mixed $NiCoFeO_x$ catalysts in three-electrode measurements and in alkaline anion exchange membrane electrolysis. In a 5 cm^2 electrolyzer, $Co_{57}Ni_{14}Fe_{29}N_x$ operated at 2.05 V at 1 A cm^{-2} and maintained stable performance for more than 240 hours. Electrochemical measurements and electron microscopy before and after electrolysis indicate that the TMNs act as precatalysts, undergoing surface oxidation to produce a catalytically active mixed-metal oxide layer while retaining a highly conductive nitride-rich core. This evolving oxide/nitride architecture provides a route to combine active surface chemistry with efficient bulk charge transport.

Ongoing work is expanding these materials beyond OER to the oxygen reduction reaction for fuel-cell applications and is investigating how composition, structure, and surface reconstruction influence catalytic selectivity and kinetics. Machine learning approaches are also being integrated with systematic catalyst synthesis and characterization to accelerate materials discovery, identify relationships between synthetic variables and performance, and develop a more predictive understanding of multimetallic nitride electrocatalysts.

SWRM 2026 SW181

Modification of the active site microenvironment for enhanced direct oxidation of methane to methanol

Frederick M. MacDonnell*, macdonn@uta.edu, Oluchukwu Igboenyesi, Wilaiwan Chanmanee, Upasana Singh, Brennan McKinney, Madelyn Johnston. Department of Chemistry and Biochemistry, The University of Texas at Arlington, Arlington, Texas, United States*

The direct conversion of methane to methanol (DMTM) with dioxygen is a highly desirable and conceptually simple reaction, but highly problematic in practice. Methanol is more susceptible to further oxidation than methane, so over-oxidation is very difficult to prevent. The most commercially viable approaches for DMTM involve simple fixed-bed reactors with gas-phase reactants, producing methanol from methane, air, and steam and operating at modest temperatures and pressures (100-500 C and 1-30 atm). We are studying such a system in which the fixed-bed catalyst is modified so that it allows facile entry of the reactants (CH_4 and O_2) but rejects and excludes polar substances, like the product methanol and water, thus protecting the methanol from further oxidation. We coat an active, solid nickel-oxide/ceria on alumina catalyst with a thin film-like layer of a Teflon-like material. This film is composed of a self-assembled monolayer of perfluorooctylsulfonate (PFOS) or related agent which bonds to the alumina support and limits permeability of reactant gases to the catalytic NiO sites to non-polar compounds, like O_2 and CH_4. The methanol product is polar and is repelled in this environment and therefore ejected into the bulk gas stream away from the catalytic sites. Moreover, it is unable to easily re-enter any catalytic site thereby protecting it from further oxidation. Initial studies reveal a 9-fold improvement in methanol production and selectivity for catalysts treated with this Teflon-like coating over the control catalyst and is competitive with the current start-of-the-art DMTM processes in the literature. We believe that the system is far from optimized and may yield substantive improvements in DMTM technology and add solid experiment data to verify this concept of product exclusion or sequestration from the catalytic sites of oxidation.

SWRM 2026 SW182

From lattice to Lorentz: Programming metal-free water splitting with donor–acceptor COF junctions

Sreeprasad Sreenivasan*, sreenivasan@utep.edu, Lissette Garcia Enriquez. Chemistry and Biochemistry, The University of Texas at El Paso, El Paso, Texas, United States*

Developing efficient metal-free electrocatalysts for overall water splitting requires coordinated control of active-site energetics, interfacial charge transfer, and near-electrode mass transport. In this presentation, we show how these three factors can be integrated within a metal-free covalent organic framework (COF) platform. We construct amide-linked COFs from benzene donor and triazine

acceptor units and integrate them with carbon nanotubes (CNTs) to form electronically coupled COF–CNT heterojunctions. The donor–acceptor framework provides spatially differentiated catalytic environments, with benzene-proximal sites favoring the hydrogen evolution reaction (HER) and triazine-proximal sites promoting the oxygen evolution reaction (OER). Density functional theory, electrostatic-potential mapping, X-ray photoelectron spectroscopy, and Kelvin probe measurements reveal framework polarization and interfacial charge redistribution, while CNT integration establishes a built-in interfacial electric field. The resulting heterojunction produces an approximately 0.20 V shift in contact-potential difference and improves interfacial charge delivery. Operando electrochemical impedance spectroscopy further distinguishes high-frequency junction-charging behavior from lower-frequency Faradaic and transport processes. We then examine how an external magnetic field further regulates this metal-free catalytic interface. Applying a 300 mT static magnetic field decreases the overpotentials for both HER and OER by tens of millivolts. Field-dependent impedance measurements and bubble imaging indicate that magnetohydrodynamic convection promotes bubble detachment and electrolyte renewal, while an additional high-frequency perturbation emerges specifically under oxygen-evolution conditions. Under the applied field, the optimized heterostructure exhibits an OER onset overpotential of approximately 261 mV and requires 366 mV to reach 10 mA cm-2 in alkaline electrolyte. Together, these results show that reticular donor–acceptor chemistry, conductive-junction engineering, and external-field modulation can collectively regulate interfacial electrostatics and near-electrode transport. This mechanistically integrated approach provides a strategy for overcoming kinetic and transport limitations in bifunctional, metal-free water-splitting electrocatalysts.

SWRM 2026 SW183

Solvent-free mechanochemical passivation of Ti3C2Tx MXene surfaces guided by machine learning

Julie P. Vanegas[1]*, julie.vanegas@utrgv.edu, Ethan Hernandez*[3]*, Amber L. Garcia*[2]*, Yaneiska Ruiz-Torres*[4]*. (1) Physics ans Astronomy, The University of Texas Rio Grande Valley, Edinburg, Texas, United States(2) Mechanical Engineering, The University of Texas Rio Grande Valley, Edinburg, Texas, United States(3) The School of Integrative Biological and Chemical Sciences (SIBCS), The University of Texas Rio Grande Valley, Edinburg, Texas, United States(4) Chemistry, Universidad Ana G. Méndez, San Juan, Puerto Rico, United States*

Two-dimensional transition metal carbides are limited less by their intrinsic properties than by the instability of their surfaces: ambient oxidation converts Ti3C2Tx to titanium dioxide and erodes performance long before a device is assembled. Wet-chemical strategies for capping these surfaces introduce their own penalty, since solvent-intensive protocols alter the native termination layer and generate liquid waste. We present reactive high-energy ball milling (RHEBM) as a solvent-free route to passivate Ti3C2Tx in a single processing step. Six ligands spanning distinct binding motifs (dopamine, thioglycolic acid, cysteine, gallic acid, citric acid, and ethylenediamine) were milled under controlled energy input and examined by XPS, XRD, FTIR, Raman, and TEM to resolve grafting chemistry, retention of surface terminations, and preservation of layer structure as functions of milling parameters. Plane-wave DFT adsorption energies for the same ligand set were used to train a machine learning pipeline combining Gaussian process regression, active learning, and SchNet representations, and SHAP analysis identified the electronic and steric descriptors that govern binding strength. The model predicts a capping ligand outside the training set, which was then synthesized and evaluated experimentally. The result is a descriptor-based framework for selecting passivating chemistries on carbide and nitride surfaces, replacing empirical screening with targeted, waste-free synthesis.

SWRM 2026 SW184

GC-PID determination of BTEX in foods and food extracts

***Jennifer L. Maclachlan**, pidgirl@gmail.com, John N. Driscoll. PID Analyzers, LLC, Sandwich, Massachusetts, United States*

Benzene, toluene, ethylene and xylenes (BTEX) are volatile aromatic hydrocarbons associated with motor-vehicle emissions, petroleum handling, and petrochemical operations and are widely distributed at trace concentrations in the environment. These compounds may enter food-production environments through contaminated air, water, raw materials, processing operations, and packaging, while benzene may also be formed within certain foods and beverages during processing or storage. Our previous investigations using gas chromatography with photoionization detection (GC-PID), with sample concentration when required, have demonstrated the utility of this technique for measuring low-parts-per-billion (ppb) to parts-per-trillion (ppt) concentrations of BTEX in ambient air and other matrices. We have observed BTEX in diverse environments, including trace concentrations in beverage-grade carbon dioxide, ambient air associated with gasoline-handling activities, and fence-line air near petroleum and petrochemical operations. The modern commercial GC photoionization detector developed by Driscoll and colleagues at HNU Systems in the mid-1970s provides high sensitivity and selectivity toward readily photoionized aromatic compounds; early characterization demonstrated a benzene detection limit of less than 2 pg and approximately 30-fold greater sensitivity than flame-ionization detection under the conditions evaluated. The present work extends GC-PID analysis to food-related matrices through development of a method for determining low-ppb concentrations of BTEX in selected solvents, liquids, and extracts of food samples. The study will evaluate sample preparation, extraction and/or concentration procedures, chromatographic separation, detector response, method detection limits, and potential matrix effects to determine the applicability of GC-PID as a selective and sensitive approach for trace BTEX analysis in foods and food-related materials.

SWRM 2026 SW185

Assessment of odor reducing agents against volatile odorous compounds and determination of absorption cross-sections of odor analytes for pseudo-absolute quantitation using headspace-gas chromatography-vacuum ultraviolet spectroscopy

***Hala Muhiar**[1], hmuhiar3@gmail.com, Michael Pecore[2], Emmanuel Varona-Torres[2], Kevin Schug[1]. (1) Chemistry and Biochemistry, The University of Texas at Arlington, Arlington, Texas, United States(2) Weaver Consultants Group, Fort Worth, Texas, United States*

Waste handling operations (WHOs) emit trace gases consisting of volatile organic compounds, including ketones, aldehydes, alcohols, aromatics, carboxylic acids, and sulfur- and amine-containing compounds, most of which have an unpleasant odor. This presents living concerns to communities residing near these facilities. Specific odor reducing agents have been used to control these odors. In this study, a selection is evaluated and compared to assess their ability to counteract odorous compounds. This research focuses on evaluating the performance of five odor reducing ingredients against eleven volatile odorous compounds of differing compound classes, which are commonly emitted from WHOs, using headspace-gas chromatography-vacuum ultraviolet spectroscopy (HS-GC-VUV). The HS autosampler is equipped with an inert pressure loop system. The VUV detector

measures the absorbance of compounds at the 125-240 nm wavelength range, where it observes unique absorption character, allowing for the differentiation of isomers and increased specificity. More specifically, GC-VUV can quantify the number of analyte molecules detected based on an analyte's absorption cross-section, referred to as pseudo-absolute quantitative analysis. For analytes lacking a recorded absorption cross-section in the VUV detector spectral library, absorption cross-sections were determined experimentally. For sample preparation, a concentrated odorous compound standard was spiked into an aqueous odor reducer solution in a headspace vial. It was assessed how the odorous compound partitions between the aqueous odor reducer solution and the headspace of the vial. Ultimately, a partition coefficient (Kp) was determined. Based on evaluations made, it was found that polyethyleneimine and an amino acid mixture are effective in reducing the presence of odorous compounds (primarily sulfur-containing compounds) relative to other agents evaluated. For the case of sulfur-containing analytes, most reduction rates using polyethyleneimine and the amino acids mixture surpassed 60%, while other odor reducing agents' reduction rates were below 20%.

SWRM 2026 SW186

Oxygenate characterization of waste plastic pyrolysis oils (WPPO) using total oxygen analysis, simulated distillation, and GC-MS

***Amey Gonzalez**, seninoga@gmail.com. Analytical Services, Lummus Technology LLC, Pasadena, Texas, United States*

Characterization of oxygen-containing compounds in Waste Plastic Pyrolysis Oils (WPPOs) is critical, as oxygenates can compromise product stability, promote corrosion, and contribute to catalyst deactivation during upgrading. Although comprehensive two-dimensional gas chromatography coupled with time-of-flight mass spectrometry (GC×GC-TOF-MS) provides detailed oxygenate characterization, its cost often limits routine implementation. This study presents an alternative workflow using conventional single-quadrupole GC-MS, simulated distillation (SimDist), and elemental oxygen analysis. Offline liquid-chromatographic fractionation and solvent dilution were employed to reduce matrix complexity, improve oxygenate detection, and minimize column fouling from the heavy hydrocarbon matrix. SimDist was used to establish boiling-range distributions for whole oils and isolated fractions, while bulk oxygen concentrations were correlated with oxygenate speciation obtained by GC-MS. Results were further evaluated alongside hydrocarbon-type distributions determined by ASTM D7423 to explore relationships between oxygenate content and established compositional characterization metrics. The combined approach links oxygen content, volatility distributions, and molecular composition across a broad boiling range, providing a practical screening methodology for oxygenate characterization in WPPOs using widely available laboratory instrumentation.

SWRM 2026 SW187

Imaging microplastics single-particles via laser-assisted micro-pyrolysis FAPA ambient mass spectrometry

***Gerardo Gamez**, gerardo.gamez@ttu.edu, Ejoke Akatugba, Daniela Barroso, Baburam Chalise, Bibek Bhattarai. Chemistry and Biochemistry, Texas Tech University, Lubbock, Texas, United States*

Microplastics (MPs) have become ubiquitous in the environment, including primary MPs from commercial products and secondary MPs from plastic waste degradation, and pose a great concern for food security/safety and toxicity. Nevertheless, detection, identification, and quantitative chemical analysis of MPs is still a challenge due to their broad size range encompassing orders of magnitude (5000 µm – 1 µm), assorted chemical composition (including polymers, additives, and sorbed species), as well as their incidence in complex sample matrices. While there are a variety of existing techniques implemented for MPs chemical analysis, they suffer from several limitations, including low sample throughput, spectral overlaps, and inadequate sensitivity. Ambient mass spectrometry (AMS) allows direct sample desorption and ionization with minimal-to-no sample preparation. Flowing atmospheric pressure afterglow (FAPA) is a plasma-based AMS source that can ionize analytes with a wide polarity range with no solvent requirements. FAPA has shown the capability for fast bulk polymer and additives characterization with spatially resolved information in three dimensions when coupled with the laser-assisted micro-pyrolysis (LAMP) technique for pyrolysis. Herein, the development of LAMP FAPA MS toward imaging of MPs directly on filter substrates will be presented. The effects of laser wavelength on pyrolysis sampling of different MPs will be discussed. Also, figures of merit for MPs of different compositions, including additives, will be shown. Finally, quantitative analysis in terms of polymer mass for single MP particles will be demonstrated.

SWRM 2026 SW188

Admittance detector with fast Fourier transform signal processing in suppressed ion chromatography

Joisha Girme*, joisha.girme@mavs.uta.edu. Chemistry and Biochemistry, The University of Texas at Arlington, Arlington, Texas, United States*

The Admittance Detector (AD) more commonly known as Capacitively Coupled Contactless Conductivity Detection (C4D) enables the detection of ionic species without direct electrical contact between the electrodes and the solution. In ion chromatography (IC), eluent suppression greatly decreases eluent conductivity, resulting in a highly resistive background where conventional C4D exhibits a highly nonlinear response near the LOD and provides poor LOD. A basic C4D cell under these conditions represents a very high resistance with a small capacitance in parallel; the latter initially decreases as the solution becomes more conductive. While the ohmic current is frequency independent, the capacitive current thorough the solution increases with increasing frequency. While the relative magnitude of the ohmic current can be improved at lower frequencies, capacitive coupling of the signal through the wall decreases at higher frequencies, deteriorating the absolute signal. The very small weak ohmic current is buried in noise. Fourier transform greatly improves the SNR, permitting many inorganic ions to be easily detected in a 20 mm bore HDPE capillary following chromatographic separation with a KOH eluent and electrodialytic eluent suppression, at injected concentrations down to 1 µM. In many cases, performance equaled or exceeded the macroscale commercial bipolar pulse conductance detector operated in parallel. Detailed results, including calibration behavior and different approaches to post-acquisition filtering will be presented.

SWRM 2026 SW189

Immittance-based sensing for perfluorooctanoic acid

***Ben Sherman**, bdsherma@gmail.com. Chemistry and Biochemistry, Texas Christian University, Fort Worth, Texas, United States*

Faradaic electrochemical methods for detecting and quantifying per and polyfluoroalkyl substances (PFAS) face complications from their inherent anodic inertness and of competing cathodic processes for direct detection. As opposed to using a reporter redox species to detect perfluorooctanoic acid (PFOA), this presentation will introduce our efforts at tracking non-faradaic (capacitive) changes at specially designed electrode interfaces to sense for PFOA in simulated and real-world water samples. This approach uses polyfluorinated self-adsorbed monolayer coatings to establish fluorophilic surfaces and electrochemical immittance spectroscopy to evaluate how the surface charging behavior changes as a function of the PFOA concentration. Ongoing work has shown this approach to be effective over the ppm to ppt concentration range and topics discussed will include how the type of electrode substrate, the structure of the coating layer, and presence of non-PFAS solutes impact the measurement.

SWRM 2026 SW190

Supercritical water reaction (SCWR) as a rapid digestion method for total organic fluorine (TOF) analysis

***Arya Mojahed Naghi**, aryamojahed@gmail.com, Charles P. Shelor, Cable Warren, Andrew Wilson, Purnendu K. Dasgupta. Chemistry, The University of Texas at Arlington, Arlington, Texas, United States*

Per- and polyfluoroalkyl substances (PFAS), often termed "forever chemicals," are a pressing environmental and public health concern. Their determination is most commonly performed by liquid chromatography–tandem mass spectrometry (LC-MS/MS); however, targeted methods quantify only a few dozen of the ~15,000 identified PFAS. Sum-parameter approaches, in which all organofluorine is quantified without speciation, simplify analysis and improve coverage. Combustion ion chromatography (CIC) is the most widely used of these: PFAS are adsorbed onto activated carbon, combusted at ~1000 °C, and the resulting HF is trapped and measured by ion chromatography (IC). The extraction step is slow and limited to PFAS that adsorb efficiently, typically long-chain species. Extractable organofluorine (EOF) methods recover a broader range of PFAS, but the extracts carry a higher burden of co-extracted organic matter that must be fully mineralized before fluoride can be measured. We present a rapid digestion method for total organic fluorine analysis using a miniature supercritical water reaction (SCWR) reactor. A small sample plug (~0.5 mL of a ~3 mL coil) is introduced together with a known volume of air to reduce fluid density and reach higher reaction temperatures. The reactor is heated to 700 °C in 10 minutes at an optimized pressure of 7500 psi (~510 atm), monitored continuously to confirm supercritical conditions, and the digest is analyzed for fluoride by IC. Under these conditions, C–F bond cleavage proceeds by hydrolysis rather than oxidation, releasing fluoride quantitatively and capable of working in anoxic conditions or containing a high organic load such as in EOF. Using trifluoroacetic acid (TFA) and trifluoromethanesulfonic acid (TFMS) as model short-chain compounds, we optimized reaction conditions and obtained high degradation and defluorination efficiencies, reproducible across replicate runs. Digestion of TFA and TFMS in methanol–water mixtures, representative of EOF extracts, retained both efficiency and reproducibility, demonstrating that the method tolerates a substantial organic-solvent load. These results establish SCWR digestion as a fast, sorbent-free route to total organic fluorine determination compatible with EOF workflows.

SWRM 2026 SW191

Fluorine-free conjugated polymer-based optical nanosensor arrays for trace PFAS detection and discrimination

***Joshua Tropp**, jtropp@ttu.edu. Chemistry and Biochemistry, Texas Tech University, Lubbock, Texas, United States*

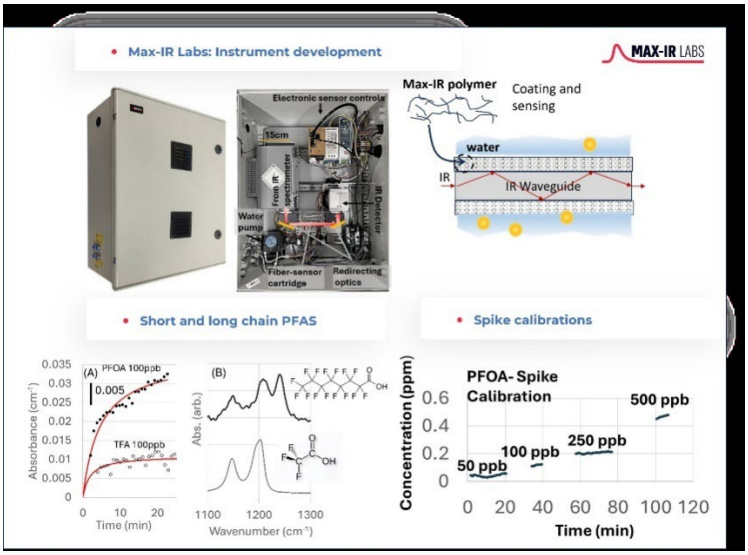
Conjugated polymers (CPs) and conjugated polyelectrolytes (CPEs) are a unique class of organic materials that can act as optical and electronic signal transducers for chemical sensing. Their delocalized electronic structures enable collective responses along the polymer backbone, providing signal amplification and high sensitivity toward molecular analytes. Per- and polyfluoroalkyl substances (PFAS) are persistent environmental contaminants that accumulate in terrestrial and aquatic systems and can enter humans through contaminated food and water. Although sensitive chromatographic methods exist for PFAS analysis, these techniques require specialized instrumentation, extensive sample preparation, and centralized laboratory analysis, motivating the development of rapid methods suitable for on-site screening. The use of CPs/CPEs for PFAS sensing has recently emerged; however, many reported platforms incorporate fluorinated materials to promote fluorophilic interactions with PFAS. Here, we instead investigate fluorine-free colorimetric and fluorescent CP/CPE sensor arrays for trace PFAS detection and discrimination. Cationic conjugated polymers bearing systematically varied ammonium-containing side chains were synthesized to modulate electrostatic and secondary interactions with anionic PFAS. Changes in polymer optical properties following PFAS exposure were characterized using UV-Vis absorption, steady-state fluorescence, and fluorescence lifetime measurements. Differential optical responses across the polymer array were further used to discriminate among structurally related PFAS analytes. These studies establish structure-response relationships governing PFAS-induced optical signaling and provide design principles for fluorine-free sensors capable of low-picomolar detection in aqueous media. The resulting approach provides a foundation for rapid, low-cost optical screening of PFAS without incorporating additional persistent fluorinated materials into the sensing platform.

SWRM 2026 SW192

Sensor for inline chemical monitoring for water and wastewater

***Chase Hazboun**, chase.hazboun@max-ir-labs.com, Trey Daunis, Jennifer Dussor, **Katy Roodenko**, katy.roodenko@utdallas.edu. Max-IR Labs, Dallas, Texas, United States*

Max-IR Labs is developing the ISMIR™ sensor platform for continuous, inline chemical monitoring in water and wastewater. The platform combines infrared spectroscopy with selective chemical preconcentration to enable sensitive detection of water-quality parameters, including naturally occurring ions such as sulfate, nutrients, and contaminants, directly in complex water matrices. Current applications include monitoring of nitrate and other nutrients for wastewater process control, as well as detection of emerging contaminants such as PFAS. By providing continuous measurements without relying on frequent grab sampling and laboratory analysis, ISMIR™ enables operators to better understand changing water chemistry, optimize treatment processes, and improve resource and operational efficiency. The presentation will highlight the sensor technology, recent validation results, and applications of inline chemical monitoring for water and wastewater treatment.



SWRM 2026 SW193

Continuously rejuvenated copper electrode for carbohydrate analysis

***Shane Wilson**, srwilson775@hotmail.com, Purnendu K. Dasgupta, Charles P. Shelor. Chemistry, The University of Texas at Arlington, Arlington, Texas, United States*

Routine HPAEC-PAD carbohydrate analysis relies on fixed Au working electrodes that are periodically replaced as their performance deteriorates. Here, we report a continuously renewed Cu electrode for constant-potential amperometric detection following high-performance anion-exchange chromatography. Rather than preserving a fixed electrode surface, the exposed Cu is intentionally consumed during operation while a spring-loaded tungsten carbide plunger continuously advances fresh wire into the detection region. With an optimized outlet-shim geometry, detector-induced dispersion for directly injected fructose was comparable to that of a commercial disposable Au electrode (FWHM = 2.8 and 2.4 s, respectively). Limits of detection for glucose, fructose, and sucrose were 0.14, 0.17, and 0.40 ppm (0.79, 0.97, and 1.17 µM), respectively. The detector was further evaluated using inulin, exemplifying the detector's ability to resolve 100 discernible peaks. During repeated analysis over 14 days, representative peak responses were highly reproducible during the first four days (average RSD = 1.63%). Absolute response drifted over time, but the normalized response remained essentially constant over 14 days. Continuous advancement therefore converts Cu consumption from a source of electrode deterioration into the mechanism for maintaining the analytical surface, enabling continuous constant-potential carbohydrate detection without relying on periodic replacement of a fixed electrode.

SWRM 2026 SW194

Electrochemical profiling of beef sarcoplasm: From meat quality monitoring to native electron-transfer kinetics

***Silan Bhandari**[1], silan.bhandari@okstate.edu, Sachinthani A. Devage[1], Ranjith Ramanathan[2], Sadagopan Krishnan[1]. (1) Chemistry, Oklahoma State University Department of Chemistry, Stillwater,*

Oklahoma, United States(2) Animal and Food Sciences, Oklahoma State University Department of Animal and Food Sciences, Stillwater, Oklahoma, United States

Meat discoloration, driven by oxidation of myoglobin to metmyoglobin, is a major determinant of consumer acceptance and economic loss in the beef industry, yet conventional methods such as Raman, NMR, FTIR, and mass spectrometry are costly and impractical for routine or point-of-need use. Electrochemical methods offer a simple, rapid, low-cost alternative for probing these redox-active biomolecules directly within native tissue extracts. Building on prior identification of myoglobin-associated redox peaks in beef sarcoplasm, we present an electrochemical investigation spanning practical meat-handling conditions to the fundamental electron-transfer behavior of the native sarcoplasmic matrix. Using cyclic and square wave voltammetry, we tracked redox signals in beef longissimus lumborum sarcoplasm across repeated freeze–thaw cycling and extended nine-day storage. Increased currents at characteristic peaks (0.82 ± 0.01 V and −0.25 ± 0.01 V vs Ag/AgCl) correlated strongly with spectrophotometrically determined metmyoglobin content ($r = 0.99$, $p < 0.01$). Over nine days of storage, peak currents at −0.26 V and +0.38 V rose by 68.9% and 270.3%, respectively, markedly greater than changes observed over shorter durations, while frequency-dependent peak shifts indicated quasi-reversible electron transfer; both measures correlated closely with metmyoglobin accumulation ($r = 0.98$, $p < 0.001$). Spiking experiments with purified myoglobin confirmed it as the dominant redox contributor. Extending this work, we report the first direct electrochemical characterization of a sarcoplasmic film adsorbed onto a polyethylenimine-modified graphite electrode, revealing a heterogeneous electron-transfer rate constant of 27.1 ± 2.2 s^{-1} and an oxygen binding affinity (K_M=722 ± 62 μM) closely matching isolated myoglobin. Together, these findings establish electrochemistry as a portable, cost-effective platform for point-of-need meat quality monitoring and advance fundamental understanding of redox-active protein behavior within native tissue matrices.

SWRM 2026 SW195

Drag-and-drop PowerPoint slides for digital quizing and active learning in organic chemistry

Robert Comito[1]*, rjcomito@central.uh.edu, Sachin Nedungadi*[2]*. (1) Chemistry, University of Houston, Houston, Texas, United States(2) University of Nebraska Omaha, Omaha, Nebraska, United States*

Organic chemistry is a conceptually rich topic that demands critical thinking and problem solving skills. Regular practice questioning remains the most effective way to teach this subject. However, essential problem types like mechanism, synthesis, and bonding are graphically demanding, and are challenging to reduce to standard digital quizzing formats. This problem limits the use of scaffolding and active learning in large chemistry service classes, where paper-and-pencil methods are not practical. Furthermore, reducing organic chemistry problems to simple "clicker" questions reinforces the unfortunate perception of this topic as a memorization course. This presentation describes the use of drag-and-drop PowerPoint slides to test mechanism, synthesis, and bonding concepts in a fully digital format. Students are given a prompt slide with movable objects, which they can rearrange and annotate to generate a response. Distribution and collection are done over standard course management systems. We used this method in seven semesters of undergraduate and graduate organic chemistry, including under remote instruction during the COVID-19 pandemic. From this experience, this presentation will provide best practices for using the slides, which are published in the *Journal of Chemical Education*. We also report detailed survey evaluation, which supports our claims that the slides are easy to use and effective as a learning activity.

SWRM 2026 SW196

School of Integrative Biological and Chemical Sciences at UT Rio Grande Valley: A unique school offering diverse and flexible master's degrees in chemistry, biology, and in between

***Yonghong Zhang**, yonghong.zhang@utrgv.edu. School of Integrative Biological and Chemical Sciences, The University of Texas Rio Grande Valley, Edinburg, Texas, United States*

The University of Texas Rio Grande Valley (UTRGV) is a public research university with its main campus in Edinburg, Texas, and multiple other campuses throughout the Rio Grande Valley. It is the southernmost member of the University of Texas System. The School of Integrative Biological & Chemical Sciences (SIBCS) at UTRGV is dedicated to advancing scientific knowledge through cutting-edge research, transformative teaching, and impactful service to the university, the Rio Grande Valley, and the scientific community, in alignment with UTRGV's mission and core values. The challenges of our rapidly changing world present a greater need for scientific understanding, data-driven analytical skills, biotechnology innovations, and critical thinking than ever before. By exploring life and material sciences, from the fundamental building blocks of matter through the many levels of living organisms and their environment, the School offers three master's degrees in chemistry, biology, and biochemistry & molecular biology. These graduate programs' unique course offerings, research opportunities, and ethical standards provide crucial preparation for graduate students (both domestic and international) pursuing career paths in research, the health professions, industry, education, public policy, and other emerging fields.

SWRM 2026 SW197

Geometry-governed symmetry-breaking charge separation and photocatalysis of benzoperylenetriimide dimers

***Ram Ratan Kaswan**, ramkaswan@my.unt.edu. Chemistry, University of North Texas, Denton, Texas, United States*

An in-depth understanding of the structure–property relationships in multichromophoric systems undergoing excited electron transfer is essential for designing reliable photocatalytic and optoelectronic devices. However, creating architectures to govern electron-transfer events in a controlled manner remains challenging due to synthetic challenges and suboptimal conditions. Here, we report two novel benzoperylenetriimide (PTI) dimers, PTI-PTI and PTI-Ph-PTI, utilizing an easily reducible PTI. The former dimer features a direct connection through the bay positions of the PTI, whereas the latter has a phenyl ring spacer. Their ability to undergo symmetry-breaking charge separation (SB-CS) and subsequent performance in photocatalytic electron pooling is probed. For the PTI-PTI dimer, which is rigid and orthogonal, SB-CS was not observed due to a lack of electronic communication between the PTI moieties, namely, a perfect "null-exciton" system. In contrast, the flexible PTI-Ph-PTI dimer showed clear evidence of SB-CS due to its ability to communicate between the macrocycles. Steady-state and time-resolved emission studies revealed significant quenching, especially in PTI-Ph-PTI compared to the monomer PTI, indicating initial signs of SB-CS. The redox gap obtained from electrochemical studies confirmed that the SB-CS state can be populated from the singlet excited state in both polar and nonpolar solvents without appreciable energy loss, a much-sought-after property. Additionally, DFT calculations supported experimental results, showing an asymmetric distribution of electron density in frontier orbitals. Subsequent femtosecond pump–probe studies provided conclusive evidence of charge separation in the PTI-Ph-PTI dimer, independent of the solvent polarity. The lifetimes of the charge-separated states were found to be 119 and 228 ps in

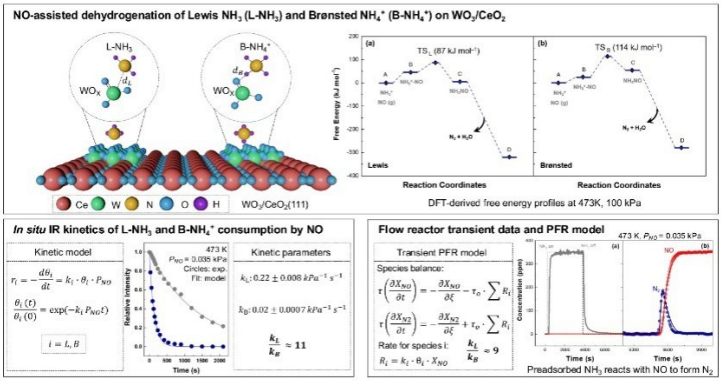
benzonitrile and toluene, respectively, which were sufficient to engage them in photocatalytic studies. Consequently, the PTI-Ph-PTI dimer was used for photocatalytic electron-pooling experiments from an application perspective. Higher yields of electron-pooling were observed compared to the monomer, indicating the potential application of this class of systems in developing future photocatalytic systems that function at higher efficiency. Importantly, how “perfect orthogonal rigidity” prohibits SB-CS and its photocatalytic activity, helping future design of symmetric dimers to observe SB-CS, is borne out from this study.

SWRM 2026 SW198

Kinetic competence of Lewis and Brønsted acid sites in the low-temperature selective catalytic reduction of NO_X

***Xinyu Li**, xinyuli@ttu.edu, Wenshuo Hu. Chemical Engineering, Texas Tech University, Lubbock, Texas, United States*

The relative reactivities of NH_3 adsorbed at Lewis acid sites (L-NH_3) and NH_4^+ formed at Brønsted acid sites (B-NH_4^+) during low-temperature selective catalytic reduction (LT-SCR) of NO_X remain a long-standing question, hindering mechanistic understanding and the development of structure–function relationships for rational catalyst design. Here, we combine flow-reactor measurements, in situ infrared spectroscopy, first-principles calculations, and mechanism-based reactor modeling to quantitatively evaluate the kinetic competence of L-NH_3 and B-NH_4^+ on dispersed WO_3 domains supported on CeO_2. Density functional theory calculations identify NO-assisted dehydrogenation of adsorbed NH_3 to form NH_2NO as the kinetically relevant step for reactions involving both surface species. Rate expressions derived from these mechanistic pathways were incorporated into transient plug-flow reactor (PFR) models to describe the time-dependent evolution of surface NH_3 species observed by infrared spectroscopy, and the transient NO consumption and N_2 formation measured in the flow reactor. Independent regression analyses of the spectroscopic and reactor data consistently show that, at 473 K, the rate constant per adsorbed NH_3 species for the reaction of L-NH_3 with NO is approximately one order of magnitude larger than that for B-NH_4^+. Infrared measurements further show that B-NH_4^+ is about three times more abundant than L-NH_3 on WO_3/CeO_2. Consequently, despite its lower abundance, L-NH_3 contributes nearly three times higher than B-NH_4^+ to the overall reaction. These results demonstrate that both Lewis- and Brønsted-bound NH_3 are kinetically competent, but that Lewis-bound NH_3 makes the larger contribution to LT-SCR reactivity on WO_3/CeO_2. More broadly, this work illustrates how transient kinetics, in situ spectroscopy, theoretical calculations, and reactor-scale modeling can be integrated to quantify site-specific reactivity, connect measurable surface intermediates with catalytic turnovers, and guide the design and mechanistic interpretation of SCR catalysts.



SWRM 2026 SW199

Atomistic structures of a sustainable polymer: AI-accelerated *ab initio* bottom-up polymer structure prediction of amorphous

***Yizhi Song**, songyeetz@gmail.com, Bharatha K. Gunawardana, Kriti Alam, Teresa Shah, Deepa Ranabhat, Hsin-Yu Ko. Department of Chemistry, University of North Texas, Denton, Texas, United States*

Poly(1,3-dioxolane) (pDXL) is a chemically recyclable polyether whose chain length can be precisely controlled to the ultra-high-molecular-weight (UHMW) limit to achieve enhanced mechanical performance, making it a promising material for more sustainable polymer development. However, its amorphous condensed-phase structures—like those of many other polymers—hinder molecular-level understanding of its material properties and, hence, subsequent rational chemical modifications. In this work, we apply a recently developed AI-accelerated ab initio bottom-up polymer structure prediction framework designed to generate amorphous pDXL at atomistic resolution. Specifically, we simulate the living polymerization of pDXL under experimental synthetic conditions using machine-learning force fields (MLFFs) trained with reliable van der Waals (vdW)-corrected hybrid density functional theory (DFT). We present the features and variability of the non-empirically generated ensemble of amorphous pDXL structures as a function of chain length and compute their X-ray/neutron scattering properties.

SWRM 2026 SW200

Unveiling the exceptional electron-acceptor ability of C_{60} in phenothiazine-C_{60}-based multi-modular donor-acceptor conjugates

***Chamari Viyanga K. Ileperuma**[1], chamariviyangaileperuma@my.unt.edu, Pankaj K. Gupta[2], Rajneesh Misra[2], Francis D'Souza[1]. (1) Department of Chemistry, University of North Texas College of Science, Denton, Texas, United States(2) Department of Chemistry, Indian Institute of Technology Indore, Indore, India*

The superior electron-accepting behavior of fullerene (C_{60}), even in the presence of strong electron-acceptor entities, is demonstrated in a series of multi-modular push-pull systems carrying a donor, phenothiazine, and C_{60}, coupled with strong electron acceptors, tetracyanobutadiene (TCBD) or dicyanoquinodimethane (DCNQ), between the donor and phenothiazine entities. Owing to the strong

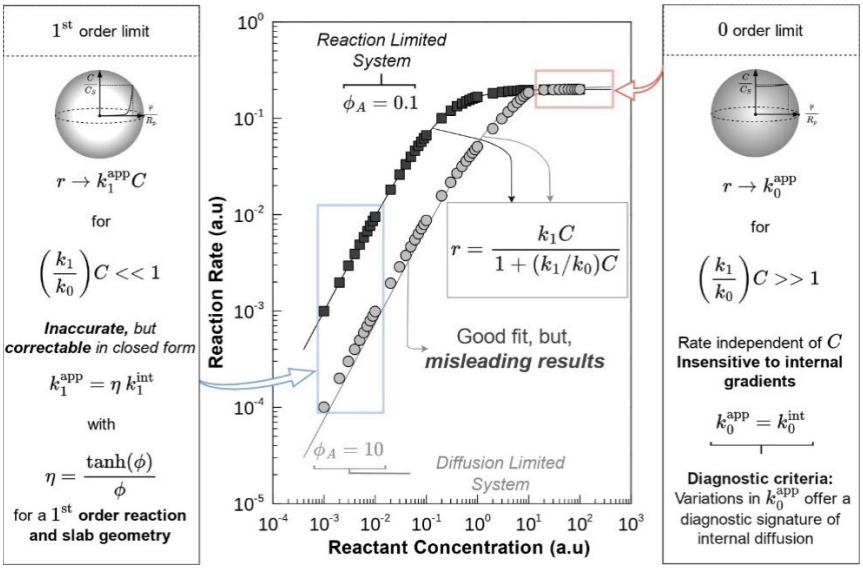
push-pull nature of the closely spaced entities, strong intramolecular charge transfer was observed, extending the optical coverage into the near-infrared region. Electrochemical studies revealed multiple redox processes owing to the presence of multiple redox-active molecular entities. DFT and TD-DFT studies helped assess the electronic structures and the excited states responsible for charge transfer, and, importantly, the role of molecular segment(s) within the multi-modular system as electron push or pull groups. Femtosecond pump-probe spectroscopy confirmed the occurrence of excited-state charge transfer and separation, with C_{60} as the terminal electron acceptor. These findings will pave the way for designing new multi-redox entities involving push-pull systems for the next generation of efficient energy harvesting, photocatalytic, and optoelectronic applications.

SWRM 2026 SW201

Diffusional effects on Langmuirian kinetics in heterogeneous catalysis

Paulo Morgado*, pmorgado@ttu.edu, Wenshuo Hu. Chemical Engineering, Texas Tech University, Lubbock, Texas, United States*

Diffusional effects within catalyst aggregates can profoundly alter observed reaction kinetics. Although closed-form treatments are established for simple rate laws, analogous expressions for ubiquitous Langmuir-type kinetics remain unavailable because the intra-aggregate mole balances are not analytically solvable. Here, we show that diffusional effects can be insidious for Langmuirian kinetics: diffusion-limited rates may still be regressed by intrinsic Langmuirian formalisms, but the resulting first- (k_1^{app}) and zero-order (k_0^{app}) parameters do not reflect the intrinsic values of the catalyst properties. These deviations depend on reactant concentration, increase with the Thiele modulus (φ), and defy closed-form relations. As Langmuirian kinetics approach the low-concentration first-order limit, k_1^{app} becomes related to its intrinsic counterpart through established effectiveness-factor expressions. Apparent zero-order constants approach intrinsic values as concentration increases and saturation is established, because zero-order rates are independent of concentration and therefore insensitive to diffusion-induced gradients. These findings enable diagnosing diffusional effects on Langmuirian rate parameters without deep numerical analysis. Systematic variations in k_0^{app} with reactant concentration provide a potential diagnostic signature of internal transport effects. Such variations indicate the parameter may no longer be intrinsic, warranting examination of diffusional limitations. To recover intrinsic rate constants, measurements in the first-order regime enable closed-form correction of k_1^{app}, whereas measurements in the zero-order regime directly yield k_0^{int}. Reanalysis of reported n-heptane hydroisomerization over bifunctional metal–acid catalysts demonstrates the framework's relevance. The data support the hidden failure mode, systematic variations in k_0^{app} as a diagnostic for internal diffusion, and the low-concentration strategy for recovering k_1^{int}. The complementary high-concentration strategy for recovering k_0^{int} is established through reaction-transport analysis.



SWRM 2026 SW202

Towards sustainable computing: Kubernetes for efficient security and portability for computational chemistry

***Kriti Alam**, kritialam@my.unt.edu, Bharatha K. Gunawardana, Yizhi Song, Hsin-Yu Ko. Chemistry, University of North Texas, Denton, Texas, United States*

Computational chemistry software often demands both portability and security. Traditional HPC scheduling (e.g., Slurm on fixed allocations) delivers strong performance but tends to fall short on portability across heterogeneous computational architectures and on security, since shared resources are readily accessible to many users. Here we develop a Kubernetes-based framework that addresses both concerns, using containers for portability and isolated resource allocation for security. The framework has shown promising results in training efficient machine-learning force fields (MLFFs) for polymers running across the diverse computational architectures available within the National Research Platform (NRP).

SWRM 2026 SW203

Examining long-lived excited charge separation in silicon(IV) phthalocyanine with axially bound C_{60} incorporated via azobenzene linkers

***Andrew Dawson**[1], andrewdawson2@my.unt.edu, Victor Sobrino-Bastán[2], Luis Martin-Gomis[2], Angela Sastre Santos[2], Francis D'Souza[1]. (1) Chemsitry, University of North Texas, Denton, Texas, United States(2) Química Orgánica, Universidad Miguel Hernandez de Elche Instituto de Bioingenieria, Elche, Valencian Community, Spain*

A very important characteristic of modern artificial photosynthetic systems used in energy-conversion applications is accelerated charge separation and long-lived charge-separated states.[1] Phthalocyanines have been used extensively as strong electron-donating groups in donor-acceptor systems; however, p-block element-hosting phthalocyanines have not yet been fully investigated.[2-3]

A novel silicon(IV) phthalocyanine, a SiPc-derived donor-acceptor, has been synthesized, with two C_{60} electron-accepting groups attached to the axial positions of the SiPc *via* azobenzene spacers. *Trans*-to-*cis* isomerization, which adjusts the donor-acceptor distance, was achieved upon photoirradiation. Strong fluorescence quenching was observed in the *trans*-C_{60}-azo-SiPc-azo-C_{60} compared to the SiPc control, suggesting the occurrence of excited-state nonradiative processes upon photoexcitation. Electrochemical and spectroelectrochemical studies were performed to determine the redox potentials and to help identify the electron-transfer products, $SiPc^{\bullet+}$ and $C_{60}^{\bullet-}$. The subsequently constructed energy diagram indicated that electron transfer occurs from ^{1}SiPc* to C_{60} in the triad, then relaxes to the ^{3}SiPc* state before returning to the ground state. DFT and TD-DFT calculations, analyzed using MultiWFN, also supported this electron-transfer mechanism. Femtosecond transient absorption studies verified electron transfer from ^{1}SiPc* to C_{60} in the triad, with the products, $SiPc^{\bullet+}$ and $C_{60}^{\bullet-}$, being spectrally identifiable. In the donor-acceptor triad, the ^{1}SiPc* had lifetimes of 86.81 and 65.91 ps in toluene and benzonitrile, respectively, which were significantly shorter than those of the SiPc-control. The final lifetimes of the radical ion pair $SiPc^{\bullet+}$-$C_{60}^{\bullet-}$ in the triad, based on nanosecond transient absorption studies, were determined to be 589.5 and 561.4 ns for $SiPc^{\bullet+}$ and $C_{60}^{\bullet-}$ signals, respectively, in toluene, and 433.8 and 488.0 ns for $SiPc^{\bullet+}$ and $C_{60}^{\bullet-}$ signals, respectively, in benzonitrile. The lifetime of the ^{3}SiPc* formed during charge recombination was 6.04 and 5.95 µs in toluene and benzonitrile, respectively, close to that of the SiPc-control in each solvent. The long-lived charge-separated states enable this triad to serve as a platform for further photocatalytic and optoelectronic applications.

SWRM 2026 SW204

Intramolecular charge transfer in phosphorus(V) porphyrin-based push-pull systems for efficient charge transfer

Hasanka Rathnayaka[1]*, hasankarathnayakamudiyanselage@my.unt.edu, Rajesh Manne*[2]*, Prashanth Poddutoori*[2]*, Francis D'Souza*[1]*. (1) Department of Chemistry, University of North Texas College of Science, Denton, Texas, United States(2) Department of Chemistry & Biochemistry, Regents of the University of Minnesota, Minneapolis, Minnesota, United States*

Natural photosynthesis provides a highly efficient and elegant model for converting solar energy into chemical energy, using complex biological pathways to drive reactions essential for life. Inspired by these processes, researchers have developed molecular donor–acceptor complexes to understand and control the excited-state dynamics of charge transfer and charge separation. In this work, we investigated a P(V) porphyrin-based molecular series to determine the relationship between molecular structure, solvent environment, and photoinduced charge-transfer dynamics. Steady-state spectroscopic measurements revealed significant absorption features related to the electronic interactions between the porphyrin and donor/acceptor components. To further understand excited-state behavior, femtosecond transient absorption (fs-TA) spectroscopy was used to monitor the ultrafast evolution of the photoexcited states.
The fs-TA measurements showed different spectral changes over time, including ground-state bleaching, stimulated emission, and excited-state absorption, helping us understand the formation and evolution of charge-transfer states. Excitation at 500 nm (corresponding to the charge-transfer absorption band) enabled direct investigation of the early-time excited-state dynamics. The observed transient features and their time evolution indicate the involvement of intramolecular charge-transfer (ICT) states, followed by subsequent excited-state relaxation. Furthermore, comparing transient behavior in solvents of different polarity provides evidence for the influence of the surrounding environment on charge-transfer stabilization and excited-state dynamics. The combination of ultrafast spectroscopy and steady-state characterization provides a detailed picture of the competing

pathways of charge separation, energy relaxation, and charge recombination in these P(V) porphyrin systems. These results improve understanding of how molecular structure influences charge-transfer processes and may help design more efficient porphyrin-based systems for solar energy conversion and artificial photosynthesis.

SWRM 2026 SW205

Screening of potentially toxic elements in children's toys across the USA–Mexico border region using X-ray fluorescence spectroscopy

*Jesus A. Rodriguez-Loya[1], Maricarmen Lerma[1], Juan P. Flores-Margez[2], **Abraham Dagda Torres**[1], adagdatorres@miners.utep.edu, Jorge L. Gardea-Torresdey[1]. (1) Chemistry and Biochemistry, The University of Texas at El Paso College of Science, El Paso, Texas, United States(2) Ciencias Químico Biológicas, Universidad Autonoma de Ciudad Juarez Departamento de Ciencias Quimico Biologicas, Ciudad Juarez, Chihuahua, Mexico*

Children's environmental health demands universal attention, as early-life exposure to toxic substances can lead to lifelong, irreversible impairments. Due to their ongoing physical development, exploratory curiosity, frequent mouthing behaviors, and penchant for wearing colorful accessories, children face heightened exposure risks through everyday toys. Additionally high-volume retail trade across binational corridors often facilitates the circulation of consumer goods subjected to differing safety baselines. To evaluate this exposure pathway, our research team collected 333 toys from prominent retail centers across the El Paso, USA (n = 109) and Ciudad Juárez, Mexico (n = 224) border corridor, sampled in proportion to each city's pediatric population under 14 years of age. Using non-destructive X-ray fluorescence (XRF) spectroscopy, intact toy surfaces were screened for lead, cadmium, arsenic, chromium, nickel, zinc, and titanium. Nearly four out of five toys (77.8%) contained at least one potentially toxic element (PTE), with approximately one in eight (12.0%) containing three or more elements simultaneously. Priority toxic elements including lead, arsenic, and cadmium were detected in 2.7%, 5.4%, and 4.5% of samples, respectively. Ultimately, in a shared regional market like Paso del Norte, harmonized binational standards and proactive cross-border surveillance are imperative to eliminate regulatory gaps and safeguard children's health.

SWRM 2026 SW206

Effects of polyethylene branch structure and zeolite framework on catalytic pyrolysis

***K SADASHIVA PATIL**, ksadashivapatil@gmail.com, SriBala Gorugantu. William A. Brookshire Department of Chemical and Biomolecular Engineering, University of Houston System, Houston, Texas, United States*

Catalytic pyrolysis of polyolefins using zeolites has shown promise for converting waste plastics into high-value products like naphtha and aromatics. However, current mechanistic insights are reported for linear polymers or model compounds over a single framework. Mixed polyolefin waste contains both linear and branched polyethylenes and interactions between catalyst and polymer branches generate intermediates whose access to Brønsted acid sites depends on pore topology. The coupled effects of branching and framework have not been studied systematically, which limits catalyst selection and the prediction of product distributions for mixed feedstocks. This work aims to identify how branch type, length and pore topology determine polyolefin cracking under pyrolysis conditions.

HDPE, LDPE and LLDPE are studied by thermogravimetric analysis (TGA) and in-situ catalytic pyrolysis at 400, 450, and 500 ºC over three commercial acidic zeolites: FAU (CBV 720), MFI (CBV 2314), and MOR (CBV 21A). Over MOR, HDPE and LLDPE deconstruction initiates at similar onset temperatures (~365 ºC), while over FAU and MFI, LLDPE decomposes nearly 50 ºC above HDPE. LDPE showed the lowest onset over all the three zeolites (313-320 ºC), attributed to the tertiary carbons that ease protolytic initiation. Densely spaced short branches in LLDPE do not confer the same advantage, suggesting that branch spacing rather than branch content controls how readily primary fragments reach internal acid sites. Py-GCxGC-FID/TOF-MS has been used to resolve the branch-architecture effects on product selectivity under fast-pyrolysis conditions. Restricted access to internal acid sites shifts product distributions toward higher carbon numbers in LLDPE. Medium pores in MFI favor successive b-scissions towards C3-C5 olefins, while supercages in FAU accommodate bimolecular hydrogen transfer that promotes conversion of olefins to paraffins and aromatics. This architecture dependence suggests that diffusion path length limits the conversion of densely branched fragments pointing toward hierarchical zeolites design for mixed polyolefin pyrolysis.

SWRM 2026 SW207

Structure determination in the classroom: Investigating supramolecules using NMR

Lakshmi Chockalingam Kasi Viswanath*, lakshmijeho@gmail.com. Chemistry, Utah Valley University, Orem, Utah, United States*

Nuclear magnetic resonance (NMR) spectroscopy is an essential tool for structural elucidation of supramolecular systems, offering students a powerful, hands-on method for connecting molecular structure to spectroscopic data. Subphthalocyanines and porphyrins, two structurally distinct classes of macrocycles, present unique and instructive NMR features, including characteristic ring current effects, symmetry dependent splitting patterns, and diagnostic shifts arising from peripheral substitution and metal coordination, making them well suited for illustrating core principles of NMR interpretation. In this work, the synthesis of subphthalocyanine and porphyrin derivatives is presented as a platform for teaching NMR based structure determination in an upper division chemistry course. Students are guided through spectral interpretation to assign proton environments, evaluate molecular symmetry, and confirm successful functionalization of these supramolecular systems. By engaging with structurally complex, non-textbook compounds derived from ongoing research, students develop practical skills in spectral interpretation while gaining insight into the unique electronic environments generated by aromatic macrocycles. This approach strengthens students' analytical reasoning and prepares them to apply spectroscopic techniques to authentic, research-level chemical problems.

SWRM 2026 SW208

From single-ligand binding to multicomponent flavor recognition: A computational study of protein–volatile interactions

Saranya Yamunan*, saranyayamunan@gmail.com, Shiru Lin. Chemistry & Biochmeistry, Texas Woman's University, Denton, Texas, United States*

Protein–volatile interactions play an important role in flavor retention and release. Although individual protein–flavor interactions are well characterized, less is known about how multiple distinct volatiles alter binding environments and behavior in protein systems. Using β-lactoglobulin as a model protein, this study examines 2-undecanone, 2-pentylfuran, and 1-octen-3-ol, representing ketone, furan, and alcohol functionalities, under increasing mixture complexity via AutoDock Vina molecular docking and GROMACS explicit-solvent molecular dynamics. Single- and multiligand docking compared protein-recognition patterns, while 100 ns molecular dynamics evaluated protein stability and ligand behavior over time. Docking revealed a progression from an overlapping recognition region for individually docked volatiles to combination-dependent redistribution and spatial separation as mixture complexity increased. Molecular dynamics showed protein conformational stability with dynamic changes in ligand proximity. Together, these results suggest that protein–volatile recognition depends on mixture composition and may not be fully represented by isolated ligand systems. Multiligand molecular dynamics and grand canonical Monte Carlo simulations will further evaluate dynamic behavior and preferential occupancy. This framework could support faster, rational flavor formulation, improving aroma balance, consistency, and sensory quality in protein-rich foods and beverages.

SWRM 2026 SW209

Sustainable recovery of lithium from discarded lithium-ion battery black mass using hydrometallurgical leaching and electrodialysis

Kalpana Dumre[2]*, kxd5658@mavs.uta.edu, Charles P. Shelor*[2]*, Oluwatosin Atitebi*[1]*, Eric Jones*[1]*. (1) Department of Industrial, Manufacturing, and Systems Engineering, The University of Texas at Arlington, Arlington, Texas, United States(2) Department of Chemistry and Biochemistry, The University of Texas at Arlington, Arlington, Texas, United States*

Lithium-ion battery (LIB) demand has grown exponentially in recent decades. LIBs contain many critical minerals including lithium which are often sourced from abroad including countries of concern. End of use LIBs represent an alternative feedstock to reduce reliance on foreign minerals, but new sustainable and economical approaches are still required. We are currently developing integrated recycling technology that combines both hydrometallurgy and electrodialysis for efficient recovery and purification of lithium from mechanically processed LIB black mass. First, old nickel-manganese-cobalt (NMC) LIBs from an electric vehicle were safely discharged followed by disassembly and removal of the internal components (cathode, anode and separator), which were then crushed and sieved to produce black mass- an intermediate powder produced during the pretreatment of end-of-life LIBs. The black mass was then subjected to hydrometallurgical leaching using sulfuric acid and hydrogen peroxide. Response surface methodology (RSM) with a central composite design was used to optimize concentrations of acid, peroxide, and the ratio of black mass to extraction volume (pulp density). The lithium recovery ranged from 20 g/kg to 35 g/kg. No single set of conditions was suitable for all metals highlighting the need to optimize conditions based on LIB chemistry. The recovery cost for lithium was estimated at $8.20/kg, ~ 60% lower compared to current market value of lithium ($21.94/kg), highlighting the potential economic viability of the proposed method. Electrodialysis was then used to recover lithium from the black mass leachate. Under the influence of an electric field, lithium and other cations are extracted through a semi-permeable cation exchange membrane. This results in purification and conversion into the commodity chemical lithium hydroxide in single process while other metals are precipitated and recovered as their insoluble hydroxides. Faradaic efficiencies of up to 57% are obtained with >70% lithium recovered.

SWRM 2026 SW210

Radical SAM enzymes: Generating and controlling the 5′-deoxyadenosyl radical

Broderick Joan[1]*, joan_broderick@tamu.edu, William Broderick*[1]*, Brian M. Hoffman*[2]*. (1) Chemistry, Texas A&M University, College Station, Texas, United States(2) Chemistry, Northwestern University, Evanston, Illinois, United States*

Radical *S*-adenosyl-l-methionine (SAM) enzymes use a [4Fe-4S] cluster and SAM to initiate radical reactions via initial formation of the organometallic intermediate Ω, which undergoes Fe–C bond homolysis to generate the highly reactive primary carbon 5′-deoxyadenosyl radical (5′-dAdo●) intermediate. The 5′-dAdo● then abstracts an H-atom from substrate to initiate substrate-based radical chemistry. The 5′-dAdo● can also be generated in the absence of substrate by using cryogenic blue light photolysis, which results in photoinduced electron transfer from the reduced [4Fe-4S]$^{+}$ cluster to the SAM sulfonium to generate 5′-dAdo● cryo-trapped in the active site. Electron paramagnetic resonance and electron-nuclear double resonance spectroscopy have revealed new insights into how the enzyme active site chaperones the reactive 5′-dAdo● species. Specifically, the 5′-dAdo● exhibits significant ^{57}Fe, ^{13}C, ^{15}N, and ^{2}H hyperfine couplings to the adjacent, isotopically labeled, methionine-bound [4Fe–4S]$^{2+}$ cluster co-generated with 5′-dAdo● during homolytic cleavage of cluster-bound SAM. The ENDOR-derived distances from C5′(dAdo●) to the labeled [4Fe-4S] cluster and methionine yields a model for active-site positioning of 5′-dAdo● with a short, nonbonded C5′-Fe distance (~3 Å). This distance involves substantial motion of 5′-dAdo● toward the unique Fe of the [4Fe–4S]$^{2+}$ cluster upon S–C(5′) bond-cleavage, plausibly an initial step toward formation of the Fe–C5′ bond of the organometallic intermediate Ω.

SWRM 2026 SW211

Characterization of the cytosolic labile iron pool in *Saccharomyces cerevisiae*

Salina Aryal, Alexia C. Kreinbrink, ***Paul A. Lindahl****, lindahl@chem.tamu.edu. Chemistry and Biochemistry/Biophysics, Texas A&M University System, College Station, Texas, United States*

Iron is essential for virtually all cells, as this transition metal has amazing catalytic abilities, and as such is required at the active sites of numerous enzymes. Consequently, iron must be imported from the environment and transported through the cell for installation into these proteins. Ironically, those same outstanding catalytic properties can damage cells, especially if iron is weakly coordinated e.g. as aqueous Fe(II) which can engage in Fenton Chemistry. This presents a conundrum for cells, as the iron during transport must be weakly bound such that it can be readily installed into recipient proteins but not so weak as to promote this damaging chemistry. The labile iron pool (LIP) serves this trafficking role in the cell, receiving iron that has been imported from the environment, and delivering it to various client apo-proteins. As its name suggests, the iron in the LIP is *labile*, and this has made characterization difficult. Indeed, LIPs have been recognized to be present in cells for half a century, but their composition remains uncertain though it is clear that Fe(II) is coordinated to low-molecular-mass non-proteinaceous ligands. The Lindahl lab has a novel liquid chromatography system inside a refrigerated glove-box that is interfaced to an inductively-coupled plasma mass spectrometer, and have used this LC-ICP-MS system to characterize the LIP in cytosol isolated from the simplest and best understood eukaryotic cell, budding yeast *Saccharomyces cerevisiae*. We have grown cells under various conditions, including high vs low iron, fermenting vs respiring metabolism, and aerobic vs hypoxic atmospheric conditions, to probe the effect on the LIP and thus better understand its

function in the cell. In this talk, our most recent results regarding the nature of this LIP will be discussed.

SWRM 2026 SW212

Chemistry at and beyond the oxo-wall

***Jason Shearer**, jshearer@trinity.edu. Chemistry, Trinity University, San Antonio, Texas, United States*

High-valent transition metal-oxo complexes are important reactive intermediates implicated in a wide variety of biological and synthetic transformations such as hydroxylation, epoxidation, and water splitting reactions. Many well characterized high-valent early first-row transition metal-oxo complexes have been isolated or trapped at low temperatures, which has allowed for the extensive study of such species. In contrast, there is a paucity of detailed studies on high-valent late first-row transition metal oxo-compounds that have been reported in the literature. For example, there is only one example of a well characterized tetragonally coordinated Co(IV)-oxo species that has been reported in the literature. This is a consequence of Ballhausen and Gray's oxo-wall concept. Owing to the population of antibonding M-O molecular orbitals as one transverses the transition metal elements, late transition metal oxo compounds possess reduced M-O bond orders and increased electron density on the oxygen atom. As a consequence, late transition-metal oxo complexes possess nucleophilic M-O moieties and are kinetically unstable. Thus, a "wall" exists between group 8 and group 9 metals making the generation and stabilization of M-O complexes beyond the oxo-wall extraordinarily difficult, if not untenable. We will present our efforts to explore the chemistry of tetragonally ligated high-valent Co-oxo and -imido species that apparently violate the oxo-wall concept. The implication of the electronic structure on the oxidation chemistries promoted by such species will also be discussed.

SWRM 2026 SW213

Radical chemistry of metal–alkyl bonds

***Kurtis Carsch**[1], kcarsch@utexas.edu, An T. Ho[1], Ning Deng[1], Thomas R. Cundari[2]. (1) Chemistry, The University of Texas at Austin, Austin, Texas, United States(2) Chemistry, University of North Texas, Denton, Texas, United States*

Metal–alkyl bonds fragment along two competing radical pathways. Homolysis (SH1) releases a free alkyl radical with loss of stereochemistry while bimolecular homolytic substitution (SH2) directly transfers the alkyl fragment to an external radical acceptor in a concerted approach. While methylcobalamin-dependent metalloenzymes such as TokK and CysS are proposed to methylate unactivated carbons through SH2 processes, synthetic systems largely reflect SH1 pathways for cobalt(III)–alkyl model complexes. More broadly, the structural and electronic factors that promote one pathway over the other remain undefined.
Recently, we have initiated a research program to elucidate the underlying factors related to radical alkylation reactivity with well-defined (salen)cobalt(III)–alkyl and (porphyrin)rhodium(III)–alkyl complexes to recapitulate reactivity of the enzymatic cofactors. Notably (salen)Co(III)–CH3 is thermally robust and shows no evidence for metal–carbon homolysis, and this complex can methylate persistent radical traps. Hammett analysis of methyl transfer indicates an electrophilic alkyl source, and Eyring analysis indicates an ordered transition state. Computations indicate the absence of

homolysis is a consequence of the strong metal–carbon bond.
Concurrently, photochemistry of (porphyrin)rhodium complexes carries this reactivity into bond formation, enabling productive formation of C(sp2)–C(sp3), C(sp3)–C(sp3), and C(sp3)–B bonds. Together, kinetic, spectroscopic, and computational analyses define how ligand field, axial ligation, and steric pressure impact the SH1/SH2 reactivity, opening routes to selective methylation that uses methane itself as the methyl source.

SWRM 2026 SW214

Harnessing the oxidizing power of nitric oxide at copper

*Subhadip Saha[1], Pokhraj Ghosh[2,3], **Timothy H. Warren**[1], thw@jhu.edu. (1) Chemistry, Johns Hopkins University, Baltimore, Maryland, United States(2) Chemistry, Southern Methodist University, Dallas, Texas, United States(3) Chemistry, Michigan State University, East Lansing, Michigan, United States*

Nitric oxide (NO) is widely recognized as a critical signaling molecule in biology, yet its capability as a potent oxidant remains underexplored. Thermodynamically, the 2 NO/N_2O couple (E° = +1.18 V vs. NHE) rivals the oxidizing power of the O_2/H_2O couple (+1.23 V), with methane-to-methanol oxidation via 2 NO/N_2O more favorable than with 1/2 O_2 (ΔG° = -44 vs. -30 kcal/mol). We illustrate how mononuclear copper(I) sites can harness nitric oxide's oxidizing power by sequential assembly of NO into *cis*-hyponitrite intermediates [Cu](κ^2-O_2N_2). Using β-diketiminate copper complexes, NO binding to Cu(I) proceeds through three-coordinate {CuNO}^{11} intermediates to generate highly reactive *cis*-hyponitrite species [Cu](κ^2-O_2N_2). Via synthetic isolation of reduced species {[Cu^{II}](κ^2-O_2N_2)}$^-$, electrochemical studies establish that neutral *cis*-hyponitrites possess remarkably high reduction potentials (E_{red} ~ 0.73 V vs. NHE).
The highly oxidizing nature of copper *cis*-hyponitrites enables hydrogen atom transfer (HAT) from C-H bonds. [Cu](κ^2-O_2N_2) abstracts H-atoms from 9,10-dihydroanthracene to give anthracene, [Cu^{II}]$_2$(μ-OH)$_2$, and N_2O. These [Cu](κ^2-O_2N_2) species generated from [Cu^{I}] and 2 equiv. NO also hydroxylate C-H bonds, with $^{15}N^{18}O$ labeling confirming oxygen transfer from NO. Based on experimental and computational analyses, we outline mechanistic pathways for HAT and C-O bond formation. Copper *cis*-hyponitrites thus emerge as functional analogs to high-valent metal-oxo oxidants [M]=O, revealing anoxic pathways for nitrosative stress relevant to biological copper sites and primordial oxidation chemistry that predates atmospheric oxygen.

SWRM 2026 SW215

Know your NO: Managing health with reactive oxygen and nitrogen species

***Alex R. Lippert**, alippert@smu.edu. Southern Methodist University, Dallas, Texas, United States*

Reactive oxygen and nitrogen species like hydrogen peroxide and nitric oxide are central and carefully regulated signaling molecules in respiratory and cardiovascular health, offering great potential as biomarkers to identify, monitor, and manage disease. Hydrogen peroxide in the exhaled breath is elevated with lung inflammation that occurs with asthma and chronic obstructive pulmonary disease, while bioavailable nitric oxide decreases with age as a landmark of cardiovascular risk. Despite the potential prognostic power of these biomarkers, robust technologies to measure these reactive molecules in a clinical setting are lacking. This talk will tell the story of an academic and

entrepreneurial journey to tackle this challenge and develop breath and blood monitoring devices for respiratory and cardiovascular disease.

SWRM 2026 SW216

Role of scaffold ligand dynamics to modulate electron transfer activation parameters in dinuclear copper(I/II) complexes

***Michael J. Rose**, mrose@cm.utexas.edu. Chemistry, The University of Texas at Austin, Austin, Texas, United States*

We report the syntheses, structures, computational analysis, spectroscopy and electron transfer (ET) properties of dimeric Cu(I) and Cu(II) complexes derived from rigid and dynamic scaffold-based ligands. The effect of the dynamic motion of metalloenzyme and biomimetic metal complexes has become increasingly of interest in recent years, as the precise role of 'dynamics' and dynamic motion in and around metal-based active sites continues to be hotly debated. In this work, we utilize two tetradentate pyrazolylmethylpyridine–based ligands constructed upon either a rigid (anthracene) or dynamic (thianthrene) scaffold. Both scaffolds provided dimeric {Cu(I)-Cu(I)} or {Cu(II)-Cu(II)} structures that provided a platform to compare ET reaction rates. Following extensive structural, computational and spectroscopic characterization, ET rates between complexes were compared by stopped-flow kinetics, NMR-based Marcus cross-relation and electrochemistry (cyclic voltammetry). Consistent with the structural 'entatic state' hypothesis of yore, Eyring analysis revealed that the rigid anthracene-based complex exhibited faster reduction ($k_{obs} \approx 10\ s^{-1}$) and lower DG‡ (16.1 kcal/mol) compared with the dynamic thianthrene-based complex ($k_{obs} \approx 5\ s^{-1}$; $\Delta G^{‡} = 16.5$ kcal/mol). Notably, the transition state of the dynamic system exhibited strong entropic influence ($\Delta S^{‡} = –8$ e.u.; $–T\Delta S^{‡}_{25C} = 2.5$ kcal/mol; $\Delta H^{‡}/–T\Delta S^{‡}_{25C} = 6$) versus the rigid system ($\Delta S^{‡} = –0.5$ e.u.; $–T\Delta S^{‡}_{25C} = 0.1$ kcal/mol; $\Delta H^{‡}/–T\Delta S^{‡}_{25C} = 117$), consistent with a role for the larger pool of ground state conformers and greater molecular motion in the dynamic system. Overall, this study demonstrates that the 'rigidity' versus 'dynamicity' is a critical and under-appreciated determinant of transition state energetics that requires further study in the context of metalloenzymes and biomimetic metal complexes, and represents the thematic 'third coordination sphere' that can yet be leveraged to understand and enhance reactivity.

SWRM 2026 SW217

Interception of Cu(II)-SNO and HONO intermediates in H_2S-mediated reduction of Cu(II)-nitrite

***Pokhraj Ghosh**[1], pghosh@smu.edu, Anagha Kuruvayil[1], Saikat Mishra[1], Aruzhan Abdikaiym[2], Brad S. Pierce[2]. (1) Chemistry, Southern Methodist University, Dallas, Texas, United States(2) Chemistry, The University of Alabama at Birmingham College of Arts and Sciences, Birmingham, Alabama, United States*

Nitric oxide (NO) and hydrogen sulfide (H_2S) are biologically important gasotransmitters that participate in interconnected signaling pathways regulating life processes such as vasodilation, neurotransmission, and immune responses. Nitrite serves as an important reservoir of NO and can react with H_2S to generate transient sulfur–nitrogen species, including thionitrite (SNO^-) and perthionitrite ($SSNO^-$). Despite growing evidence for NO/H_2S chemical crosstalk, the mechanistic pathways by which biologically-relevant metal-bound nitrite reacts with H_2S and the identities of the

resulting intermediates remain incompletely understood.
Using the neutral ligand 2,6-bis[1-(2,6-diisopropylphenylimino)ethyl]pyridine (L), we isolate and structurally characterize the Cu(II)-nitrite complex [LCu(κ^2-O_2N)]PF_6 (λ_{max} = 392 nm, ε = 2174 M^{-1} cm^{-1}; λ_{max} = 655 nm, ε = 310 M^{-1} cm^{-1}). Reaction of this complex with 2 equiv of H_2S generates NO (56%) together with N_2O. To probe sulfur-nitrogen intermediates involved in this transformation, we independently synthesize and isolate in the solid state Cu(II)-thionitrite complex [LCu(κ^1-SNO)]ClO_4 (λ_{max} = 375 nm, ε = 950 M^{-1} cm^{-1}) and characterize it with its ^{15}N isotopolog, by UV–vis, EPR, ^{15}N NMR, and FTIR spectroscopies. The ^{15}N NMR exhibits a marked downfield resonance at δ 1014 ppm relative to the free [(15-C-5)Na]$S^{15}NO$ at δ 904 ppm in CD_3CN at 22 °C. UV-vis monitoring of the reaction between [LCu(κ^2-O_2N)]$^+$ and H_2S at -60 °C reveals growth of the same 375 nm absorption feature, providing spectroscopic evidence for formation of a Cu(II)-SNO intermediate, consistent with a possible proton-assisted nucleophilic-attack pathway. In parallel, phosphine-based trapping experiments monitored by ^{31}P NMR spectroscopy, together with ESI-MS analysis, support formation of nitrous acid (HONO) through an acid–base pathway. Ongoing computational studies, together with experimental evidence for Cu(II)-SNO and HONO intermediates, support the involvement of proton-assisted nucleophilic-attack and acid–base pathways in H_2S-mediated reduction of Cu(II)-bound nitrite.

SWRM 2026 SW218

Paving the road to publications in scientific periodicals: Lessons from the past

***Nicolay V. Tsarevsky**, nvt@smu.edu. Department of Chemistry, Southern Methodist University, Dallas, Texas, United States*

Before the “introduction-methods-results-and-discussion” (IMRaD) structure of scientific papers first appeared in the latter part of the 19th century (e.g., in the work of Louis Pasteur) and became widely embraced as the “norm,” scientific publications were rather heterogenous in terms of organization and contents. The first scientific periodicals (i.e., journals, as opposed to the more frequently printed newspapers, and the less frequently published but much more detailed books and monographs) appeared in the second half of the 17th century, including *Journal de Sçavans* (first published in Paris in 1665), *Philosophical Transactions* (of the Royal Society; London, also 1665), *Miscellanea Curiosa Medico-Physica Academiae Naturae Curiosorum* (Leipzig, 1670), and *Acta Medica et Philosophica Hafniensia* (Copenhagen, 1673). In this talk, selected early examples of publications that appeared in some of the mentioned journals that deal with chemistry will be discussed in terms of topics covered, as well as style of writing. In addition, an early example (from 1672) of what today would be called a request for peer review from the editor of the *Philosophical Transactions*, Henry Oldenburg (*ca.* 1618-1677), will be presented to demonstrate that some “modern” ideas of how scientific publishing should be conducted and regulated, may be much older than it is often assumed.

SWRM 2026 SW219

***Caveat emptor*: Advice and tips for preparing scientific publications and presentations**

***Ronald Smaldone**, ronsmaldone@gmail.com. Chemistry and Biochemistry, The University of Texas at Dallas, Richardson, Texas, United States*

Scientific communication is an essential component of a successful academic career, yet many researchers receive limited formal training in how to effectively present and publish their work. In this presentation, I will share practical strategies for preparing compelling scientific presentations, manuscripts, and posters, drawing on my experience as a researcher, educator, mentor, author, and conference organizer. The presentation will examine how to identify and communicate the central message of a research project, organize scientific information for maximum clarity and impact, and tailor content to different audiences and formats.

SWRM 2026 SW220

Do's and don'ts of effective presentations

***Frank D. Blum**, fblum@okstate.edu. Chemistry, Oklahoma State Regents for Higher Education, Stillwater, Oklahoma, United States*

Communicating effectively is a core competency that is critical for a chemical professional. You want your audience to walk away with a sense of: what you are did, why you did it, and why it is important (or at least interesting). There are a few simple guidelines that can be used to enhance the transfer of information in a scientific setting, like a talk, poster, or group meeting, etc. I will review these with some examples of "do's and don'ts" that may help you to deliver more efficient presentations.

SWRM 2026 SW221

Communicating science to the outside world: Lessons on style, substance, and presentation

***Benjamin E. Blass**, benjamin.blass@temple.edu. Pharmaceutical Sciences, Temple University School of Pharmacy, Philadelphia, Pennsylvania, United States*

As scientists, we spend a great deal of time in laboratories of various types attempting to push the boundaries of human knowledge and create novel technologies capable of improving the human condition. Moving our discoveries beyond the lab, however, requires skilled oration and a finely tuned writing style that is capable of convincing others that our scientific achievements are worthy of attention, investment, and, in the face of AI generated slop, real. If someone were to discover a cure for pancreatic cancer, but was unable to convince others that the finding had value, then the "cure" would be useless to society. This discussion will focus on lesson learned on how to craft high quality papers and presentations that are required to build a career and move scientific discoveries beyond individual research teams and institutions.

SWRM 2026 SW222

Brave enough to be visible: Personal branding and the confidence to communicate your chemistry

***Jennifer L. Maclachlan**, pidgirl@gmail.com. PID Analyzers, LLC, Sandwich, Massachusetts, United States*

Practical strategies will be discussed for identifying and communicating areas of expertise, developing an authentic professional voice, translating complex chemistry for different audiences, using storytelling and visual communication to make technical information memorable, and extending the reach of presentations and publications through professional networks and digital and social media. The presentation will also consider how consistency, credibility, relationship building, and thoughtful use of emerging communication tools can strengthen a scientist's professional presence over time. Effective scientific communication is not self-promotion for its own sake. It is a means of connecting people with ideas, establishing trusted expertise, and increasing the likelihood that good science will be seen, understood, discussed, and remembered. Chemists at every career stage can learn to communicate their chemistry with greater clarity and confidence—and develop a professional identity that makes both the scientist and the science more visible.

SWRM 2026 SW223

Balancing innovation protection and scientific publication: Challenges and opportunities for industrial researchers

***MASUD MONWAR**, monwam@cpchem.com. Bartlesville R&T Center, Chevron Phillips Chemical Co, Bartlesville, Oklahoma, United States*

Protecting the confidentiality of innovation is essential for preserving a company's competitive advantage and ensuring long-term business success. At the same time, publishing research and innovation outcomes can enhance the visibility and reputation of both the organization and the individual researchers. Balancing these seemingly competing objectives is often challenging; however, with a thoughtful and strategic approach, it is possible to achieve both goals while creating value for the company and its innovators.
Developing effective strategies to protect proprietary knowledge while fostering recognition within the broader scientific community can be a complex venture. Success in this effort requires collaboration among researchers, intellectual property professionals, business leaders, and management teams, whose combined expertise can help navigate the associated risks and opportunities. Although the process can be demanding, the professional, scientific, and business benefits often justify the effort. This presentation will examine the challenges and opportunities associated with publishing as an industrial researcher, as well as the potential rewards that arise from successfully balancing innovation protection with scientific engagement.

SWRM 2026 SW224

Use of artificial intelligence to facilitate scientific communication

***H.N. N. Cheng**, hncheng100@gmail.com. (Retired) Southern Regional Research Center, USDA Agricultural Research Service, New Orleans, Louisiana, United States*

Artificial intelligence (AI) has rapidly transformed the way scientific information is created, refined, and shared. Since the introduction of ChatGPT in 2022, a wide range of powerful AI platforms has emerged, offering researchers new tools to support nearly every stage of scientific communication. In publications, AI can assist with literature searches, organization of ideas, drafting and revising manuscripts, improving clarity, and checking for consistency. For presentations, AI can help design effective slides, generate visual explanations, and support rehearsal and delivery. AI also holds

promise for broadening the reach of scientific communication by helping scientists tailor messages to diverse audiences, including students, collaborators, stakeholders, and the public. When used thoughtfully and responsibly, these tools can enhance productivity, improve the precision and accessibility of scientific writing, and allow researchers to focus more fully on the creative and intellectual aspects of their work. As AI capabilities continue to evolve, its influence on scientific publishing and presentation practices will only grow, making it an increasingly valuable resource for researchers, educators, and professionals. This talk will provide an overview of current AI tools relevant to scientific communication and offer practical guidance on using them effectively, ethically, and responsibly.

SWRM 2026 SW225

Synthesis, modification, and control of quantum materials using electrochemistry

Joshua Bocarsly[1,2]*, jdbocars@central.uh.edu. (1) Chemistry, University of Houston, Houston, Texas, United States(2) Texas Center for Superconductivity, University of Houston, Houston, Texas, United States*

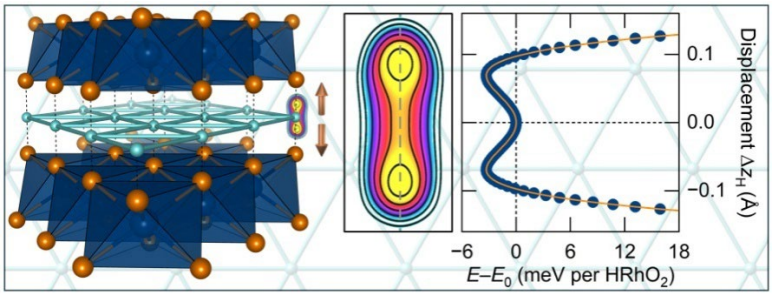
Quantum materials such as high-temperature superconductors, magnets, spin glasses, and topological insulators promise to revolutionize human society by enabling applications ranging from quantum computing to lossless power transmission lines and maglev trains. However, a consistent roadblock in this field is the challenge of obtain materials with well-controlled electron count, crystal structure, and chemical composition. Here, I will discuss our efforts in using electrochemical ion (de)intercalation to directly modify the composition and electron count of several magnets and superconductors. In addition to *ex situ* measurements of the electrochemically synthesized materials, we use a suite of powerful *in situ* methods to directly follow the electrochemical processes and characterize novel magnetic and superconducting phases as they form.

SWRM 2026 SW226

Strong, yet split hydrogen bonding with ice rules in delafossite (H/D)RhO_2

Matthew Wright*, matthew-alex-wright@hotmail.com, Anthony K. Cheetham, Ram Seshadri. Materials, University of California Santa Barbara, Santa Barbara, California, United States*

Despite remaining enigmatic, strong hydrogen bonding provides an advanced design handle for tailoring the properties of functional materials. Here, 3*R*–(H/D)RhO_2 delafossites (prepared by ion exchange of Na^+ from $NaRhO_2$) contain H/D in linear coordination with O, linking $Rh^{III}O_2$ layers. Bragg and real-space X-ray and neutron scattering analysis, vibrational and solid-state NMR spectroscopy, and density functional theory (DFT)–based electronic structure calculations have been employed to understand the nature of the hydrogen bonding. Despite short distances between H/D and the two O to which they are bonded, a clear double-minimum corresponding to a shorter and longer (H/D)–O distance is established. The triangular lattices formed by H/D appear to display ice-like disorder, corroborated by low-temperature heat capacity measurements.



SWRM 2026 SW227

Mixed ligand *f*-element coordination polymers with 2-bromoterephthalate and aliphatic dicarboxylate spacers

Ralph A. Zehnder*, ralphzehnder@me.com. Chemistry & Biochemistry, Angelo State University, San Angelo, Texas, United States*

The creation of *f*-element open frameworks may assist with overcoming technical challenges in actinide chemistry such as the improvement of sequestering *f*-element and *d*-block ions. This may be useful for the advanced nuclear fuel cycle or the creation of improved nuclear waste matrices.
Using slow diffusion protocols at room temperature (RT) we synthesized a series of lanthanide 2-bromoterephthahlate glutarates ($Ln_2(Glut)_2(TPBr)(H_2O)_4{\cdot}4H_2O$), with Ln = La, Ce, Pr, Nd. Determining the single crystal X-ray structures of the obtained coordination polymers demonstrates that they are isomorphous, crystallizing in the orthorhombic crystal system with space group Ibam.
We were able to extend this series to the elements plutonium and neptunium.
This work demonstrates once again that trivalent lanthanides serve well as surrogates for the creation of their trivalent actinide counterparts. We crystallized an isomorphous coordination polymer; $^{239}Pu_2(Glut)_2(TPBr)(H_2O)_4{\cdot}4H_2O$ and the corresponding ^{237}Np-analog.

SWRM 2026 SW228

Ultrafast energy flow in supported TMDC heterostructures

Md Shaikot Alam Shakil*, mshakil4@cougarnet.uh.edu, Ting-Hsuan Wu, Ding-Shyue Yang. Chemistry, University of Houston System, Houston, Texas, United States*

Understanding the electronic coupling and energy flow across layered two-dimensional heterostructures (HSs) is crucial to the exploitation of carrier and phonon transports as well as thermal management in next-generation optoelectronic devices. By using reflection ultrafast electron diffraction, we directly examine photoinduced out-of-plane structural dynamics of supported MoS_2/WS_2 bilayer HSs and their individual monolayers. Experimental evidence reveals the launch of ultrafast carrier-coupled intralayer atomic motions due to interlayer charge transfer across the van der Waals (vdW) heterojunctions that is absent for individual monolayers. Also, different pathways of energy flow as a result of carrier–phonon coupling and phonon scattering are reported with the corresponding characteristic times. On longer timescales, relaxation of thermalized atomic motions can be sufficiently described by a thermal transport model. A higher thermal boundary conductance (TBC) across MoS_2/WS_2 HSs is obtained compared to those at the monolayer–substrate interfaces. These results further shed light on the optical, phonon, and interfacial thermal properties of vertically-stacked vdW HSs.

SWRM 2026 SW229

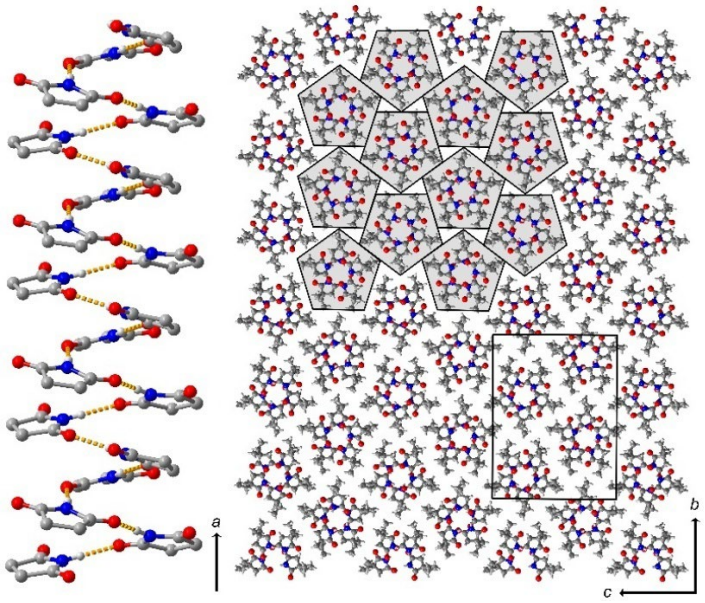
Packing pentagons

***Tomce Runcevski**, truncevski@smu.edu. Southern Methodist University, Dallas, Texas, United States*

Fivefold motifs are everywhere in nature, from viral capsids to biological assemblies, yet they are nearly absent from the catalog of molecular crystals. True C5 rotational symmetry is forbidden in 3D space groups, and regular pentagons cannot tessellate a plane without leaving voids. Aristotle would have recognized the problem: *Natura abhorret a vacuo*. A crystal that insists on fivefold order must find something to put in the empty space it creates. Even the densest periodic pentagonal arrangement, the ice-ray packing, has been reported at crystallographic length scales in only a handful of cases.

Here we show that a simple asymmetric molecule fills the void on its own. In crystals of the anticonvulsant drug ethosuximide, directional hydrogen bonding assembles pseudo-fivefold helices with a high-Z′ repeat, and conformational and enantiomeric disorder collects at the helix periphery. That disorder occupies exactly the geometric voids that pentagonal tessellation demands, and the ice-ray packing is stabilized in a bulk periodic solid. Pseudo-fivefold helices are themselves exceptionally rare in molecular solids, so this one material carries two of the least common structural motifs in crystallography at once.

Hierarchical bonding makes the lattice profoundly anisotropic, and the crystals grow as whiskers with aspect ratios that rival synthetic inorganic nanowires. They are compliant along their soft direction, stiff along the helix axis, and they bend and recover without fracture. This is the mechanical signature of a flexible material, the class now being pursued for optical waveguiding, actuation, and damage-tolerant devices, arriving here from a packing motif that crystallography has treated as forbidden territory. Pentagonal packing is not a geometric curiosity. It is an unexploited design handle for the mechanical behavior of molecular solids, and here we show what becomes available once the void is filled.



Ice-ray pentagonal packing of five-fold helices

SWRM 2026 SW230

Synthesis-enabled discovery and crystal chemistry of rare earth silicon pnictides

Gayatri Viswanathan[1,2,3], *gviswanathan8730@gmail.com, Gordon J. Miller*[1], *Kirill Kovnir*[1,2]. *(1) Department of Chemistry, Iowa State University of Science and Technology, Ames, Iowa, United States(2) Ames National Laboratory, Ames, Iowa, United States(3) Rice Advanced Materials Institute, Rice University, Houston, Texas, United States*

Metal tetrel pnictides represent a versatile, underexplored platform for functional solids in energy conversion applications, including nonlinear optics, thermoelectrics, and quantum materials. Featuring a flexible covalent tetrel-pnictide backbone, these compounds accommodate diverse metal cations and form complex structures, often with noncentrosymmetric space groups or atypical structural motifs. However, accessing this rich phase space is hindered by an inherent reactivity mismatch between volatile pnictogens and refractory components. Traditional high-temperature solid-state synthesis routes favor the formation of thermodynamically stable binary pnictides and often fail to capture elusive metastable phases with fascinating crystal chemistry.
By leveraging unconventional synthesis approaches – such as arc-melted precursors, molten salt fluxes, and topotactic transformations – we alter kinetic reaction pathways to bypass thermodynamic barriers and open access to underexplored phase spaces. Guided by variable-temperature *in situ* powder X-ray diffraction, we investigated phase dynamics within ternary *Ln*-Si-*Pn* and quaternary *Ln*-*M*-Si-*Pn* systems (*Ln* = La, Ce; *M* = Mn, Au; *Pn* = P, As), revealing temperature-dependent polymorphism and complex phase competition. Targeted synthesis approaches then enabled the isolation and structural characterization of several new compounds, revealing novel structures and unusual metal coordination environments, including two-coordinate linear Mn for the first time in an extended solid ($La_6MnSi_4As_{14}$) and a homologous intermetallic series with Au square-net nanosheets ($LaAu_nSiP$; n = 1-3). Transport and magnetic property measurements elucidate structure-composition-property relationships across this underexplored class of materials, enabled by predictive and unique synthesis approaches.

SWRM 2026 SW231

Reversible and asymmetric phase-transition pathways in MnSb conversion-type anodes revealed by synchrotron X-ray diffraction

Jason J. Zhou[1,2], *jasonstark0326@gmail.com, Joshua Bocarsly*[1,2]. *(1) University of Houston System, Houston, Texas, United States(2) University of Houston Texas Center for Superconductivity, Houston, Texas, United States*

Lithium-ion batteries with increased capacity are needed to enable next-generation energy storage. Conversion-type anodes can store significantly more lithium than intercalation-type layered materials such as graphite. However, the mechanisms of conversion systems remain obscure and are generally incompletely reversible. As a result, known conversion electrodes suffer severe loss of capacity in the first cycle. This presentation focuses on the conversion anode MnSb, which has been shown to accommodate up to 3 equivalents of Li according to the formula MnSb + 3Li -> Mn(nano) + Li3Sb. We show that, by modifying the potential window, this material can achieve ~100% first cycle reversibility. We use *ex situ* and *in situ* synchrotron diffraction to understand this unique behavior. The conversion reaction is found to occur through an asymmetric mechanism, with a different reaction pathway on lithiation vs. delithiation. During lithiation, MnSb transforms to LiMnSb and then to a mixture of Li_3Sb and Mn nanoparticles. On delithiation, a new solid-solution intermediate occurs along

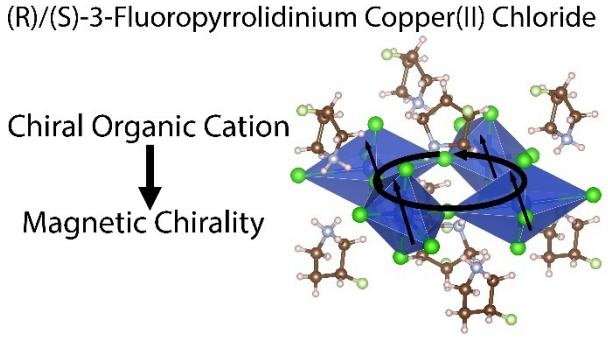
the delithiation pathway, which appears to be important in enabling the reverse reaction to proceed to completion. This reaction asymmetry reveals distinct kinetic and thermodynamic pathways and establishes MnSb as a useful model for understanding reversible conversion chemistry. More broadly, the results demonstrate how solid-state synthesis, electrochemistry, and in situ and ex situ synchrotron diffraction can complement each other to reveal the vague phase transition pathways of conversion-type electrode materials and to guide the material design of next-generation high-performance batteries.

SWRM 2026 SW232

Chirality transfer to the magnetic sublattice in the hybrid perovskite (R)-/(S)-3-fluoropyrrolidinium copper(II) chloride

Daniel B. Straus[1]*, dstraus@gmail.com, Zheng Zhang*[1]*, Mingyu Xu*[2]*, Jose L. Gonzalez Jimenez*[2]*, Stephen Zhang*[3]*, Weiwei Xie*[2]*, Xianghan Xu*[4]*. (1) Chemistry, Tulane University, New Orleans, Louisiana, United States(2) Chemistry, Michigan State University, East Lansing, Michigan, United States(3) Chemistry, Princeton University, Princeton, New Jersey, United States(4) Physics, University of Minnesota Twin Cities, Minneapolis, Minnesota, United States*

Incorporating chiral organic cations into organic−inorganic hybrid materials has been shown to enable the inorganic sublattice to display chiroptical properties. We report a new two-dimensional magnetic (S = 1/2) chiral metal halide perovskite, (R)- and (S)-(C4H9FN)2CuCl4 (where (C4H9FN)+ is 3-fluoropyrrolidinium), which consists of Cu−Cl inorganic layers separated by (C4H9FN)+ organic cations. The presence of the chiral (C4H9FN)+ organic cation induces the formation of chiral magnetic order, even though the inorganic sublattice itself is nearly structurally centrosymmetric. We also report the racemic variant, containing an equal amount of (R)- and (S)- cations, which shows no evidence of chiral magnetic order. When the magnetic susceptibility is measured perpendicular to the inorganic Cu−Cl layer propagation direction, an antiferromagnetic phase transition at Neel temperature TN = 2.23 K is observed in both the chiral and racemic materials, and the existence of the magnetic phase transition is supported by specific heat capacity measurements. Field-induced magnetic chirality is observed through the existence of a second-order magnetoelectric effect in the chiral variant, while no magnetoelectric signal is observed for the racemic material, indicating the absence of magnetic chirality. Our findings demonstrate that materials exhibiting chiral magnetic order can be created through the incorporation of a chiral cation into an organic−inorganic hybrid magnetic material, potentially allowing for the design of tailored materials that combine chiral magnetism with other desirable optical and electronic properties that come from structural chirality.



SWRM 2026 SW233

Early adventures in hyperpolarized metabolic imaging

***A. D. Sherry**, dean.sherry@utsouthwestern.edu. The University of Texas Southwestern Medical Center, Dallas, Texas, United States*

The AIRC was fortunate to obtain one of the earliest commercial DNP systems in 2006, the HyperSense from Oxford Instruments. Prior to 2006, the majority of ^{13}C tracer studies in the AIRC focused on isotopomer analysis of ^{13}C NMR spectra collected after steady-state perfusion of isolated, perfused hearts or livers with a ^{13}C enriched substrate. DNP studies using the HyperSense, primarily using HP-[1-^{13}C]pyruvate, provided new insights into metabolism that simply were not possible without real-time kinetic data. That instrument alone advanced the careers of several young scientists (Shawn Burgess, Matthew Merritt, Karlos Moreno, Charlie Khemtong, Crystal Harrison, and Lloyd Lumata) and established the AIRC as one of the leading centers in the world performing HP-^{13}C experiments. This lecture will focus on some of those early studies and the new insights that hyperpolarized ^{13}C provided.

SWRM 2026 SW234

Opportunities for new probes in clinical ^{13}C imaging

***Craig Malloy**[1,2], craigrmalloy@gmail.com, Jae Mo Park[2], Mai Huynh[2], Zoltan Kovacs[2]. (1) VA North Texas Health Care System, Dallas, Texas, United States(2) The University of Texas Southwestern Medical Center, Dallas, Texas, United States*

Fluxes in biochemical pathways are abnormal in chronic diseases such as cancer, diabetes, heart disease and inherited disorders. A challenge in understanding biochemistry *in vivo* is the complexity of the system. Radiotracers are used for clinical metabolic imaging, yet provide little information about individual metabolic pathways. The use of ^{13}C as the tracer with detection by NMR provides pathway-specific information. However, the s/n in a biological ^{13}C NMR study is poor and for this reason hyperpolarization technologies have been developed. Dynamic nuclear polarization of [1-^{13}C]pyruvate enables ^{13}C imaging of pyruvate oxidation to CO_2 and reduction to lactate. Imaging of pyruvate metabolism in the brain, heart, liver, skeletal muscle and other tissues has been investigated in patients. These studies prove that clinical translation is feasible and also point out the need for new biomarkers. Three examples follow. *First,* probes are needed for β oxidation. Among patients with coronary artery disease, oxidation of pyruvate tended to be lower throughout the heart compared to healthy controls. Since the heart preferentially oxidizes long chain fatty acids, detection of pyruvate oxidation is an incomplete picture of mitochondrial function. Probes that are water soluble and are sensitive to flux through β oxidation are needed. *Second,* gluconeogenesis is an important target. [1-^{13}C]pyruvate can be oxidized via pyruvate dehydrogenase to acetyl-CoA for energy production, or it can be carboxylated to oxaloacetate for gluconeogenesis. Both pathways yield $^{13}CO_2$ and therefore imaging this product does not specifically detect gluconeogenesis. Imaging gluconeogenesis in the liver and kidney would enable investigation of controversies about the pathophysiology of type 2 diabetes, relevant to the pharmaceutical industry in this era of GLP1 agonists. *Third*, monitoring specific reactions in the citric acid cycle is relevant to cancer metabolism. Imaging an isocitrate dehydrogenase gene mutation by detection of 2-hydroxyglutaric acid strongly links to a more favorable outcome in gliomas. During therapy for cancer, hyperpolarized [1,4-$^{13}C_2$]fumarate detects the loss of integrity of cancer cell membranes by entry into the cell or leakage of fumarase out of the

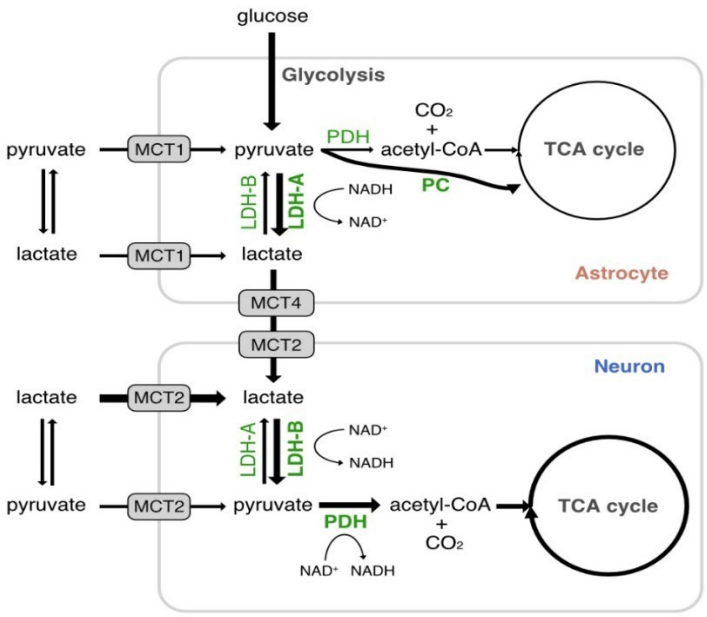
cell. Hydration of fumarate generates malate, a biomarker of cell necrosis. Both processes involve the citric acid cycle and illustrate the need for probes detecting specific reactions in the citric acid cycle.

SWRM 2026 SW235

Hyperpolarized ^{13}C MRI for imaging brain metabolism

***Jae Mo Park**, jaemo.park@utsouthwestern.edu. Advanced Imaging Research Center, The University of Texas Southwestern Medical Center, Dallas, Texas, United States*

Glucose and lactate are primary substrates in cerebral energy metabolism. Hyperpolarized (HP) ^{13}C MRI is a noninvasive approach for probing cerebral metabolism by detecting HP products from HP ^{13}C-labeled agents. In particular, HP [1-^{13}C]pyruvate has been successful because of its central position linking glycolysis, lactate metabolism, and mitochondrial oxidation. In the brain, its conversion to [^{13}C]bicarbonate provides a sensitive measure of PDH activity and mitochondrial metabolism. However, the cellular origin of bicarbonate and the contribution of lactate as an alternative substrate remain important considerations for interpreting HP measurements.
Recent studies combining HP ^{13}C MRI with *ex vivo* metabolomics analysis demonstrate that pyruvate and lactate both efficiently deliver ^{13}C into neuronal oxidative metabolism. Isotopic tracing and spatial metabolomic analyses support neuronal PDH as the predominant source of bicarbonate, with comparable incorporation of ^{13}C into mitochondrial intermediates from pyruvate and lactate. Despite these metabolic similarities, HP [1-^{13}C]pyruvate provides greater sensitivity for detecting PDH-mediated bicarbonate production because of its longer T1, smaller endogenous pool, and efficient transfer into oxidative metabolism. HP [1-^{13}C]lactate, in contrast, provides complementary information by directly probing lactate utilization and assessing altered LDH-B activity. In glioma, HP [1-^{13}C]lactate produces increased pyruvate and reduced bicarbonate production, providing a metabolic signature of altered redox balance and impaired mitochondrial oxidation.
Beyond brain tumors, HP MRI can characterize metabolic remodeling associated with neuroinflammation and traumatic brain injury. These studies establish HP pyruvate and lactate as probes for investigating cerebral metabolic function and demonstrate their potential for metabolic phenotyping of neurological disease.



SWRM 2026 SW236

Quantitative analysis of pyruvate delivery and spatial characteristics in hyperpolarized [1-13C]pyruvate cardiac MRI

***Fatemeh Khashami**, fatemeh.khashami@utsouthwestern.edu. AIRC, The University of Texas Southwestern Medical Center, Dallas, Texas, United States*

Background: Hyperpolarized (HP) [1-13C]pyruvate MRI enables real-time assessment of substrate delivery and metabolism in the human heart. Quantitative measurement of myocardial lactate and bicarbonate requires reliable characterization of the left ventricular (LV) blood-pool pyruvate signal. However, large variation in pyruvate signal intensity and spatial distribution between studies makes it difficult to define a consistent vascular reference.
Methods: A quantitative spatial analysis was applied to previously acquired human cardiac HP [1-13C]pyruvate MRI data from 106 HP injections at 3 Tesla [1]. Pyruvate images were summed across the dynamic acquisition, and voxel intensities within the LV region were ranked from highest to lowest. The ranked signal distribution was fitted with an exponential model to describe the spatial decrease from the high-intensity LV blood-pool core toward lower-intensity boundary voxels. The resulting spatial parameters were evaluated as quantitative measures of pyruvate delivery and compared with downstream myocardial lactate and bicarbonate signal-to-noise ratio. Ranked LV pyruvate intensities showed a consistent spatial decay pattern across human studies. The observed exponential model provided a simple quantitative description of differences in LV pyruvate signal distribution among studies. The normalized spatial-distribution parameter showed a positive association with downstream lactate and bicarbonate signal quality, suggesting that the spatial pattern of pyruvate delivery contains useful information for subsequent metabolic measurements. This analysis also supports subject-specific voxel selection and spatial quality assessment using the pyruvate data alone.

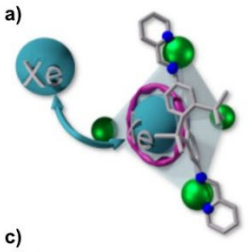
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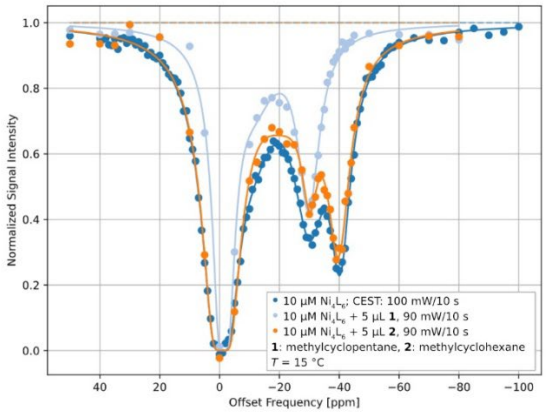
HyperCEST NMR reveals size-selective guest binding in hidden diastereomers of paramagnetic MOPs

***Leif Schröder**[1,2], leif.schroeder@dkfz.de, David Sabasch[1,2], Jabadurai Jayapaul[1]. (1) Translational Molecular Imaging, Deutsches Krebsforschungszentrum, Heidelberg, BW, Germany(2) Physics and Astronomy, Universitat Heidelberg, Heidelberg, BW, Germany*

Metal-organic polyhedra (MOPs) are self-assembling host structures with applications ranging from chemical engineering to biomedical drug delivery by enabling encapsulation of various guests. Their intriguing features include tunable facial portal diameters and cavity sizes. The ionic radius of the chosen metal center is the commonly known parameter to control selective guest access but experimental evidence for the reversible formation of host-guest complexes in solution is challenging for paramagnetic species like Co(II) and especially Ni(II). Previous work has shown that guest exchange can also greatly vary between the three possible diastereomers of M_4L_6 tetrahedra, thus pointing towards further tuning of portal and/or cavity size. Here, we present an NMR approach based on displacement of hyperpolarized ^{129}Xe to probe binding of methylcyclopentane (**1**) or -hexane (**2**) to a previously NMR-inaccessible $[Ni_4L_6]^{4-}$ MOP (Fig. 1a; L^{2-} = 4,4′-bis[(2-pyridinylmethylene)amino][1,1′-biphenyl]2,2′-disulfonate). Chemical exchange saturation transfer reveals signals from all

diastereomers (*T*, C_3, S_4) between ~-15 ppm and -40 ppm (Fig. 1b) and demonstrates that guest selectivity occurs without changing the metal ion. Addition of **1** cancels the most prominant signal at -40 ppm which is presumably from Xe inside the MOP *T* conformation. Contrary, **2** does seem to cause significant Xe displacement (Fig. 1b). Spectroscopic data is further supported by complementary T_1 relaxation measurements demonstrating a significant but incomplete shielding from paramagnetic impact on ^{129}Xe only upon addition of **1** (Fig. 1c). Again, addition of **2** does not prevent Xe from entering the cavities as revealed by fast relaxation. Further experiments are ongoing to quantify the exchange parameters and to map the size-selective guest binding behavior in more detail.





c)

Solution	T_1 of dissolved ^{129}Xe [s]
H_2O	116 ± 3
10 µM Ni_4L_6	10.7 ± 0.2
40 µM $NiCl_2$	30.6 ± 0.5
10 µM Ni_4L_6 + 5 µL **1**	83.0 ± 2.0
10 µM Ni_4L_6 + 5 µL **2**	13.3 ± 0.1

1: methylcyclopentane; **2**: methylcyclohexane

a) Schematic model of the investigated Ni_4L_6 MOP. **b)** z-spectra illustrating CEST responses at -40, -30 and around -15 ppm. Addition of **1** causes primarily loss of the most prominent signal at -40 ppm, whereas addition of **2** does not seem to block host access. **c)** T_1 relaxation times in 1 mL sample solutions demonstrating Xe displacement upon addition of **1**.

SWRM 2026 SW238

Cucurbit[6]uril-tethered DNA conjugates as potential ^{129}Xe hyperCEST biosensors

SOUMEN PRADHAN*, soumenp@smu.edu. CHEMISTRY, Southern Methodist University, Dallas, Texas, United States*

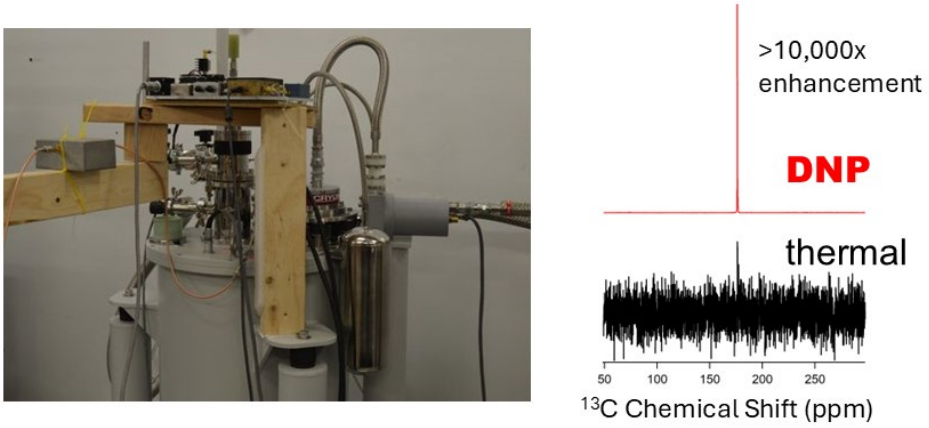
Cucurbit[6]uril, CB[6], is an important host due to its aqueous molecular recognition, metal-free click chemistry, as well as its Xe binding ability. Curiously, the full potential of CB[6]-based systems, especially in biomedical and bioimaging applications, has not been realized yet, mainly due to the difficulty in installing appropriate synthetic handles, which would allow efficient conjugation to biomolecules. Here, we demonstrate the first synthesis of a CB[6]-monoazide (CB[6]-N_3) derivative that can be readily attached to DNA via strain-promoted azide-alkyne cycloaddition. Further, the orthogonal molecular recognition properties of the DNA and CB[6] domains of the covalent conjugates were harnessed to develop (a) A host-DNA rotaxane via CB[6] facilitated click chemistry and (b) a pseudorotaxane DNA duplex that can detect an input sequence via tandem DNA strand displacement and CB[6]-mediated xenon hyper-CEST signaling.

SWRM 2026 SW239

Optimization of dissolution dynamic nuclear polarization-enhanced NMR and MRI signals

Lloyd L. Lumata*, lloyd.lumata@utdallas.edu. Physics, University of Texas at Dallas, Richardson, Texas, United States*

Dynamic nuclear polarization (DNP) via the dissolution method can generate liquid-state NMR signal enhancements of >10,000-fold by 1) transferring the high electron spin aligment to the target nuclear spins at high magnetic field and low temperature and 2) rapidly dissolving the frozen polarized sample using superheated water or other solvents to produce hyperpolarized liquids at room or physiologically tolerable temperature. Hyperpolarized metabolic tracers such as 13C-pyruvate and other substrates can then be used for in vitro NMR spectroscopy or in vivo magnetic resonance imaging (MRI) to track and evaluate the abnormal biochemistry in cancer and other pathologies vis-a-vis the metabolic behavior of the surrounding normal cells and tissues. In order to get the highest hyperpolarized NMR and MRI signal sensitivity, optimization can be made in DNP sample preparation and instrumental conditions. In this talk, a number of optimization methods and techniques on obtaining the highest dissolution DNP-enhanced NMR and MRI signals will be discussed in light of the close interplay of the electron and nuclear spins at cryogenic temperature during the DNP process, and the ways to mitigate the polarization losses of the hyperpolarized NMR signals at room temperature after dissolution.



A homebuilt dissolution dynamic nuclear polarization (DNP) instrument used in the Lumata Research Lab and representative hyperpolarized and thermal equilibrium NMR signals showing a massive NMR signal enhancement of >10,000-fold.

SWRM 2026 SW240

Accessible metabolic 13C magnetic resonance with rapid parahydrogen-based hyperpolarization

Andreas B. Schmidt*, andreas.schmidt@uniklinik-freiburg.de. Medical Physics, Radiology, University Medical Center Freiburg, Freiburg, Germany*

Parahydrogen-based hyperpolarization provides a highly accessible and high-throughput route to generate heteronuclear spin polarization for metabolic NMR and MRI. In this contribution, I will present recent results from our research group in Freiburg demonstrating the versatility of parahydrogen hyperpolarization across different experimental settings. Applications range from

metabolic studies in cells to preclinical in vivo imaging of tumors, illustrating the potential of the approach for probing metabolism in living systems. Finally, I will present our first applications combining parahydrogen-based hyperpolarization with low-field MRI, providing a pathway toward more accessible, compact, and mobile metabolic imaging.

SWRM 2026 SW241

High-throughput pyruvate-to-lactate flux profiling in leukemia and breast cancer using all-benchtop SABRE hyperpolarization and 1.4 T ^{13}C NMR spectroscopy in cellular and PDX models

***Eduard Y. Chekmenev**, chekmenev@wayne.edu. Chemistry, Wayne State University, Detroit, Michigan, United States*

NMR hyperpolarized (HP) [1-^{13}C]pyruvate is garnering attention, owing to its ability to enable non-invasive monitoring of critical biochemical pathways, including glycolysis and the TCA cycle with exceptional specificity and temporal resolution. HP [1-^{13}C]pyruvate captures dynamic metabolic fluxes in real time, enabling early detection of disease signatures, including cancer, as well as highly sensitive monitoring of therapeutic response. In this work, we demonstrate our progress toward developing next-generation clinical assay for metabolic flux sensing of HP [1-^{13}C]pyruvate, using non-cryogenic all-benchtop technology: SABRE hyperpolarization with low-field NMR spectrometer. Our approach utilizing peak lactate signal and k_{PL} enabled a statistically significant differentiation of parental versus drug-resistant leukemia cell lines (Fig. 1) in four parent-resistant pairs, as well as the ability to distinguish among multiple leukemia subtypes. Moreover, performing this metabolic assay with variable pyruvate concentration (0.1-20 mM) allows for robust measurement of Michaelis-Menten kinetics (Fig. 1): these results demonstrate the feasibility of detecting drug resistance in leukemia cells and feasibility of differentiating metastatic vs. non-metastatic cell lines. The pilot study with cancer cells derived from patient derived xenograft leukemia model of leukemia show the feasibility of performing Michaelis-Menten kinetics flux sensing too, thus, paving the way to clinical studies with patient derived materials.

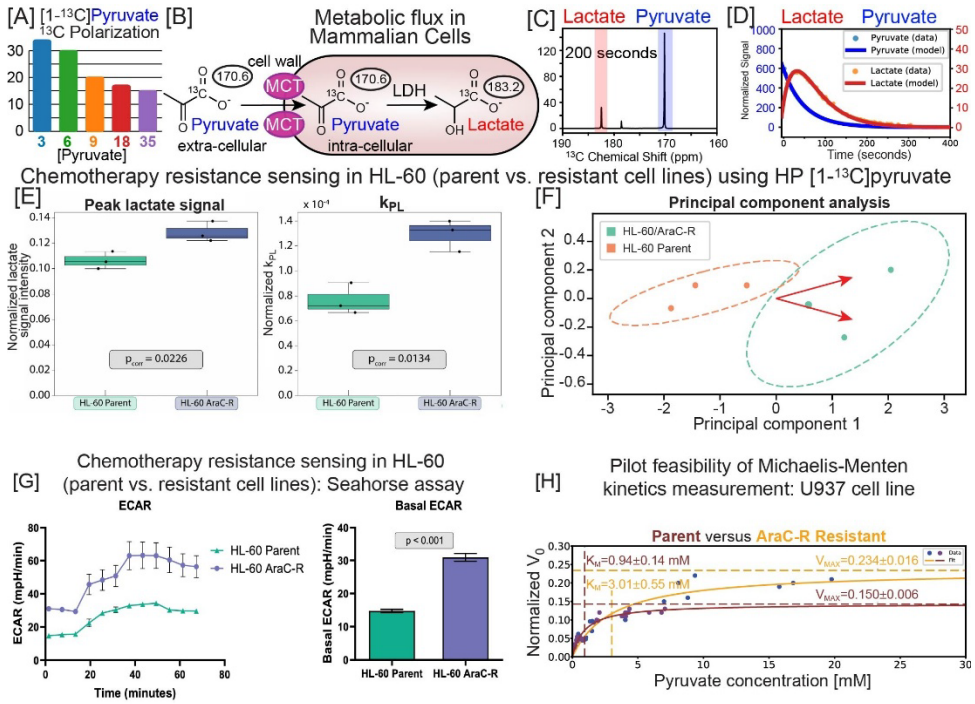


Figure 1. [A] ^{13}C polarization via SABRE-SHEATH; [B] Metabolic flux schematic; [C] Example of $^{13}C\{^{1}H\}$ benchtop NMR spectroscopy. [D] Example of dynamics of ^{13}C signals. [E,F] Chemotherapy resistance sensing in HL-60 cell lines (parent vs. AraC-resistant). [G] Corresponding statistically significant basal ECAR levels determined using Seahorse bioanalyzer. [H] Pilot feasibility of Michaelis-Menten kinetics measurement in parent vs. chemotherapy resistant U937 leukemia cells.

SWRM 2026 SW242

Study of T_1 and T_2 relaxation times of sodium cytosine monophosphate in the presence of bimetallic complexes of a furan-based polyamine macrocycle

***Devyn Ericksen**, devyn.ericksen@enmu.edu, Md Mhahabubur Rhaman. Physical Sciences, Eastern New Mexico University, Portales, New Mexico, United States*

Magnetic Resonance Imaging (MRI) with Gd(III)-based contrast agents (CAs) is widely used clinically to acquire anatomical information about tissue to differentiate between healthy and diseased tissue, though these agents carry significant risks, including severe allergic reactions, nephrotoxicity, and deposition in the brain. However, it is important to diagnose diseases at the molecular, protein, or chemical-messenger levels to prevent and cure them. In this regard, Gd(III)-based contrast agents are unsuitable due to their lack of molecular-level specificity across various pathological conditions. That's why, to expand the capabilities of MRI for disease diagnosis, we need bioresponsive MRI CAs that respond to biological signals or pathological abnormalities, or interact with molecular biomarkers via selective binding, and even respond to various pH and oxidative stress conditions. This field demands further study of various metal-ion complexes with versatile ligands. In that case, first-row transition metal ions such as Fe(III), Mn(II), Co(II), Ni(II), and Cu(II) have received considerable attention due to their diverse chemistry, comparatively low toxicity, and moderate magnetic susceptibility. In our research, a furan-based polyamine macrocycle was synthesized via the Schiff base reaction of 2,5-furandicarboxaldehyde and *N*-methyl-2,2'-diaminodiethylamine in high-dilution methanol, followed by a sodium borohydride reduction. This macrocyclic ligand contains two furans and six amine functional groups. It was used to prepare paramagnetic bimetallic complexes of several

first-row transition-metal ions. T_1 and T_2 relaxation times of various ^{1}H NMR peaks and phosphate peaks of sodium cytosine monophosphate were measured in the presence of these complexes and compared with those of a similar Gd(III) complex. Acknowledgment: This work was primarily supported by Eastern New Mexico University's internal grant PIRR3. Ms. Devyn, an undergraduate student, was supported by the Green & Silver Predisential scholarship. This project acknowledges the New Mexico Legislature for funding the Nuclear Magnetic Resonance Spectrometer.

SWRM 2026 SW243

DNP NMR reveals environment-dependent conformational ensemble of disordered proteins

Rupam Ghosh[1]*, rupam.ghosh@utsouthwestern.edu, Yiling Xiao*[1]*, Dominique Lagasca*[1]*, David Diaz*[1]*, Kendra Frederick*[1,2,3]*. (1) Biophysics, The University of Texas Southwestern Medical Center, Dallas, Texas, United States(2) Center for Alzheimers and Neurodegenerative Diseases, The University of Texas Southwestern Medical Center, Dallas, Texas, United States(3) O' Donnell Brain Institute, The University of Texas Southwestern Medical Center, Dallas, Texas, United States*

Dynamic nuclear polarization (DNP) enhances the sensitivity of magic-angle-spinning (MAS) NMR, enabling structural studies of biomolecules at concentrations and in environments that are challenging for conventional solid-state NMR. Extending DNP-enhanced MAS NMR to complex cellular environments, however, remains challenging because of low protein concentrations, heterogeneous molecular composition, and natural abundant signal. This approach becomes further challenging for intrinsically disordered proteins (IDP) like tau which sample multiple conformations based on its environment. In solution NMR, disordered proteins yield population-weighted, exchange-averaged peaks that mask the underlying conformational ensemble. However, freezing at 100K prevents interconversion and traps the underlying conformation populations. Using DNP MAS NMR, the conformational ensemble from frozen IDP can be quantitatively assessed using NMR peak shape analysis. Here, we demonstrate that DNP-enhanced MAS NMR combined with quantitative NMR peak-shape analysis can detect and characterize conformational populations of an IDP in increasingly complex biological environments. We apply this approach to tau under in vitro conditions, in cellular lysates, and in intact mammalian cells. Across these environments, DNP-enhanced MAS NMR resolves distinct conformational preferences and reveals changes in conformational sampling associated with the cellular environment and stoichiometric interactions. These results demonstrate that hyperpolarization enhanced MAS NMR can report quantitatively on conformational ensembles of disordered proteins in complex environments. This work establishes a framework for using DNP-enhanced MAS NMR to interrogate the conformational landscapes of disordered proteins directly within biological environments, including intact cells.

SWRM 2026 SW244

Structural context modulates the conformational ensemble of the intrinsically disordered amino terminus of α-synuclein

Rania Dumarieh*, rania.dumarieh@utsouthwestern.edu, Dominique Lagasca, Sakshi Krishna, Jaka Kragelj, Yiling Xiang, David Diaz, Kendra Frederick. Biophysics, The University of Texas Southwestern Medical Center, Dallas, Texas, United States*

Intrinsically disordered regions play crucial roles in biological systems yet often elude conventional biophysical characterization. We employed a freezing approach coupled with solid-state NMR to capture conformational distributions across timescales. Using segmentally isotopically labeled α-synuclein (α-syn), we examined the conformational ensembles of the six alanines, three glycines, and a single site (L8) in the disordered amino terminus under three conditions: in 8 M urea, as a frozen monomer in buffer, and within the disordered regions flanking the amyloid core. Spectra differed significantly across conditions and deviated from statistical coil predictions. In 8 M urea, monomeric α-syn showed the most restricted conformational sampling, rarely accessing α-helical or β-strand chemical shifts. In buffer, sampling broadened, favoring α-helical conformations with lesser random coil character. The disordered regions flanking the amyloid core showed the most extensive sampling, with broad peaks spanning the full chemical shift range and a marked increase in extended β-strand conformations. These results demonstrate that intrinsically disordered regions adopt distinct conformational ensembles shaped both by the chemical environment and by adjacent sequence context — differences that may explain why the monomer and the amyloid form of α-syn interact with different biomolecules inside cells.

SWRM 2026 SW245

Study of T_1 and T_2 relaxation times of water in the presence of bimetallic complexes of a furan-based polyamine macrocycle

***Alesha Foster**, aleshafoster07@gmail.com, Md Mhahabubur Rhaman. Physical Science, Eastern New Mexico University, Portales, New Mexico, United States*

Though Gadolinium-based contrast agents (CAs) are routinely used in clinical magnetic resonance imaging (MRI), they carry many risks, including severe allergic reactions, nephrotoxicity, and deposition in the brain. Demand for gadolinium-free MRI CAs motivated inorganic chemists to explore paramagnetic transition-metal complexes as potential alternatives. Consequently, the first-row transition-metal complexes, such as Mn(II), Fe(III), Co(II), Ni(II), and Cu(II), are of interest as potential alternatives to Gd(III)-based contrast agents to improve efficiency and reduce toxicity. These metal ions are inexpensive, chemically versatile, less toxic, and have moderate magnetic susceptibility. Instead of free metal ions, organometallic complexes exhibited lower toxicity and greater magnetic susceptibility, depending on their electronic structures. In our research, a furan-based polyamine macrocycle was synthesized via the Schiff base reaction of 2,5-furandicarboxaldehyde and N-methyl-2,2'-diaminodiethylamine in high-dilution methanol, followed by a sodium borohydride reduction. This macrocyclic ligand contains six amine and two furan functional groups. It was used to make bimetallic complexes. T_1 and T_2 relaxation times of water were measured in the presence of these complexes and compared with those of a similar Gd(III) complex. In addition, T_1 and T_2 relaxation times at various ^{1}H NMR peaks of the serum albumin protein will be measured. In this oral presentation, the principles of T_1 and T_2 relaxation times, the synthesis of bimetallic complexes, NMR instrumentation, and comparisons of results will be explained. Acknowledgment: This work was primarily supported by Eastern New Mexico University's internal grant PIRR3. Ms. Foster acknowledges the Sponsor Project at Eastern New Mexico University for providing the graduate assistant position and travel support. This project acknowledges the New Mexico Legislature for funding the Nuclear Magnetic Resonance Spectrometer.

SWRM 2026 SW246

Investigating thiol-containing biomolecules in parahydrogen-induced hyperpolarization at low-field NMR

Gabriel Rocha[1], *gabriel.rocha@utsouthwestern.edu, Quy S. Luu*[2], *Stefan Gloeggler*[2]*. (1) Biomedical Engineering, The University of Texas Southwestern Medical Center, Dallas, Texas, United States(2) Advanced Imaging Research Center, The University of Texas Southwestern Medical Center, Dallas, Texas, United States*

Parahydrogen-induced polarization (PHIP) allows for a massive increase in NMR signal detection. This enables higher sensitivity for tracking concentrations and biological functions that conventional NMR methods are not equipped to detect. Introducing PHIP to more chemically complex processes, such as bio-molecules with functional groups that take part in exchanges or other associated chemical pathways, gives an opportunity to investigate further into certain bio-chemical systems. Thiol-containing molecules, specifically, are involved in multiple key body compounds and can allow a more in-depth analysis on its functionality and overall affect on PHIP chemistry and behavior of hyperpolarization. This work aims to study and incorporate thiol-containing molecules into PHIP experiments and determine overall affects on hyperpolarization and NMR behavior at low field.

SWRM 2026 SW247

Exploring new PHIP-SAH precursor for real-time metabolic magnetic resonance spectroscopy

Leander Konstantin K. May[1,2], *leander.may@mpinat.mpg.de, Lena Börschmann*[1,2], *Denis Moll*[1,2], *Lisa M. Fries*[1,2], *Gonzalo G. Rodriguez*[1,2], *Charlotte von Petersdorff-Campen*[1,2], *Maria D. Santi*[1,2], *Sergey Korchak*[1,2], *Andrei Leonov*[3], *Patrick Giavalisco*[4], *Stefan Gloeggler*[1,2,5]*. (1) NMR Signal Enhancement, Max-Planck-Institut fur Multidisziplinare Naturwissenschaften, Göttingen, NDS, Germany(2) Universitatsmedizin Gottingen Center for Biostructural Imaging of Neurodegeneration, Göttingen, NDS, Germany(3) Max-Planck-Institut fur Multidisziplinare Naturwissenschaften Abteilung NMR-basierte Strukturbiologie, Göttingen, NDS, Germany(4) Metabolomics Core Facility, Max-Planck-Institut fur Biologie des Alterns, Cologne, NRW, Germany(5) Advanced Imaging Research Center | Departement of Biomedical Engineering, The University of Texas Southwestern Medical Center, Dallas, Texas, United States*

Parahydrogen-induced polarization (PHIP) is a robust technique that enhances magnetic resonance signals through nuclear spin hyperpolarization. While [1-^{13}C]pyruvate remains the predominant hyperpolarized metabolite in clinical translation efforts, broadening the range of traceable metabolic pathways is essential. By utilizing specially tailored metabolic precursors, the field can expand its impact and facilitate the monitoring of novel metabolic routes linked to cancer and neurodegenerative conditions, such as Alzheimer's disease.
Our work focuses on the development of new PHIP by sidearm hydrogenation (SAH) substrates using strategic deuteration methodologies together with targeted incorporation of the sidearm for hydrogenation (Fig. 1, **A**). Our workflow allows fast generation (60 – 90 s) of highly polarized biocompatible probes (up to 39% for α-ketoisocaproate (αKIC), the keto acid of essential amino acid leucine; Fig. 1, **B**), ready for use in *in vitro* or *in vivo* studies (Fig. 1, **C**).

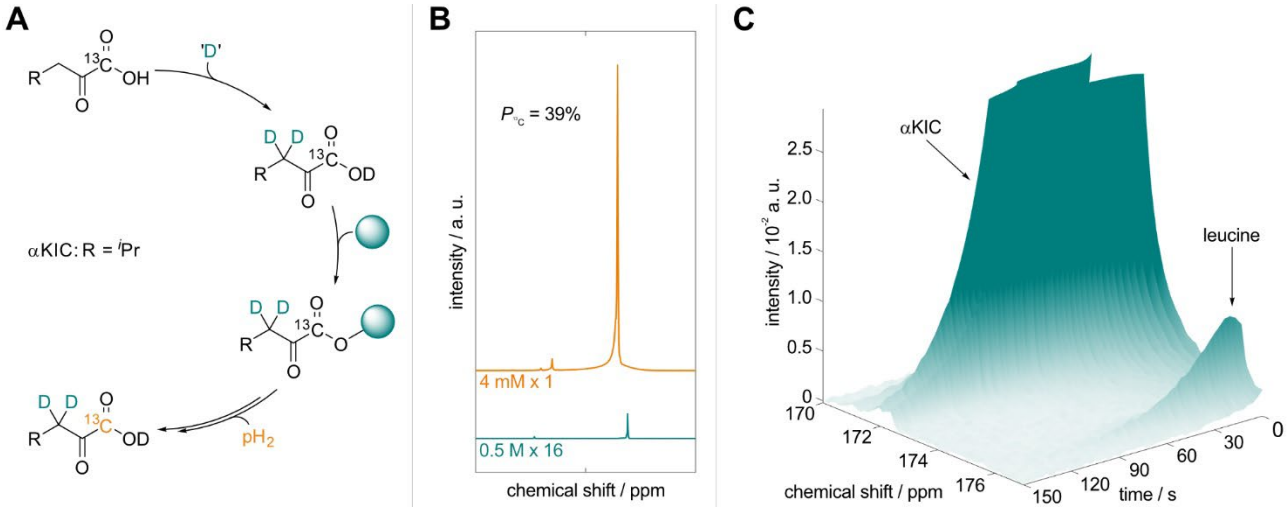


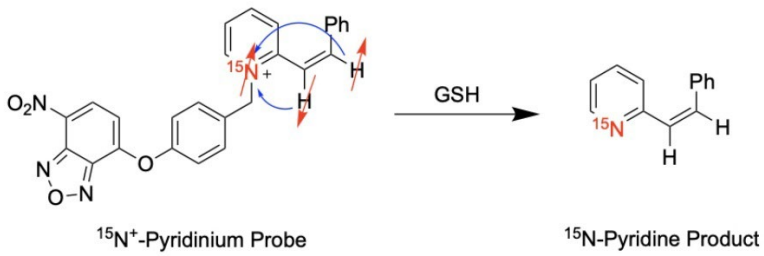
Fig. 1. A Schematic depiction of the synthesis procedure to obtain PHIP-SAH precursors for hyperpolarization experiments using parahydrogen (pH_2). **B** Comparison of hyperpolarized αKIC (orange, ~4 mM, ~0.2 mL buffered D_2O, 310 K, 1 scan) and thermal polarized sodium [1-^{13}C]pyruvate (cyan, 0.5 M, 0.2 mL D_2O, 298 K, 4 scans, 4 x scale) ^{13}C NMR spectrum. **C** Excerpt of the ^{13}C spectra recorded as a pseudo-2D experiment of the enzymatic conversion of hyperpolarized αKIC to leucine by cancer cells. Intensity relative to the highest aKIC signal.

SWRM 2026 SW248

Reaction-encoded hyperpolarized ^{15}N molecular probes for glutathione detection

***Guoshu Xie**, guoshu.xie@utsouthwestern.edu, Stefan Gloeggler. AIRC, The University of Texas Southwestern Medical Center, Dallas, Texas, United States*

Hyperpolarized magnetic resonance offers a powerful platform for the detection of biochemical transformations, yet reaction-based ^{15}N probes capable of sensing intracellular redox processes remain scarce. Here we propose a parahydrogen-hyperpolarizable ^{15}N-pyridinium molecular probe for the detection of glutathione (GSH), the most abundant intracellular thiol and a central regulator of cellular redox homeostasis. The probe couples an NBD-based, GSH-responsive trigger to a ^{15}N-labeled styrylpyridinium reporter designed for parahydrogen-based signal enhancement. Reaction with GSH cleaves the sensing unit and converts the ^{15}N-pyridinium reporter into its corresponding ^{15}N-pyridine product, producing a pronounced, nuclear magnetic resonance (NMR) spectrally resolved ^{15}N chemical-shift response. The styrylpyridinium scaffold further enables efficient transfer of parahydrogen-derived spin order to the ^{15}N nucleus, substantially enhancing magnetic resonance sensitivity. This reaction-encoded sensing strategy unites chemical selectivity with hyperpolarized ^{15}N detection, establishing a modular platform for monitoring biologically relevant thiol chemistry by magnetic resonance.



SWRM 2026 SW249

Building the spliceosome: Molecular control of RNA–protein complex assembly in gene expression and disease

***Byung Ran So**, byungran.so@uta.edu. Chemistry and Biochemistry, The University of Texas at Arlington, Arlington, Texas, United States*

RNA–protein complexes play central roles in regulating gene expression. The spliceosome is a macromolecular RNA–protein complex that removes introns from precursor messenger RNA (pre-mRNA) to generate mature mRNA. Composed of five small nuclear ribonucleoproteins (snRNPs), U1, U2, U4, U5, and U6, along with numerous splicing factors, the spliceosome undergoes highly coordinated assembly and remodeling during pre-mRNA splicing. Although much is known about the functions of individual snRNPs in splicing, how cells regulate their assembly and abundance remains less well understood. Our laboratory investigates the molecular mechanisms governing snRNP biogenesis and how disruption of this process affects RNA processing. We identified a previously unrecognized role for the U1 snRNP-specific proteins in regulating snRNP assembly through interactions with the Survival of Motor Neuron (SMN) complex, a chaperone essential for snRNP assembly. Moreover, we found that cancer-associated mutations in non-coding U1 snRNA disrupt the formation of not only U1 snRNP but also other snRNPs and sequester the SMN complex, revealing consequences beyond their established effects on splicing. We recently identified that activation of the oncogenic transcription factor MYC selectively alters the relative abundance of snRNPs, creating an imbalance that is accompanied by widespread changes in alternative splicing and 3′-end RNA processing. Together, our studies reveal that snRNP assembly and abundance are dynamically regulated and provide new insight into how RNA–protein interactions, non-coding RNA mutations, and oncogenic signaling influence RNA processing and gene regulation.

SWRM 2026 SW250

Structure-guided design of amido cyanines (AmCy) for high-performance near-infrared imaging

***Syed Usama**, syedmuhammad.usama@utsa.edu, Jared Head, Rabia Haque. Chemistry, The University of Texas at San Antonio, San Antonio, Texas, United States*

High-performance biomedical imaging necessitates fluorophores with optical properties within clinically-relevant imaging windows (above 800 nm) for deep-tissue penetration and minimal background autofluorescence. Heptamethine cyanines have remained the ubiquitous scaffold for the design of translatable fluorophores owing to their modular synthesis and tunable emission within the near-infrared region (NIR). Among these, Indocyanine Green (ICG) and IRDye800 stand out given their numerous clinical and preclinical bio-imaging applications. Despite their widespread utility, however, these fluorophores often suffer from poor *in vivo* performance due to photodegradation, aggregation-induced fluorescence quenching, and nonspecific tissue accumulation, limiting their application for long-term and quantitative imaging. Previous studies have focused on developing second-generation alternatives utilizing established heptamethine scaffolds, only partially addressing these limitations. Therefore, innovative design strategies that harness cyanine tunability are needed for high-performance NIR platforms. To address these limitations, we report herein a new class of heptamethine amido cyanines (AmCy7) highlighted by a meso-amido moiety incorporating a 5-carbon bio-conjugatable linker. Through rational design of the meso-substituent, favorable bathochromic shifts were achieved for a series of AmCy7 dyes with optical properties tuned to clinically-relevant

808 nm laser excitation. Further, incorporating aryl-sulfonated indolenines enhanced aqueous solubility while maintaining excellent optical properties, allowing for the generation of a library of biocompatible AmCy7 fluorophores with varying *N*-alkyl substitutions. Among the series, a lead compound, AmCy800, demonstrated remarkable resistance to photobleaching during prolonged irradiation, minimal aggregation in biological media, and consistent imaging performance in physiologically relevant environments over common NIR standards. Overall, this work leverages the versatility of cyanine design in the development of AmCy7 fluorophores as a promising platform for next-generation NIR imaging agents with improved performance for biomedical and clinical applications.

SWRM 2026 SW251

Quantifying and controlling beta-strand hydrogen bonds in peptides and proteins

Robert W. Newberry*, rnewberry@utexas.edu. The University of Texas at Austin, Austin, Texas, United States*

Protein structure is stabilized by a variety of noncovalent interactions, but many remain incompletely understood. For example, recent evidence implicates hydrogen bonds within individual beta-strands as key determinants of protein structure; however, these interactions have never been experimentally quantified, due in part to limitations in available experimental methods. To overcome this challenge, we adapt protein engineering approaches typically used for probing side-chain interactions to provide the first experimental quantification of these backbone interactions. Our data suggest that these intra-strand interactions are a key feature of protein structure that can be exploited for design and engineering efforts. To capitalize on that potential, we exploit differences in the stereoelectronics of peptide-bond isosteres to enhance these interactions selectively, which we apply to the development of peptides with enhanced activity against the misfolding and aggregation of proteins involved in neurodegeneration.

SWRM 2026 SW252

Chemical reactivity as a quantitative readout of RNA molecular recognition in cells

Lauren Hagler*, laurendhagler@gmail.com. Chemistry, Texas A&M University, College Station, Texas, United States*

RNA molecules form dynamic structural ensembles that govern their interactions with proteins, ligands, and other biomolecules. In cells, these interactions occur within a complex environment that can reshape RNA folding, accessibility, and binding behavior. Chemical probing methods such as DMS-MaPseq provide nucleotide-resolution measurements of RNA reactivity directly in this environment, but these measurements are most often interpreted qualitatively to describe where RNAs are folded or accessible rather than to predict how strongly they bind, function, or change across cellular condition. Our goal is to extend chemical probing beyond structural annotation, using changes in chemical reactivity to quantitatively measure molecular recognition in cells. Across diverse RNA-binding systems, we combine DMS-MaPseq with controlled perturbations of binding-partner concentration, designed RNA libraries, and functional assays. By measuring the magnitude and concentration dependence of these reactivity changes across sequence variants, we can quantify interaction strength and determine how RNA sequence, structural stability, local geometry, and

conformational accessibility shape binding in the cellular environment. Together, this work establishes in-cell chemical probing as a quantitative approach for measuring RNA molecular recognition and for connecting nucleotide-resolution reactivity measurements to predictive models of RNA binding and function.

SWRM 2026 SW253

Boron chemistry in organic synthesis, bioconjugation, and drug discovery

***Shiqing Xu**, shiqing.xu@tamu.edu. Texas A&M University, College Station, Texas, United States*

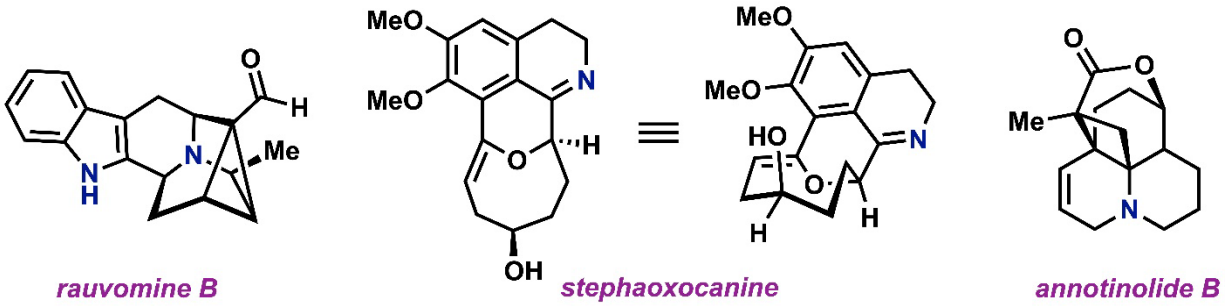
Organoboron compounds are highly versatile building blocks in modern organic synthesis due to their broad applicability in diverse transformations. These compounds have also attracted growing interest in chemical biology and drug discovery because of their unique chemical properties of reversible interactions with biological nucleophiles. This lecture will highlight our recent efforts to develop new boron-based reactions and synthetic strategies for the efficient construction of structurally diverse, drug-like boron-containing scaffolds. It will also describe our progress in developing selective boron-based covalent chemistry for bioconjugation and drug discovery. These efforts aim to establish organoboron compounds not only as versatile synthetic building blocks, but also as promising molecular frameworks for the development of chemical probes and therapeutic leads.

SWRM 2026 SW254

Chemical investigations inspired by unusual alkaloids

*Ankush Banerjee, Fan Xu, Jake Aquilina, Bhawyanth Duvvuru, Kristiana Kasper, **Myles Smith**, myles.smith@utsouthwestern.edu. The University of Texas Southwestern Medical Center, Dallas, Texas, United States*

Complex alkaloids bearing unusual structural features serve as challenging proving grounds for modern chemical methods and inspiration for the development of new synthetic strategies. Here, we showcase our recent work towards the total synthesis of unique alkaloids from the rauvomine, *Lycopodium*, and stephaoxocane families.



SWRM 2026 SW255

Strategy-driven complex bioactive molecule synthesis

***Filippo Romiti**, filippo.romiti@utdallas.edu. Chemistry and Biochemistry, The University of Texas at Dallas, Richardson, Texas, United States*

Organic synthesis is pivotal to medicine, materials science, agriculture, and more. In response to the necessities of these disciplines, synthesis provides entry to any required compound that would be otherwise inaccessible. However, the efficiency of a synthesis directly affects cost effectiveness, material throughput, and waste stream. The development of outside-the-box synthesis strategies dotted with catalytic steps and novel chemical methods is paramount to achieving an “ideal” synthesis. Thus, strategic advances and new synthesis logics for the rapid construction of molecular complexity are vital to organic chemistry and the disciplines that depend upon it. We focus on the development of novel succinct strategies and new chemical transformations to enable reliable access to meaningful quantities of complex natural products and their unnatural analogues with potentials for the treatment of cancer, neurological disorders, and infectious diseases. The terpenes and alkaloids we target are promising lead compounds for the development of new medicines, but their unknown or unclear mechanism of actions and the lack of a dependable way to access them has severely hindered their therapeutical development. We aim to solve this issue while also expanding and innovating the toolbox available to medicinal and synthetic chemists. In fact, our targets are not only important from a biological standpoint, but they also represent state-of-the-art challenges for complex molecule synthesis. Thus, these total synthesis efforts fuel the invention of new chemicals methods and serve as a proving ground for our new logics and existing transformations to solve critical synthesis problems in complex settings. To aid achieving these goals, we conceive novel and versatile synthesis logics that are amenable to the preparation of multiple members of a family of bioactive natural products as well as unnatural analogues.

SWRM 2026 SW256

Patterns within patterns: Shaping light and chemistry in space and time

***Alex R. Lippert**, alippert@smu.edu. Southern Methodist University, Dallas, Texas, United States*

Light and matter have an intimate pattern of relationships that manifest as color, form, and energy to animate life as we know it. As practical chemists, light can gift us with elegant control over chemical reactivity that is difficult to achieve using dark techniques. In our laboratory, we use digital light processing technology to precisely pattern light with control of color and intensity with a high degree of precision in space and time. Juxtaposing this luminous patterning technique with innovative chemistry and optical engineering has enabled inventive new 3D displays, microscopic 3D printing, liquid crystalline artwork, and other endeavors which we will discuss in this talk.

SWRM 2026 SW257

Bright NIR-II/SWIR emissive polymer-based nanoassemblies

***Joshua Tropp**, jtropp@ttu.edu. Chemistry and Biochemistry, Texas Tech University, Lubbock, Texas, United States*

The development of bright, scalable, and functionally adaptable near-infrared emissive materials is important for bioimaging, sensing, optical communication, and anticounterfeiting, particularly in the second near-infrared (NIR-II) and shortwave infrared (SWIR) regions. However, many organic NIR-II emitters are limited by low brightness, poor photostability, or synthetic complexity that hinders scalable preparation. Here, we investigate how nanoscale self-assembly transforms structurally simple polyisoindigo (PIG)-based donor–acceptor conjugated polymers into highly emissive NIR-II/SWIR functional materials. PIG copolymers incorporating structurally diverse donor units were synthesized and assembled by nanoprecipitation into surfactant-stabilized conjugated polymer nanoparticles (CPNs). The resulting nanoassemblies exhibit strong NIR/SWIR emission centered between 950 - 1200 nm with emission extending throughout the NIR-II/SWIR region. Assembly of the polymer chains into nanoscale particles produces dramatic increases in molar brightness relative to the molecularly dissolved polymer state, with enhancements exceeding 10^5-fold. The resulting particles exhibit brightness competitive with leading organic and inorganic NIR-II emitters while retaining a comparatively simple and scalable molecular design.
The nanoassemblies additionally exhibit strong photostability and colloidal stability in aqueous media, while maintaining high optical performance in strongly scattering environments. In tissue-mimicking phantoms, PIG nanoparticles retain higher signal and signal-to-background ratios than organic small-molecule standards with increasing imaging depth. Despite their high photostability, the conjugated polymer backbone undergoes oxidative degradation following exposure to hydrogen peroxide and UV irradiation, as evidenced by loss of visible/NIR absorption and substantial decreases in polymer molecular weight. This behavior suggests a reactive oxygen species-assisted backbone-scission pathway and provides an opportunity to design transient optical nanomaterials where long-term persistence is undesirable. Together, these results demonstrate how nanoscale organization of simple donor–acceptor conjugated polymers can generate emergent optical properties, transforming scalable molecular building blocks into bright, stable, and degradable NIR-II/SWIR functional nanoassemblies.

SWRM 2026 SW258

Low-energy excitation leading to symmetry-breaking charge separation in near-infrared-absorbing bisstyryltriphenylamine–BODIPY dimers

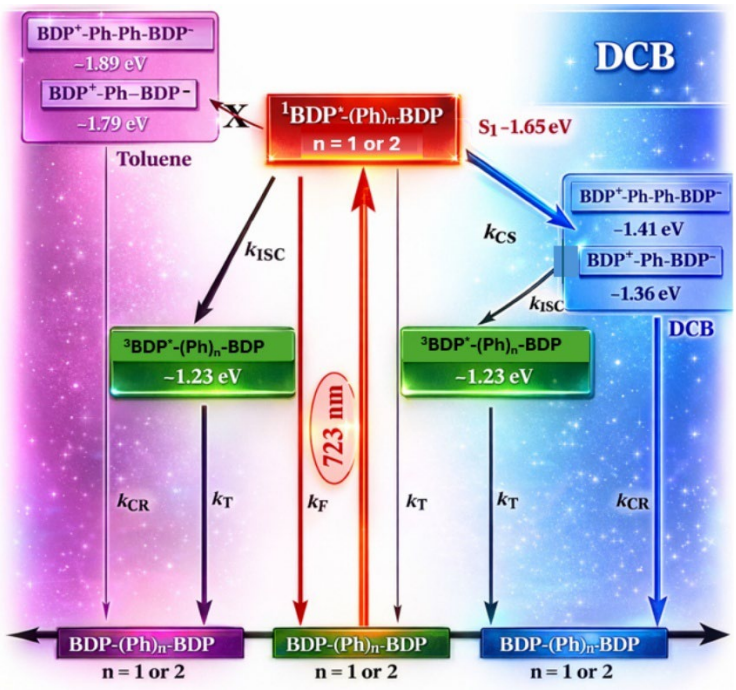
Swatej Sabbarwal*, swatejsabbarwal@my.unt.edu, Ram Ratan Kaswan, Austin Willard, Jorge Galwan, Aida Yahagh, Francis D'Souza. Chemistry, University of North Texas, Denton, Texas, United States*

BODIPY chromophores have attracted significant attention because of their diverse applications in optoelectronics. In particular, symmetry-breaking charge separation (SB-CS) in BODIPY systems has been widely investigated as a means of mimicking natural photosynthesis by generating radical ion pairs upon photoexcitation. However, most BODIPY derivatives reported for SB-CS absorb mainly in the visible region, whereas natural chlorophylls harvest light in the far-red and near-infrared (NIR) regions. This spectral limitation restricts efficient utilization of lower-energy photons for charge separation. Herein, we report a new class of NIR-absorbing bisstyryltriphenylamine-BODIPY dimers that undergo efficient symmetry-breaking charge separation following NIR excitation. Steady-state spectroscopic and femtosecond transient absorption studies reveal the ultrafast formation of the charge-separated (CS) state after photoexcitation. Electrochemical measurements indicate that this process is thermodynamically favorable, with the excited-state energy exceeding the redox potential required for charge separation. In addition, quantum chemical calculations support the presence of a low-lying charge-transfer state and strong electronic communication between the two BODIPY units, consistent with their nearly coplanar geometry. These findings demonstrate that these dimers are

promising platforms for symmetry-breaking charge separation and NIR light harvesting and provide useful guidelines for the design of next-generation molecular systems for efficient photoinduced energy and charge conversion.

References

1. Sabbarwal, S.; Kaswan, R. R.; Galvan, J.; Willard, A.; Yahagh, A.; D'souza, F. Low-Energy Excitation Leading to Symmetry-Breaking Charge Separation in Near-Infrared-Absorbing Bisstyryltriphenylamine–BODIPY Dimers. *J. Am. Chem. Soc.* **2026**.



SWRM 2026 SW259

Evolution of push-pull donor-acceptor systems for NIR-active optoelectronic applications

Sainyam Sikka[1]*, sainyamsikka@my.unt.edu, Rajneesh Misra*[2]*, Francis D'Souza*[1]*. (1) Chemistry, University of North Texas College of Science, Denton, Texas, United States(2) Chemistry, Indian Institute of Technology Indore Discipline of Chemistry, Indore, MP, India*

Push-pull π-conjugated donor-acceptor molecular systems have emerged as invaluable materials for optoelectronics, photovoltaics, and photonic energy-conversion applications. In our previous study, we synthesized and studied a new class of push-pull architectures based on bis(N,N-dimethylaminophenyl)–benzothiadiazole molecular systems, incorporating potent electron acceptors such as tetracyanobutadiene (TCBD) and dicyanoquinodimethane (DCNQ), to establish fundamental structure–activity–photodynamics relationships.[1] These systems demonstrate extended absorption into the visible and near-infrared (NIR) regions, enhanced ICT, and photoinduced charge-transfer and charge-separation processes. These findings provided the molecular-design basis for the present study, in which we further evolved the donor–acceptor framework to examine how donor identity, molecular symmetry, branching, and acceptor strength govern the electronic and excited-state properties of push–pull architectures.[2] Building upon the earlier acceptor-centered design, we developed a new series of triphenylamine-based D–A systems incorporating phenothiazine (PTZ) donor units and TCBD or DCNQ acceptors in both symmetrical and asymmetrical molecular configurations. These strong interactions lead to broad absorption extending into the near-infrared

(NIR) region, along with enhanced ICT character and lower optical band gaps. Density functional theory (DFT) and time-dependent DFT (TD-DFT) studies assessed the thermodynamic feasibility of ICT in these molecular systems by providing insights into frontier molecular orbitals, optimized geometries, and the spatial redistribution of excited-state electron density, indicating ICT. Femtosecond transient absorption spectroscopy, combined with global target analysis, was used to investigate excited-state dynamics, showing clear evidence of ultrafast excited-state charge transfer followed by charge separation along with associated timescales and relaxation pathways. This work further reveals that multibranched symmetrical systems provide better electronic delocalization and charge-transfer characteristics than asymmetric systems. Together, these techniques show strong correlations between molecular structure, electronic coupling, and excited-state charge-transfer dynamics, making them effective NIR-active push-pull materials for next-generation optoelectronic and photonic applications.

SWRM 2026 SW260

Supramolecular control of lanthanide coordination in multinuclear sandwich complexes for two-photon upconversion

Anne E. Gorden[1]*, anne.gorden@ttu.edu, Pooja Dogra*[1]*, Jessica Wallace*[2]*, Biswash Guragain*[1]*, John Gorden*[1]*, Jorge Monteiro*[3]*, Ana de Bettencourt-Dias*[2]*. (1) Chemistry and Biochemistry, Texas Tech University, Lubbock, Texas, United States(2) University of Nevada Reno, Reno, Nevada, United States(3) Cal Poly Humboldt, Arcata, California, United States*

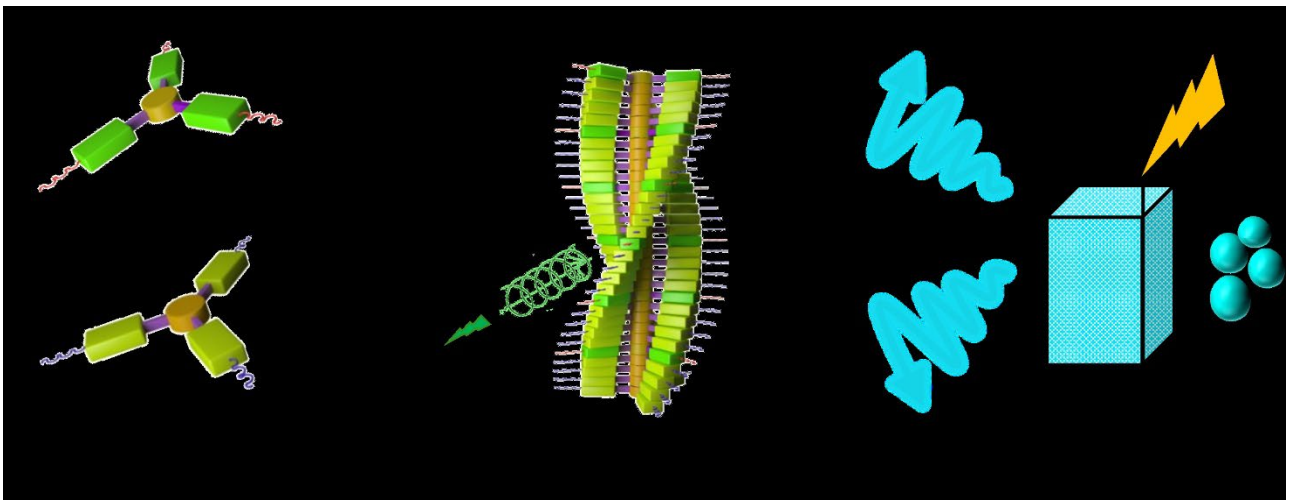
Lanthanide ions possess flexible coordination geometries and high coordination numbers, providing unique opportunities for constructing molecular and supramolecular architectures with tunable structures and properties. We are exploring how ligand design can control the coordination and self-assembly of lanthanide complexes, with an emphasis on Schiff-base frameworks that organize multiple lanthanide ions into well-defined structures. Here, we employ modular, conjugated ligands in which the donor set, electronic properties, and ligand backbone can be varied to direct supramolecular assembly. These ligands form dinuclear (Ln2L3) triple-decker sandwich architectures in which ligand stacking, coordination geometry, and short lanthanide–lanthanide distances are intimately coupled. Small changes to the ligand backbone, including incorporation of pyridyl or pyrazinyl donors, alter the metal coordination environments and interactions between stacked ligands, providing molecular handles for tuning the resulting supramolecular structures. Functionalization of the ligand periphery can further modify solubility while maintaining the underlying self-assembled architecture. These structural features can be leveraged to influence lanthanide-centered photophysical properties, including two-photon upconversion. Together, these studies establish ligand-centered design principles for controlling the structure, organization, and properties of multinuclear lanthanide assemblies.

SWRM 2026 SW261

Circularly polarized luminescent cyanostilbenes: Efficient design strategies to tune self-sorting and chiral amplification in self-assemblies

Bhawani Narayan*, bhawanin91@gmail.com. Chemistry, Huston-Tillotson University, Austin, Texas, United States*

Circularly Polarized Luminescence (CPL), the differential spontaneous emission of left/right circularly polarized light by chiral luminescent species, is an important tool to elucidate the excited state conformation of chiral emissive species. Circularly Polarized Luminescence (CPL) is rare in solution state self-assembled organic π-conjugated chromophores due to the inherently low g_{lum} and concentration quenching effects. However, cyanostilbene chromophores are emissive in self-assembled solutions by virtue of 'Aggregation Induced Enhanced Emission (AIEE)'. In this work, we would present two efficient design strategies by which self-assembled CPL emissive cyanostilbenes can be either tuned to result in amplification of CPL or undergo homochiral polymerization in solution-state self-sorted stacks. In the first strategy, we utilized the C_3-symmetric 1,3,5 benzene tricaboxamide (BTA) core. With the aid of synergistic hydrogen bonding interactions from the BTA core and pi-pi interactions of the cyanostilbene chromophore units, we could achieve cooperatively self-assembled supramolecular stacks. By co-assembling achiral molecules with a minor percentage of chiral molecules, we were able to obtain CPL active assemblies with g_{lum} same as the homochiral assemblies. In the second strategy, we have realized the concept of chirality driven self-sorting. We have utilized 1,2 *trans*-cyclohexanediamide cores and tethered cyanostilbenes as the functional chromophores. Narcissistically self-sorted, CPL active, supramolecular assemblies were obtained in solution.



SWRM 2026 SW262

Aromatic heterocycle-fused porphyrins: Synthesis and impact on photophysical properties

***Hong Wang**, hong.wang@unt.edu. University of North Texas, Denton, Texas, United States*

Incorporation of heteroatom(s) into largely *π*-extended structures can provide a handle to control the electronic structure, and has become an effective and important strategy to manipulate the materials to possess desirable properties, such as electrochemical activity, optical absorption spectra, photoluminescence, redox behaviour, charge transfer, bandgap tuning, and other characteristics. Understanding how the incorporated heteroatom/heterocycles affect the conjugated systems is of paramount importance to guide new materials design. In this presentation, new synthetic methods to fuse different type of aromatic heterocycles to the porphyrin periphery will be presented. These new methods have led to the synthesis of novel *π*-extended molecular structures incorporating both porphyrins and other aromatic components including benzoimidazo-isoindoles, naphthodithiophene and azepine. Unprecedented electronic and photophysical properties have discovered for these *π*-extended porphyrins. For example, an unusual trend was observed in the florescence quantum yield upon converting thiophene-attached benzoporphyrin to naphthodithiophene-fused porphyrin.

Azepine-fused porphyrin displayed unusually short fluorescence lifetime (0.7 ns), noting that the fluorescence and phosphorescence lifetime for conventional free base porphyrins is 9-10 ns. Porphyrin oligomers including dimers and trimers based on benzoimidazo-isoindole-fused porphyrins have also been prepared. While ZnD1-C_{60} exhibited long-lived CS state (~30-40 microseconds), ZnFBD1 system displayed efficient singlet-singlet energy transfer (>95% efficiency). Different scenario occurred in the trimer system. Zn-Trimer-1 showed strong exciton coupling and titration of Zn-rimer-1 with C_{60} suggested cooperativity of the three porphyrin components, which is in sharp contrast to that was observed with ZnD1-C_{60} system. These results showcase the significant impact of heteroatom/heterocycles and the importance of the conjugated *π*-spacer in governing the energy and electron transfer events. The characterizations of these pi-extended porphyrins including time-resolved emission and transient absorption spectroscopy, cyclic voltammetry, DFT calculations will also be presented.

SWRM 2026 SW263

Structural modulation of metalloporphyrins for electrocatalytic conversion of nitrate and carbon dioxide pollutants into value-added products

***Alankar Kafle**, alankar.kafle@unt.edu, Kamal Dhakal, Swatej Sabbarwal, Thomas R. Cundari, Francis D'Souza. Chemistry, University of North Texas College of Science, Denton, Texas, United States*

With rapid modernization and a growing human population, the atmospheric concentrations of CO_2 and NO_3^- continue to rise due to rising fossil fuel consumption, expanding industrialization, and agricultural activities, leading to serious environmental issues. Nitrogen-containing metalloenzymes serve as nature's catalytic machinery for driving carbon and nitrogen cycles, supporting ecosystem productivity and maintaining environmental sustainability. Carbon monoxide dehydrogenase (CODH) and formate dehydrogenase (FDH) facilitate natural CO_2 fixation, while nitrogenase and related metalloenzymes drive the biological conversion of dinitrogen. Although natural biological processes can fix and remove these pollutants, the increase due to anthropogenic activity far exceeds their capacity; therefore, there is an urgent need for a sustainable approach to manage these pollutants. In this context, electrocatalytic conversion of these pollutants into value-added products can be pursued as a viable strategy. In the search for efficient electrocatalysts, synthetic molecules containing active sites similar to metalloenzymes may offer analogous reactions and can be explored as highly efficient electrocatalysts. Among these, metalloporphyrins present a well-defined active site resembling metalloenzymes, enabling efficient electrocatalytic conversion of CO_2 and nitrate. Understanding structure-activity relationships is essential for developing highly efficient electrocatalysts; therefore, electrocatalytic activity must be investigated by modulating the metal centers and ligand substituents. In this contribution, we will discuss the systematic evaluation of electropolymerization, compositing with graphitic materials, and tuning peripheral functional groups as successful strategies for the development of improved NO_3RR and CO_2RR electrocatalysts.

SWRM 2026 SW264

Symmetry breaking charge separation in zinc phthalocyanine dimers self-assembled via hydrogen bonding

***Ram Ratan Kaswan**, ramkaswan@my.unt.edu, Francis D'Souza. Chemistry, University of North Texas, Denton, Texas, United States*

Photoinduced symmetry-breaking charge separation (SBCS) in a symmetrical pair of dimers is known to maximize energy conversion during the light-to-chemical energy conversion process. Although this has been shown in a few covalently linked dimers, the demonstration of such an event in self-assembled chromophore dimers has been very rare, especially dimers formed by hydrogen-bonding interactions. Here, we present a classic example of hydrogen-bonding-paired self-assembled zinc phthalocyanine dimers ((ZnPc-COOH)$_2$ and (ZnPc-Ph-COOH)$_2$) of different chromophore distances and demonstrate SB-CS resulting in ZnPc$^{\cdot+}$-ZnPc$^{\cdot-}$ electron transfer products upon far-red light illumination. The occurrence of SB-CS in the ZnPc dimers was confirmed by multiple studies, including fluorescence emission, which showed significant quenching in the dimer. Estimation of energy stored in the charge-separated states from electrochemical studies (redox gap ~1.55 eV) revealed the energy to be close to the pumping energy ($E_{0,0}$ ~ 1.80 eV), thus minimizing the energy loss during light-to-energy conversion. While DFT studies were able to assess geometry and carboxylic acid pairing strength, the TD-DFT studies were able to point out the excited states responsible for promoting excited-state electron transfer within the ZnPc dimers. Finally, femtosecond pump-probe studies provided definitive evidence of SB-CS, with electron transfer rate constants of 5×10^{11} and 0.7×10^{11} s^{-1}, respectively, for (ZnPc-COOH)$_2$ and (ZnPc-Ph-COOH)$_2$, revealing the significance of H-bond pairing in promoting efficient charge separation in the far-red-capturing ZnPc dimers.

SWRM 2026 SW265

Functional rotaxanes in lipid membranes: From photoswitchable membrane modulation to ion transport, neuromorphic behavior, and antibacterial activity

*Udyogi N. Conthagamage[1], Victor Garcia-Lopez[4], Stijn van der Ham[2], Hanumantha R. Vutukuri[2], **Jeremy Smith**[3,5], smithjc@ornl.gov, John Katsaras[5], Charles P. Collier[5], Peter Podar[6,5], Mario E. Rivera[1], Huili Yao[1]. (1) Louisiana State University, Baton Rouge, Louisiana, United States(2) Universiteit Twente Faculteit Technische Natuurwetenschappen, Enschede, Netherlands(3) Biochemistry & Cellular and Molecular Biology, The University of Tennessee Knoxville College of Arts and Sciences, Knoxville, Tennessee, United States(4) Chemistry, Louisiana State University, Baton Rouge, Louisiana, United States(5) Oak Ridge National Laboratory, Oak Ridge, Tennessee, United States(6) The University of Tennessee Knoxville Tickle College of Engineering, Knoxville, Tennessee, United States*

Lipid membranes are vital structural components in biology, safeguarding cells and organelles, regulating substance exchange, controlling integral membrane protein activity, and supporting cellular functions. Developing chemical tools to modulate membrane structure and dynamics offers innovative ways to regulate these properties and associated protein functions.
Rotaxanes are a promising platform for this purpose, as they can precisely position actuators at various membrane depths to modulate membranes. They consist of a macrocycle that randomly shuttles along an axle. When embedded in a membrane, the axle serves as a membrane spanning track, allowing precise macrocycle movement. Decorating the macrocycle with photoswitches enables easy, light-induced, site-specific membrane modulation.
Our work shows the synthesis of a novel rotaxane featuring a macrocycle with appended azobenzene photoswitches, together with its efficient photoswitching behavior in solution and in model lipid bilayers with different fluidities. Photoswitching between the *E* and *Z* isomers of the rotaxane regulates membrane permeability, allowing for controlled release of hydrophilic cargo. This regulation

arises from photoisomerization-induced repositioning of the macrocycle within the membrane in each isomeric state. This light-regulated membrane permeability enables reversible switching of the electrical properties of the rotaxane-embedded membrane. Photoisomerization switches the membrane between a memristive state, with voltage-dependent ion transport due to increased permeability, and a memcapacitive state characterized by charge buildup across the bilayer. Overall, this work introduces a new approach to emulate the history-dependent electrical behavior of neural synapses, indicating that photoswitchable rotaxanes in membranes could be valuable for bioinspired neuromorphic devices. Our research demonstrates that this rotaxane also serves as an effective antibacterial agent against *Acinetobacter baumannii*, a highly virulent and multidrug-resistant pathogen. Structure–activity analysis shows that the azobenzene-functionalized macrocycle and the positive charge distribution in the axle influence antibacterial activity. The findings also indicate a membrane-active mechanism, although further studies are needed to fully understand the antibacterial action.

SWRM 2026 SW266

Tellurium-based strategies for ion transport across biological membrane mimics

***You Jiang**, you_jiang@tamu.edu, Benyu Zhou, Francois P. Gabbai. Chemistry, Texas A&M University, College Station, Texas, United States*

Over the past two decades, we have developed a range of cationic main-group Lewis acids for the recognition and sensing of anions in aqueous media. Our investigations of boron-based systems incorporating pendant sulfonium and telluronium groups revealed that group 16 elements can interact favorably with anionic guests through σ-hole interactions. In this presentation, we will highlight recent advances from this research program, with particular emphasis on the application of tellurium-containing compounds as ion transporters across phospholipid bilayers. We will demonstrate that telluronium cations engage anions through chalcogen-bonding interactions, giving rise to distinct anion transport behaviors that have been characterized using phospholipid-based vesicle assays. Furthermore, we will show that the redox properties of tellurium can be exploited to develop stimuli-responsive transporters that are activated by biologically relevant redox agents, including glutathione. Finally, extending beyond anion transport, we will describe how redox-controlled and redox-switchable intramolecular N–Te chalcogen bonding can be harnessed to achieve stimuli-responsive transport of biologically relevant divalent metal ions.

SWRM 2026 SW267

Highly selective ionophore-based bilayer emulsion membranes

***Ronald J. Vogler**[1], rjv684@utexas.edu, Aída Fica[2], Angela Pierce[4], Katherine Kimball[1], Samuel West[1], Sneha Sinha[3], Claire Baldus[2], Manish Kumar[1,2]. (1) John J. McKetta Jr. Department of Chemical Engineering, The University of Texas at Austin, Austin, Texas, United States(2) Fariborz Maseeh Department of Civil, Architectural and Environmental Engineering, The University of Texas at Austin, Austin, Texas, United States(3) Department of Biomedical Engineering, The University of Texas at Austin, Austin, Texas, United States(4) Department of Molecular Biosciences, The University of Texas at Austin, Austin, Texas, United States*

Biological channels (e.g., membrane proteins) have shown potential for use as membrane materials for ion-separations due to the high throughput and ion-ion selectivity of these channels in biological systems. For example, our group has recently developed an emulsion-based membrane material comprised of a network of water droplets encased in oil; the water droplets are joined together by amphiphilic bilayers containing biological channels that determine the transport behavior and ion-selectivity of the membrane. In this work, we build on this droplet-network platform for ion-ion separations by investigating the use of commercially-available ionophores as alternatives to biological channels and developing a crosslinked, thin-film droplet network with enhanced mechanical stability. Unlike biological channels that form a continuous pathway for ion transport through the amphiphilic bilayer, ionophores partition into the bilayer and carry ions across the bilayer via facilitated transport. Various ionophores were studied to demonstrate the tunability of ionophore-based droplet networks towards different separations. For example, droplet networks containing valinomycin, a potassium selective ionophore had a K^+/Na^+ selectivity of 137; droplet networks containing nonactin, an ammonium-selective ionophore, had an NH_4^+/Na^+ selectivity of 124; and droplet networks containing lithium ionophore VIII had an Li^+/Na^+ selectivity of 167.
A crosslinked droplet network with enhanced mechanical stability was developed by incorporating monomers into the aqueous and oil phases of this material and photopolymerizing these monomers to form network polymers in each phase. Microscopy and non-steady-state ion-current measurements verified that the network of water droplets and the amphiphilic bilayers were preserved after crosslinking. Rheological measurements indicated that the storage and loss moduli of the crosslinked droplet network were much higher than typical values for non-crosslinked droplet networks. Furthermore, crosslinked droplet networks containing nonactin exhibited an NH_4^+/Na^+ selectivity of 54, demonstrating the potential of these crosslinked membranes for ion-ion separations.
Overall, this work demonstrates the creation of biomimetic membranes from ionophores for highly-selective ion-ion separations.

SWRM 2026 SW268

Predicting and controlling which mefenamic acid crystal forms appear in organic crystallization: Crystal growth and design

Zainab Khokhar[1,2]*, zainabbkhokharr@gmail.com. (1) Klein Independent School District, Klein, Texas, United States(2) William A. Brookshire Department of Chemical and Biomolecular Engineering, University of Houston Cullen College of Engineering, Houston, Texas, United States*

In this project, we studied a property of crystals called polymorphism using mefenamic acid in different organic solvents. Mefenamic acid is a NSAID used to treat mild pain and has three polymorphic structures: forms I, II, and III. These structures vary in stability, form I being the most thermodynamically stable and form III being the least. Mefenamic acid is an anthranilic acid derivative which places it in the fenamate chemical class, a common category of NSAIDs. Mefenamic acid is flexible, and its ablity to change conformation is caused by the rotation of a dimethyl-phenyl group around the Car-N bond. Since mefenamic acid has a low solubility in water, its use in clinical practice and bioavailability is limited since it is manufactured in a solid state. Our research searches for possible polymorphs of potential drugs (mefenamic acid), the determination of relative stability, and the definition of strategies to control polymorph transformations.

SWRM 2026 SW269

Theoretical determination of substituent effects for chromium complexed arenes

Daniyal Khan[1]*, k.daniyal@outlook.com, Tennyson Broadhurst*[2]*, Bruce Hietbrink*[3]*. (1) Keller Central High School, Fort Worth, Texas, United States(2) Academic Magnet High School, North Charleston, South Carolina, United States(3) Chemistry & Biochemistry, University of Delaware, Newark, Delaware, United States*

Previous studies have shown that substituent electronic effects can influence the stability of cationic and anionic intermediates, with electron-donating and electron-withdrawing groups producing different effects depending on their position within an aromatic system. Prior research has also demonstrated that chromium tricarbonyl coordination can stabilize both benzylic cations and anions. Building on these findings, this study investigates how six para-substituents, H, CHO, CH_3, NO_2, NH_2, and OCH_3, influence the stability of intermediates along an S_N1 substitution pathway and how chromium tricarbonyl coordination alters these effects. Substituted benzyl chloride and arene systems were compared with and without chromium tricarbonyl coordination. A total of 48 molecular structures were investigated in the gas phase, including 24 structures containing the chromium complex and 24 corresponding structures without chromium, with six substituents examined at each stage of the reaction pathway. Molecular structures were modeled using Avogadro, while density functional theory (DFT) geometry optimizations and energy calculations were performed using ORCA at the B3LYP/def2-SVP level of theory. Calculated energies were compared across substituents, reaction stages, and chromium coordination to identify trends in cation stabilization. This work provides insight into how aromatic substituents and transition-metal coordination influence the energetic properties of reactive intermediates in S_N1 chemistry.

SWRM 2026 SW270 - Withdrawn

SWRM 2026 SW271

Influence of sonication media on the particle size of Ti_3CNT_x MXene

Hasan F. Zubaer[3]*, faiaz.zubaer@gmail.com, Hariharan D*[2]*, Abdoulaye Djire*[1]*. (1) Texas A&M University Artie Mcferrin Department Of Chemical Engineering, College Station, Texas, United States(2) Indian Institute of Technology Gandhinagar Department of Chemical Engineering, Gandhinagar, GJ, India(3) College Station High School, College Station, Texas, United States*

MXenes have attracted significant interest for electrochemical energy applications because of their high electrical conductivity, two-dimensional layered structure, and tunable surface chemistry. During processing, ultrasonication can generate acoustic cavitation and shear forces capable of reducing MXene particle size; however, the influence of the sonication medium on MXene fragmentation and dispersion remains insufficiently understood. This study investigates the effect of sonication medium on the particle size, suspension stability, and structural characteristics of Ti_3CNT_x MXene. Ti_3CNT_x was synthesized from Ti_3AlCN MAX phase and subsequently dispersed in deionized water, ethanol, isopropanol (IPA), and dimethyl sulfoxide (DMSO). Equal-mass suspensions were sonicated for two hours under identical conditions, followed by vacuum filtration, oven drying, and laser diffraction particle-size analysis. Suspension stability was evaluated through time-dependent settling observations, while X-ray diffraction (XRD) was used to assess structural changes following processing. Sonication medium substantially affected the measured particle size. Relative to the untreated control (D50 = 6.89 μm), water and ethanol produced lower median particle sizes of 4.37

μm and 3.80 μm, respectively, corresponding to reductions of approximately 37% and 45%. In contrast, IPA and DMSO produced larger apparent median particle sizes of 14.14 μm and 8.90 μm, respectively. Water also exhibited the greatest suspension stability, while IPA and DMSO settled rapidly, suggesting that differences in particle dispersion and aggregation may contribute to the observed particle-size distributions. XRD confirmed retention of the characteristic Ti_3CNT_x diffraction features without detectable additional phases following sonication, indicating preservation of the primary layered crystal structure. These results demonstrate that sonication medium is a critical processing parameter for controlling Ti_3CNT_x particle size and dispersion behavior and provide a basis for optimizing MXene processing for subsequent electrochemical applications.

SWRM 2026 SW272

Time-dependent breakdown of MNenes to facilitate a sustainable future

***Lauren Page**, laurenompage@gmail.com. A and M Consolidated High School, College Station, Texas, United States*

Ammonia (NH3) is foundational to global agriculture, sustaining a human population that has far exceeded the planet's natural carrying capacity. However, the traditional Haber-Bosch process is environmentally taxing, requiring extreme temperatures and pressures while emitting approximately two tons of CO2 for every ton of NH3 produced. As a sustainable alternative, the lattice nitrogen-mediated Nitrogen Reduction Reaction (NRR) enables ammonia synthesis at ambient conditions. This study identifies Nitride MXenes—specifically Ti2N, Ti3CN, and Ti4N3—as highly effective electrocatalysts for this pathway. To optimize performance, the catalysts underwent sonication for varying durations (30 min, 60 min, 120 min, etc). Particle size analysis revealed that sonication significantly reduced particle dimensions, thereby exposing a higher density of active edge sites and significantly enhancing electrocatalytic performance. Experimentally, sonicated catalysts achieved superior Faradaic efficiency (FE) and higher ammonia yields compared to pristine materials, establishing a precedent for the preeminence of sonicated material versus pristine material and demonstrating a more efficient and sustainable electrochemical route for green ammonia production.

SWRM 2026 SW273

Effect of sonication time on MXene particle size and agglomeration

***Saim Karim**, saimkarim778@gmail.com. College Station High School, College Station, Texas, United States*

MXenes are two-dimensional materials with promising applications in energy storage and electrocatalysis due to their high electrical conductivity and large surface area. This study investigated the effect of sonication time on MXene particle size by comparing samples sonicated for 5 minutes (control), 1 hour, 2 hours, and 4 hours. Particle size analysis was used to evaluate changes in average particle size and distribution following sonication. Results revealed a non-monotonic relationship between sonication time and particle size. The 5-minute control produced the smallest and narrowest particle size distribution, while the 2-hour and 4-hour samples shifted toward larger, more concentrated particle sizes, suggesting re-agglomeration or larger flake formation. The 1-hour sample showed the greatest shift toward larger particles, indicating substantial agglomeration rather than continued exfoliation. These findings suggest that shorter sonication times are more effective for

producing fine, well-dispersed MXene particles, while extended sonication may promote fragmentation and re-agglomeration. The results provide insight into optimizing MXene processing conditions for advanced energy and electrocatalytic applications.

SWRM 2026 SW274

Decoding biophysical fragility in MYC/MAX condensate networks in MYC-driven cancer states

***Alexander N. Nguyen**, alexplayz5347@gmail.com, **Yuvraj Rathore**, uv.rathore02@gmail.com, Iva Wagner, Gul Zerze. Chemical Biomolecular Engineering, University of Houston, Houston, Texas, United States*

MYC is a major oncogenic transcription factor that partners with MAX to regulate gene expression, yet the biophysical consequences of cancer-associated MYC/MAX imbalance within biomolecular condensates remain poorly understood. Here, coarse-grained molecular dynamics simulations were employed to determine how changes in MYC/MAX abundance influence condensed-phase organization, residue-level contact networks, and component-specific partitioning thermodynamics. Three multichain systems representing MYC-rich (200:50), balanced (200:200), and MAX-rich (200:400) conditions were simulated at 310 K. Across all conditions, a sharply localized protein-dense phase persisted, indicating that substantial shifts in MYC/MAX balance can alter condensate composition without disrupting phase separation. Increasing MAX abundance progressively enhanced its enrichment within the condensed phase and produced distinct reorganization of residue-level contact-frequency patterns. Concurrently, MYC and MAX partition coefficients increased while transfer free energies became more negative, reflecting increasingly favorable partitioning into the condensed state. Collectively, these findings reveal that MYC/MAX imbalance can reshape molecular organization and thermodynamic partitioning within persistent condensates, providing a quantitative biophysical framework for understanding how dysregulated MYC/MAX balance may alter transcription-associated protein organization in cancer.

SWRM 2026 SW275

Disentangling inner filter, dilution, and quenching effects on the native fluorescence of albumin

***Han Vo**, votranhanbao@gmail.com, Samuel Chirinos, Md Sohanur Rahman, David E. Thompson. Department of Chemistry, Sam Houston State University, Huntsville, Texas, United States*

Bovine serum albumin (BSA) is a naturally fluorescent protein because it contains aromatic amino acid residues, particularly tryptophan. The fluorescence of tryptophan is highly sensitive to interactions with nearby molecules, making fluorescence spectroscopy a useful technique for studying protein–ligand interactions. In this study, we investigate the effects of dimethyl trisulfide (DMTS) on the fluorescence properties of BSA to evaluate its interaction with albumin. A series of DMTS samples, prepared with and without ethanol, was mixed with BSA using varying amounts of DMTS. UV–Vis spectroscopy was used to characterize the absorbance spectra of DMTS, BSA, and DMTS-BSA mixtures prior to fluorescence analysis. Fluorescence spectroscopy was then performed by acquiring three-dimensional (3D) and two-dimensional (2D) spectra to identify the optimal excitation and emission wavelength ranges, followed by one-dimensional (1D) emission spectra to evaluate changes in BSA fluorescence. Both UV–Vis and Fluorescence spectroscopy showed

concentration-dependent changes in signal. To determine whether these concentration dependent experiments provide evidence for albumin binding of DMTS, three effects on the signal need to be disentangled: Albumin dilution, inner filter, and fluorescence quenching. Here we present data from control experiments showing how these are disentangled. Together, these findings provide a foundation for ongoing investigation of a possible interaction between DMTS and albumin that may alter the local environment of tryptophan residues.

SWRM 2026 SW276

Molecular glues: Computational modeling of a PROteolysis TArgeting Chimeras (PROTACs) targeting Aurora kinase A for diffuse large B-cell lymphoma

*Siddharth Suhas Nalamari[2,1], **Gaurav Sharma**[1], eigensciences@gmail.com. (1) Eigen Sciences, Apex, North Carolina, United States(2) Lone Star High School, Frisco, Texas, United States*

Diffuse Large B-Cell Lymphoma (DLBCL) is an aggressive cancer characterized by rapid cell proliferation and resistance to current therapies. Aurora kinase, a key regulator of mitosis, is often overexpressed in DLBCL and contributes to uncontrolled cell division. Instead of traditional inhibition, this study explores a targeted protein degradation strategy using Proteolysis-Targeting Chimeras (PROTACs) to eliminate aurora kinase and potentially reduce treatment-related side effects. PROTACs are bifunctional molecules that recruit a target protein to an E3 ubiquitin ligase, enabling ubiquitination and proteasomal degradation. The FASTA sequence of aurora kinase was obtained from UniProt, and AlphaFold v3 was used to predict 3D structures of aurora kinase and CRBN. Binding sites of the aurora kinase were identified using P2Rank and PrankWeb. The PROTAC structure was generated from a SMILES string using the Open Babel web server, and molecular docking was performed with HDOCK 2.0 to model binary and ternary complexes. Binding affinities were calculated using PRODIGY2025, and interactions were visualized with PLIP2025 software. The chemical variants of the PROTAC were obtained using the CREM web server. Results demonstrated favorable binding energies and stable ternary complex formation with the PROTAC P1, which showed the highest number of hydrogen bonds and hydrophobic interactions. In future studies, I will investigate methods to increase the solubility and bioavailability of the selected PROTAC molecule. These results can help in developing novel treatment methods using PROTAC-mediated aurora kinase degradation as a promising therapeutic strategy for DLBCL.

SWRM 2026 SW277

Shuriken: Computational design of a multispecific hexabody targeting surface glycoproteins of six pathogenic viruses

***Rithvik Kamesh**[2,1], mail.rithvikk@gmail.com, Gaurav Sharma[1]. (1) Eigen Sciences, Apex, North Carolina, United States(2) Liberty High School, Frisco, Texas, United States*

Emerging and re-emerging viral diseases highlight the need for therapeutic platforms capable of targeting multiple pathogens. This study computationally designed and evaluated a multispecific hexabody containing nanobody-derived binding domains against the surface glycoproteins of SARS-CoV-2, influenza, Ebola, HIV-1, measles, and chikungunya viruses. Viral glycoprotein sequences and nanobody structures were obtained from UniProt and the Protein Data Bank, respectively. Protein structures and antibody complexes were modeled using AlphaFold, while nanobody–glycoprotein

interactions were assessed through HDOCK molecular docking. Binding free energies were estimated using PRODIGY, and potential linear B-cell epitopes were evaluated using BepiPred. The strongest predicted binders were 8RW9 for influenza (−17.3 kcal/mol), 5M7Q for Ebola (−14.1 kcal/mol), 8SFS for HIV-1 (−13.4 kcal/mol), 5DA0 for SARS-CoV-2 (−14.5 kcal/mol), 5M7Q for measles (−16.5 kcal/mol), and 5M7Q for chikungunya (−9.0 kcal/mol). Multiple hexabody configurations were subsequently modeled and compared using predicted template modeling (pTM) and interface predicted template modeling (ipTM) scores. Among the evaluated designs, the Original-12 configuration achieved the highest structural-confidence scores, with a pTM of 0.55 and an ipTM of 0.53. These findings demonstrate a computational framework for selecting viral glycoprotein-binding nanobodies and incorporating them into a multispecific antibody platform. However, further structural optimization, molecular-dynamics simulations, and experimental validation are required to confirm stability, binding specificity, neutralization capacity, and therapeutic safety.

SWRM 2026 SW278

Evaluating the efficacy of aggregation propensity as a predictor of oligopeptide dimerization in redox-active conditions

***Pranav Kolli**, pranavsaikolli@gmail.com. Molecular Biology and Biochemistry, University of California Irvine, Irvine, California, United States*

Peptide sequence determines its structure, function, ability to exhibit self-assembly behavior, and stimuli responsiveness. Different cysteine-containing amino acid sequences were synthesized and characterized to experimentally validate a computer model predicting peptide aggregation propensity. Oligopeptide aggregation occurs when the cysteine group in the peptide oxidizes to form a thiol-disulfide bond with another cysteine, forming a dimer. Those outputs yielded peptide sequences that are likely to aggregate based on the probability of the formation of thiol-disulfied bonds and dimerization. The oligopeptides' structure and redox activity will be tested using a variety of light spectroscopy and microscopy techniques that show peptide structure, aggregation, and morphology. The goal of the study is to identify if oligopeptide sequences that exhibit high aggregation propensity will experimentally demonstrate redox-active aggregation. Experimental validation of aggregation propensity to predict oligopeptide dimerization will contribute to identifying the most precise metrics to predict oligopeptide dimerization in redox-active conditions. Oligopeptides were synthesized via solid state peptide synthesis and undertook cleavage, precipitation,and purification. MALDI mass spectrometry and UPLC determined oligopeptide purification accuracy by distinguishing mass and distribution which can be compared to the expected protein mass. Dissipative self-assembling peptides (DSAPs) require constant chemical fuel, also producing waste products which can interfere with chemical reactions. The synthesis of self-assembling oligopeptides that demonstrate self-assembly properties provide a more energy-efficient alternative compared to DSAPs. The testing of the aggregation propensity of oligopeptide dimerization in redox-active conditions will create more precise prediction methods, leading to the development of biomaterials and nanotechnologies for improved drug release precision.

SWRM 2026 SW279

Studying the effect of calcium on the growth, viability, and inflammation induced by H2O2 of *Lactiplantibacillus plantarum* using *in-vitro* assay and minibioreactor

***Aliyah Odunowo**, odunowoaaliyah@gmail.com. Fulshear High School, Fulshear, Texas, United States*

The goal of my research was to experiment and study how the addition of calcium to *L. plantarum* ATCC 14917 would affect their growth, morphology, and viability. I also studied how that addition could help overcome the inflammation caused by reactive oxidizing species (ROS) when cultured with certain concentrations of Hydrogen Peroxide (H2O2).
I investigated the bacteria grown in rich media (MRS Broth) and metal-limited chemically defined media (CDM) with varied Ca2+(0, 10, and 25 mM) and H2O2 (0, 1, 5 mM) concentrations. I used in-vitro assays to assess their growth, viability, and morphology under oxidative stress. This process was then repeated using a minibioreactor, to simulate the flowrate in a small intestine, and to get insight into the morphology and viability of *L. plantarum* in the intestine.

SWRM 2026 SW280

Effect of chiral nanoparticles in biomolecule polymorphism

***jacqueline lam**[2], lambjacqueline28@gmail.com, Suman Pal[1]. (1) Chemistry, University of Houston System, Houston, Texas, United States(2) Dulles High School, Sugar Land, Texas, United States*

Nanomaterials have seen a large increase in industrial usage in the past few decades. Surface-functionalized nanomaterials have recently been shown to be a versatile platform to control molecular recognition, crystal growth, and biomolecular self-assembly. Regulation of the polymorphism of biomolecules is highly desirable since each polymorph differs in its structure, physicochemical and biological properties, affecting molecular stability, solubility, biological activity, disease progression, pharmaceutics, and biomaterials design. In this work, gold nanoparticles (Au NPs) modified by chiral amino acids D- and L-arginine were used to study the effect of surface chirality and chemical environment on the nanoparticle-biomolecule interactions and biomolecular crystallization. Nanoparticle interactions with glycine, glutamic acid, and oxalic acid were investigated at various pH values. Hydrodynamic size and colloidal stability of gold nanoparticles were measured using dynamic light scattering and zeta potential analysis. Crystal nucleation, growth and morphological properties were studied using optical microscopy and powder X-ray diffraction (PXRD). We found that the chiral surface modification and solution pH significantly affect nanoparticle aggregation and interfacial interactions, leading to significant changes in crystal growth and polymorphism. These results suggest the critical role of the nanoparticle surface chemistry in the regulation of biomolecular crystallization and polymorphism.

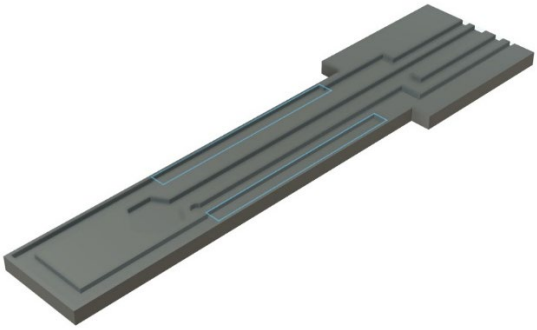
SWRM 2026 SW281

3D printing of chemical resistant electrochemical cells for nonaqueous spectroelectrochemistry

***Jose Garcia**, jetbemi@gmail.com, Naihao Chiang. Chemistry, University of Houston System, Houston, Texas, United States*

Spectroelectrochemistry (SEC) is a powerful analytical technique that combines the world of spectroscopy and electrochemistry. The use of electrochemical cells is a vital part for

spectroelectrochemistry because it allows for the oxidation or reduction reactions to occur. It also helps the spectroscopic methods to catch more reliable data to allow for studies regarding the electrochemical reaction using light. The use of 3D printing allowed for experimentation with new models and it allowed for testing to be conducted in the lab. A use of 3D printing in science is the production of reaction vessels since researchers have used 3D printing to create specialized reaction vessels for chemical experiments. This allows for the design of unique models that can facilitate complex chemical processes. The experimentation of spectroelectrochemistry allows for the discovery of how light interacts with matter on an oxidation and reduction reaction. The electrochemical cells allow for this change to occur and it allows for the chemicals to stay in their places. Also, the use of chemical resistant resin permits the creation of models that can withhold against the properties of certain chemicals. It would make them more malleable to work with and easier to replicate.





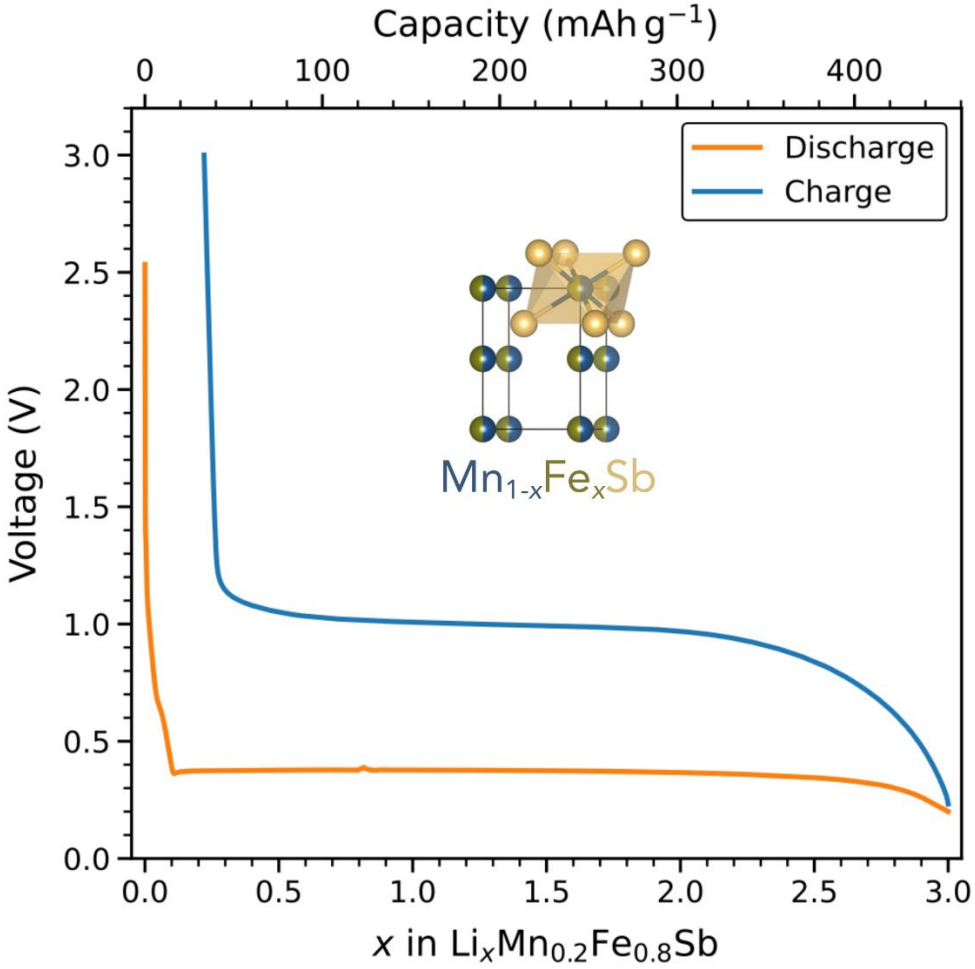
SWRM 2026 SW282

$Mn_{1-x}Fe_xSb$ as a conversion anode material for lithium-ion batteries

Aran Pirouzan[1]*, pirouzana@gmail.com, Jason J. Zhou*[2]*, Joshua Bocarsly*[2]*. (1) Obra D Tompkins High School, Katy, Texas, United States(2) Department of Chemistry, University of Houston College of Natural Sciences and Mathematics, Houston, Texas, United States*

Electrochemical energy storage has become essential for many applications, including EVs and portable electronics, leading to the widespread use of lithium-ion batteries (LIBs) because of their high energy density. Most commercial LIBs use layered electrode materials, motivating the investigation of conversion-type electrode materials with higher theoretical capacities. This study analyzes the structure and electrochemical behavior of $Mn_{1-x}Fe_xSb$ compositions as a model conversion-type electrode system. Although conversion-type electrodes offer a high theoretical capacity, their electrochemical performance is influenced by phase-transition behavior during cycling, contributing to poor cyclability. The goal of this study was to determine how $Mn_{1-x}Fe_xSb$ solid-solution composition influences phase-transition behavior and electrochemical performance by integrating MnSb and FeSb. Four $Mn_{1-x}Fe_xSb$ compositions were synthesized, characterized using X-ray diffraction (XRD), and prepared for electrochemical evaluation. XRD analysis revealed differences in the characteristics, with lower Mn content exhibiting cleaner diffraction patterns. Electrochemical evaluation of the $Mn_{1-x}Fe_xSb$ series investigated the relationship between composition, phase-transition behavior, and first-cycle reversibility. Increasing Mn content generally produced more complex phase-transition behavior and improved first-cycle reversibility. MnSb exhibited more complex phase-transition behavior with higher first-cycle reversibility, while FeSb exhibited more straightforward phase-transition behavior with lower first-cycle reversibility. Preliminary findings provide insight into how composition influences the characteristics and electrochemical behavior of

the $Mn_{1-x}Fe_xSb$ solid solution. Further investigation will clarify relationships among composition, phase-transition behavior, and electrochemical performance in conversion-type electrodes.



First-cycle voltage profile of $Mn_{0.2}Fe_{0.8}Sb$ vs. Li/Li^+

SWRM 2026 SW283 - Withdrawn

SWRM 2026 SW284

Synthesis of layered oxide cathodes materials for lithium-ion batteries

Shwetha Jayakumar[1]*, shwjay2020@gmail.com, Patcheammalle Kesavan*[2]*. (1) Young Women's Leadership Academy, Midland, Texas, United States(2) Chemistry, Midland College, Midland, Texas, United States*

Lithium-ion batteries are significant to technological development of the future due to their fast-charging capabilities, high voltage, and compact design. Layered oxide cathodes are a critical component because they are able to provide the high energy density, efficient space usage, and steady lithium ion movement. The cathode materials are synthesized using transition metal oxides initially. Then, lithium is combined with the precursor compounds to produce layered metal oxides. The layered oxide cathode materials for lithium ion batteries were synthesized using a sintering

method. The precursors used were lithium nitrate (LiNO3), manganese acetate tetrahydrate (Mn (CH3COO)2 . 4H2O), nickel acetate (Ni(CH3COO)2 . 4H2O), and cobalt nitrate (Co(NO3)2 . 6H2O) which are the most commonly used materials that produce layered oxide cathodes in lithium-ion batteries. Various compositions of cathode materials using Li(1+x) (MnNiCo)(1-x)O2 were made with x = 0.1 resulting in the total moles of lithium set equal to 1.1. Manganese, nickel, and cobalt were all set to 1-x making the total amount of moles of the three elements equal to 0.9. LMNC1 is synthesized using manganese, nickel, and cobalt with the addition of lithium using the composition of cathode materials Li(1+x) (MnNiCo)(1-x)O2 resulting in manganese rich composition having 0.45 moles, nickel composition having 0.225 moles, and cobalt composition having 0.225 moles. After weighing all the precursor compounds, it was ground in the mortar and pestle and transferred to a ceramic crucible. Then, it was sintered in the Lindbergh BLue programmable furnace set to ramp up to 900 oC and stay at that temperature for 9 hours. It was then cooled down to room temperature. The sintered materials are then ground to a powder, weighed and stored in a vial. LMNC2 is synthesized similarly to LMNC1 with a manganese - 0.55 moles, nickel - 0.175 moles, and cobalt - 0.175 moles. LMNC3 is synthesized using manganese - 0.65 moles, nickel - 0.125 moles, and cobalt - 0.125 moles. This composition underwent the same process of synthesis as LMNC1.
The characterization of these cathode materials will be done using X-Ray Diffraction (XRD) and Scanning Electron Microscopy (SEM). The resulting materials will be tested on their charge and discharge characteristics while sealed within a lithium ion coin battery cell.

SWRM 2026 SW285

Synthesis and characterization of polymer-coated iron oxide nanoparticles as potential templates for guiding organic compound crystallization

***Hy Kim**, kimjhy14@gmail.com. Cypress Ranch High School, Cypress, Texas, United States*

Crystal polymorphism is an important concept, particularly in the pharmaceutical industry, because different polymorphs can exhibit different physicochemical properties that may affect drug performance. This research investigates the potential of polymer-coated iron oxide nanoparticles (NPs) as templates for guiding crystal growth and polymorph formation. Polycrystalline magnetite (Fe_3O_4) NPs were synthesized and subsequently coated with a 3-aminophenol–formaldehyde (APF) polymer shell to form Fe_3O_4@APF core–shell structures. Several techniques, including X-Ray diffraction (XRD), Fourier-transform infrared spectroscopy (FTIR), scanning electron microscopy (SEM), transmission electron microscopy (TEM), and energy-dispersive X-ray spectroscopy (EDS) mapping, indicated the successful synthesis of Fe_3O_4 and Fe_3O_4@APF NPs. After characterization, both types of as-synthesized NPs were evaluated in glycine crystallization experiments. Preliminary results showed that the control experiments, conducted in the absence of templates and in the presence of uncoated Fe_3O_4 NPs, predominantly yielded α-glycine. Interestingly, in the presence of Fe_3O_4@APF NPs, a mixture of α- and γ-glycine polymorphs was obtained. These preliminary observations may provide insight into NP-assisted approaches for guiding crystal polymorph formation and improving control over the formation of targeted crystal forms for pharmaceutical applications.

SWRM 2026 SW286

ICP-MS determination of selected trace metals in commercial instant noodles using hot plate and microwave-assisted acid digestion

***Victor Tran**, victor.tran@tsu.edu, **Shawnise Gregory**, s.gregory2918@student.tsu.edu, Erica Preeth, Jazlynn Vallair, Kevin Anthony, Sonya C. Caston, **Tuan Phan**, tuan.phan@tsu.edu. Texas Southern University College of Science Engineering and Technology, Houston, Texas, United States*

Instant noodles are widely consumed because of their affordability, convenience, and extended shelf life; however, trace metal contamination may occur through raw ingredients, environmental exposure, food processing, or packaging materials. This study evaluated selected trace metals in five commercially available instant noodle products using inductively coupled plasma mass spectrometry (ICP-MS) following conventional hot plate and microwave-assisted acid digestion. Approximately 0.250 g of homogenized noodle samples, including seasoning packets, were digested with nitric acid and hydrogen peroxide prior to analysis. Aluminum (Al), chromium (Cr), copper (Cu), arsenic (As), cadmium (Cd), and lead (Pb) were quantified to compare digestion performance and assess trace metal occurrence. Preliminary results showed that Cu was consistently detected in all samples, whereas As and Cd were generally present at low concentrations or below the method detection limits. Aluminum exhibited the greatest variability among samples and between digestion methods, while an elevated Pb concentration was observed in one coded sample following hot plate digestion. Overall, microwave-assisted digestion provided efficient sample preparation with reduced digestion time compared with conventional hot plate digestion. Ongoing quality assurance and quality control studies, including method validation and certified reference material analyses, are being conducted to further evaluate method accuracy, precision, and recovery. These findings demonstrate the applicability of ICP-MS coupled with acid digestion for the determination of trace metals in processed food products.This research was supported by the National Science Foundation (NSF) under Award No. 2306877.

SWRM 2026 SW287 - Withdrawn

SWRM 2026 SW288

Comparison of hot plate and microwave-assisted acid digestion for ICP-MS determination of trace elements in honey

***Victoria Tran**, victoria.tran@tsu.edu, **Morgan Clark**, mclark33@student.tsu.edu, **Aliya Broadway**, a.broadway9985@student.tsu.edu, Kevin Anthony, Sonya C. Caston, **Tuan Phan**, tuan.phan@tsu.edu. Texas Southern University College of Science Engineering and Technology, Houston, Texas, United States*

Honey is widely consumed for its nutritional value and has been recognized as a potential bioindicator of environmental contamination because bees can accumulate trace elements from their surrounding environment. This study compared conventional hot plate and microwave-assisted acid digestion methods for the determination of selected essential and potentially toxic trace elements in local and commercial honey using inductively coupled plasma–mass spectrometry (ICP-MS). Five honey samples representing both local and commercial sources were digested with nitric acid and hydrogen peroxide prior to analysis. Concentrations of magnesium (Mg), aluminum (Al), chromium (Cr), manganese (Mn), iron (Fe), cobalt (Co), nickel (Ni), copper (Cu), zinc (Zn), arsenic (As), cadmium (Cd), and lead (Pb) were determined. Magnesium was the predominant essential element detected in all samples, whereas As and Cd were generally present at low concentrations or below the method detection limits. Elevated Zn and Pb concentrations were observed in one local honey sample following hot plate digestion; however, Pb was not detected in the corresponding microwave-digested

samples. Differences in elemental concentrations between the two digestion methods suggest that sample preparation can significantly influence ICP-MS results for honey matrices. Ongoing quality assurance and quality control studies, including method validation and recovery experiments, are being conducted to further evaluate analytical performance and optimize sample preparation for trace element determination in honey. This research was supported by the National Science Foundation under Award No. 2306877.

SWRM 2026 SW289

Biosorption of copper and cadmium using hydrochar derived from *Chlorella* and rice hull

***Ben Jang**, ben.jang@etamu.edu, Lacy Baxter, Alexander Nachman, Noah Smith. Chemistry and Biochemistry, East Texas A&M University, Commerce, Texas, United States*

This study investigates the removal of toxic heavy metals from water; the heavy metals of focus were Copper and Cadmium. The remediation utilized is biosorption with hydrochars derived from microwave hydrothermal carbonization (mHTC) of chlorella and rice hull. Biosorption capacity/efficacy and kinetics were analyzed for hydrochars derived from different ratios of rice hull to chlorella via mHTC at 220C. The results indicate that biosorption using hydrochar derived from different ratios of rice hull and chlorella is an effective way of heavy metal remediation. The introduction of rice hull significantly increased the efficiency of hydrochar production; certain ratios were capable of maintaining the efficacy seen with plain chlorella hydrochar and on occasion exceeding its adsorption capabilities. It is concluded that 30/70 and 40/60 are within the ‘Goldilocks’ zone that maximizes yield and biosorption efficacy.

SWRM 2026 SW290

Plastics as heavy metal vectors in landfill-mined soil: A rapid *in-situ* handheld XRF assessment from Bhalswa dumpsite, New Delhi

***Rhea Kochhar**[1,2], rheakochhar05@gmail.com, Deepak K. Haritwal[1], G.V. Ramana[1]. (1) Civil Engineering, Indian Institute of Technology Delhi Department of Civil Engineering, New Delhi, DL, India(2) Civil Engineering, Washington State University, Pullman, Washington, United States*

The reuse of landfill-mined soil for applications such as filling low-lying areas and road construction is gaining attention in developing countries like India, driven by the growing adoption of landfill mining. However, this recovered material often contains elevated levels of contaminants — including heavy metals, microplastics, and organic pollutants — that limit its suitability for reuse. Microplastics are of particular concern, as their increasing abundance and role as vectors for heavy metal transport further compound this risk. Conventional laboratory-based analysis of heavy metal concentrations on plastic surfaces is time-consuming and resource-intensive, necessitating faster field-screening alternatives. This study presents a rapid, field-based method for assessing heavy metal contamination in plastic fragments recovered from landfill-mined soil using a handheld X-ray fluorescence (XRF) analyser. The approach enables in situ, real-time screening of both mined soil and associated plastic debris, providing a practical tool for pre-reuse quality assessment. Samples were collected from a dumpsite in Bhalswa, New Delhi, India, and FTIR-ATR spectroscopy confirmed the presence of four plastic types: polyethylene (PE), polypropylene (PP), polyvinyl chloride (PVC), and polystyrene (PS). XRF analysis revealed substantial heavy metal accumulation in the soil matrix,

led by chromium (Cr, 860.04 ppm), zinc (Zn, 512.52 ppm), copper (Cu, 335.85 ppm), and lead (Pb, 141.74 ppm). On recovered plastic fragments, Cu and Zn were detected in 100% of samples, followed by Cr (96.8%), Pb (90.3%), and As (77.4%), with peak concentrations exceeding 4,000 ppm for Zn and 10,000 ppm for Cu. In contrast, native (virgin) plastic samples showed no detectable levels of As, Cd, Hg, Ni, or Pb, confirming that the elevated heavy-metal loads in landfill-derived plastics originate from surrounding waste. These findings establish handheld XRF as a valuable field-screening tool for evaluating contamination risk prior to material reuse.

SWRM 2026 SW291

Assessment of heavy metal contamination in playground dust using atomic absorption spectrometry (AAS)

***Jessica Meza**, jessica.meza@cameron.edu, Kandalama Priyasantha. Chemistry, Physics and Engineering, Cameron University, Lawton, Oklahoma, United States*

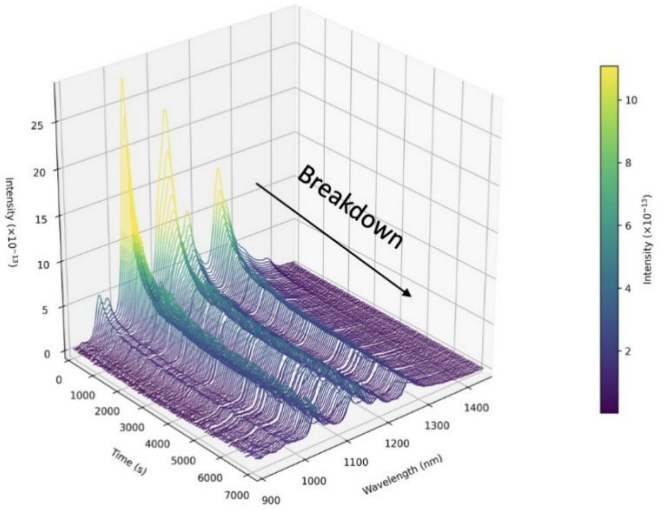
Heavy metal contamination in environmental dust is an important concern because recreational areas, particularly playgrounds, can provide opportunities for repeated exposure to contaminated particles. Children may be especially susceptible to exposure through inhalation, ingestion, and hand-to-mouth contact. This study aims to quantify selected heavy metals in dust collected from playgrounds throughout the Lawton, Oklahoma area using flame atomic absorption spectrometry (AAS).
Initial work focused on developing and optimizing an analytical method for quantitative determination of metals in environmental dust. Calibration curves were successfully constructed for the target metals, including iron (Fe), manganese (Mn), nickel (Ni), cadmium (Cd), lead (Pb), zinc (Zn), cobalt (Co), and copper (Cu). During method development, the organic phase used in the procedure did not dilute effectively with deionized water as reported in the literature. Therefore, the method was modified to incorporate an appropriate organic diluent, allowing calibration standards to be prepared in a matching solvent matrix. Evaluation of the calibration data demonstrated substantial differences in analytical response among the metals. Fe and Mn exhibited the narrowest linear calibration ranges, spanning approximately a 10-fold concentration range, while Ni demonstrated the widest linear range at approximately 200-fold. Cd exhibited the greatest calibration sensitivity, whereas Pb showed the lowest sensitivity under the experimental conditions.
Building on this optimized calibration method, the current study will apply AAS to the quantitative analysis of playground dust samples collected throughout the Lawton area. Samples will be prepared using acid digestion and analyzed for the target metals using the established calibration curves. The resulting concentration data will be used to compare metal levels among playground locations and evaluate the extent of heavy metal contamination. This work establishes an analytical framework for monitoring trace metal contamination in frequently used recreational environments and provides baseline data for evaluating potential environmental exposure in the Lawton community.

SWRM 2026 SW292

Through the lens of chirality: Breakdown of single-walled carbon nanotubes into graphene quantum dots

***Alyssa Dickens**, a.m.dickens@tcu.edu, Ugur C. Topkiran, Anton V Naumov. Physics & Astronomy, Texas Christian University College of Science & Engineering, Fort Worth, Texas, United States*

Single-walled carbon nanotubes (SWCNTs) are in growing demand for their applications in optics, electronics, and biophysics, and their widespread use leads to concerns about waste management and environmental sustainability. Current removal methods include oxidative chemical degradation through UV-assisted sodium hypochlorite. While studies claim this method reduces SWCNTs to carbon oxides and carbonate ions, our research shows graphitic structures such as graphene oxide sheets and graphene quantum dots persist in SWCNT surfactant solutions throughout and following breakdown. We monitor the breakdown process over two hours of UV-assisted sodium hypochlorite treatment using visible and near-infrared (NIR) fluorescence (480-1450 nm), Raman spectroscopy, and transmission electron microscopy (TEM). Through the use of four surfactants, sodium dodecyl sulfonate (SDS), sodium dodecylbenzene sulfonate (SDBS), sodium cholate (SC), and sodium deoxycholate (SDC), surfactant effects are observed to influence chirality-specific degradation rates. Previously believed to be the result of surface tension, small-diameter SWCNTs are expected to degrade faster than their larger-diameter counterparts. Our holistic analysis reveals that the opposite is true: SWCNTs with larger diameters break down fastest under UV-assisted sodium hypochlorite treatment. Our work explores the persistence of graphitic structures throughout UV-assisted sodium hypochlorite treatment and the influence of surfactants on chirality-specific degradation rates.



SWRM 2026 SW293

Gold nanoparticle-based biosensors for targeted detection of HPV E6 and E7 oncoproteins

***Louie Tapia**, louie.tapia01@utrgv.edu, Julie P. Vanegas, Brittany Griggs. Department of Chemistry, University of Texas Rio Grande Valley, Edinburg, Texas, United States*

Human papillomavirus (HPV) infection is a major cause of cervical cancer, with viral oncoproteins E6 and E7 disrupting tumor-suppressor pathways and promoting malignant transformation. Gold nanoparticles (AuNPs) are promising biosensing platforms because their optical properties respond to change in size, aggregation, and surface chemistry. This study investigates the synthesis of functionalizable AuNPs for targeted detection of HPV E6 and E7. AuNPs were synthesized by aqueous mechanochemistry using chloroauric acid trihydrate and 2-propargylamine as a gold precursor and surface ligand, respectively. Ball-milling conditions, including reaction time, reagent ratios, and water volume were varied to evaluate their effects on nanoparticle formation and optical properties. Samples were characterized by UV-Vis, DLS, PL, and FTIR spectroscopy. The

synthesized AuNPs are functionalized through copper(I)-catalyzed azide-alkyne cycloaddition with biotin-PEG4-azide and azido-PEG2-OH to improve stability and provide sites for biomolecular recognition. Streptavidin and biotinylated anti-HPV16 E7 antibody are incorporated for selective E7 capture, followed by an enzyme-linked detection antibody and TMB substrate for colorimetric detection. This approach aims to establish a rapid and functionalizable AuNP platform for HPV oncoprotein detection.

SWRM 2026 SW294

ROS-responsive gold nanoparticles for targeted methotrexate delivery in inflammatory diseases

***Elaina HEath**, elaina.heath@okstate.edu, Niloofar Valizadeh Dana, Jimmie D. Weaver, Yolanda Vasquez. Chemistry, Oklahoma State University The College of Arts and Sciences, Stillwater, Oklahoma, United States*

Methotrexate (MTX) is a first-line treatment for rheumatoid arthritis (RA); however, systemic administration can lead to off-target effects and dose-limiting toxicities. To improve site-specific delivery, we are developing reactive oxygen species (ROS)-responsive gold nanoparticle (AuNP) nanocarriers designed to release MTX within the inflammatory microenvironment of arthritic joints. Gold nanoparticles will be functionalized with methotrexate, amine-terminated polyethylene glycol (NH_2-PEG-SH), and a ROS-cleavable thioketal linker. PEGylation will be employed to enhance colloidal stability and reduce nonspecific protein adsorption, while the thioketal linker provides stimulus-responsive drug release under elevated ROS conditions characteristic of inflamed tissues. The thioketal linker was synthesized and characterized by ^{1}H NMR and ATR-FTIR spectroscopy. Functionalized AuNPs will be characterized using UV-Vis spectroscopy and dynamic light scattering (DLS) to evaluate nanoparticle formation, surface modification, and hydrodynamic size. Biological performance will be assessed in vitro using RAW 264.7 macrophage cell cultures to evaluate nanoparticle cytotoxicity and therapeutic potential under inflammatory conditions. This ROS-responsive AuNP platform represents a promising strategy for targeted MTX delivery and controlled drug release in RA. The development of these nanocarriers may contribute to reducing systemic toxicity while improving therapeutic efficacy, supporting future preclinical evaluation of nanoparticle-based treatments for inflammatory diseases.

SWRM 2026 SW295 - Withdrawn

SWRM 2026 SW296

Exploring Mn-based MOF, MOXI-214, as a vaccine adjuvant candidate

***Alexander J. Mathai**, alexander.j.mathai@gmail.com, Ziqi Wang, Thomas Howlett, Emily Osborn, Shahabuddin Alam, Jeremiah J. Gassensmith. Chemistry and Biochemistry, The University of Texas at Dallas, Richardson, Texas, United States*

Vaccines are among the most effective public health interventions in human history, often relying on adjuvants to create protective, long-lasting immunity. Although current adjuvants like aluminum salts

have proven effective for extracellular pathogen immunity, there remains a need for novel adjuvants that elicit stronger, more targeted immune responses against intracellular pathogens through innate immune stimulation. Manganese ions (Mn2+) are known to stimulate the cyclic GMP-AMP synthase-stimulator of interferon gene (cGAS-STING) pathway, a critical innate immune signaling pathway. Activation of this pathway induces type I interferons and inflammatory cytokines in response to foreign dsDNA, favoring development of cytotoxic T cells and other immune populations capable of eliminating infected cells and clearing intracellular pathogens. However, effective intracellular delivery of Mn2+ and other metal ions remains a major challenge, with metal-organic frameworks (MOFs) serving as a potential solution. MOFs are polycrystalline porous materials composed of metal nodes connected by organic ligands, with versatile applications ranging from atmospheric carbon capture to catalysis and use in biomedical science. Our laboratory has developed a fully manganese-based MOF, MOXI-214 (MOXI), capable of biomimetic encapsulation of biomolecules commonly found in vaccines. We propose that MOXI can deliver Mn2+ intracellularly while enabling antigen release, functioning as an integrated antigen delivery and adjuvant system. The immunostimulatory capabilities of MOXI were assessed with in-vitro studies evaluating cytotoxicity, cellular uptake, immune activation, and mitochondrial stress. Results demonstrate that MOXI is a biocompatible immunostimulatory platform inducing robust cGAS-STING activation compared to equivalent manganese controls, supporting its potential as a vaccine adjuvant candidate.

SWRM 2026 SW297

Nanoscale characterization of co-assembled peptide fibers

***Erwin Kingston**, erwinjkingston@gmail.com, James A. Hebda. Biochemistry, Austin College, Sherman, Texas, United States*

Over the life cycle of plastic based clothing microplastics shed from the fibers and eventually make their way into the water supply, contributing nearly 200,000 tons of plastic waste entering marine ecosystems annually. Natural biopolymers like cotton fibers require extensive land, water, pesticide, and fertilizer use. Peptides capable of polymerizing into higher order fibrils could be a sustainable alternative capable of biodegradation and industrial scale manufacturing. In this study, higher order fibrils formed by heterodimeric, co-assembled peptides are prepared and imaged using atomic force microscopy (AFM). Peptides were designed according to the heptad repeat motif found in self-assembling coiled-coils with complimentary charged residues, cysteine residues, and different lengths to induce sticky-end assembly. Co-assembly was previously shown to stabilize helical structure and produce nanoscale fibers as visualized by negative stain electron microscopy. Samples containing individual positive or negative peptides were compared to samples containing combining the two under varying conditions to characterize favorable assembly conditions. We showed that samples kept in buffers with salt led to difficulty with imaging the formed structures because of salt crystals. A sample preparation protocol previously used in transmission electron microscopic (TEM) imaging of the same peptides was then mirrored and applied for AFM imaging. Through this experiment we confirmed similar assemblies between both methodologies and further characterized the morphology of assembled structures. This study lays the groundwork for future investigation into the co-assembled fibers where additional characteristics relevant to their applications can be elucidated.

SWRM 2026 SW298 - Withdrawn

SWRM 2026 SW299

From bacteria to cancer therapy: Self-assembled virus-like particles for targeted enzyme delivery

***Y Nguyen**, ynn230000@utdallas.edu, Orikeda Trashi, Ikeda Trashi, Harshini Bapanapalli, Jeremiah J. Gassensmith. Chemistry and Biochemistry, The University of Texas at Dallas, Richardson, Texas, United States*

Virus-like particles (VLP) are non-infectious biomaterials designed to resemble viruses, allowing them to be engineered for targeted drug delivery. By modifying VLPs to recognize Platelet-Derived Growth Factor Receptor Beta (PDGFR-β), a receptor overexpressed in various cancers such as lung, liver, and colorectal cancers, we can enhance their ability to selectively bind to tumor cells, excluding healthy cells. One major challenge in cancer treatment is the tumor microenvironment, where cancer cells undergo high glucose metabolism, leading to excess lactate production. This buildup acidifies the surroundings, promotes tumor growth, and weakens the immune system by impairing T-cell function. To address this, we are developing a dual-enzyme VLP system encapsulating lactate oxidase (LOX) and catalase (CAT). LOX converts lactate into pyruvate and hydrogen peroxide (H2O2), helping to reduce lactate accumulation, while CAT breaks down excess H2O2 into oxygen and water, preventing oxidative damage to normal cells. By integrating these enzymes into VLPs, we aim to not only suppress tumor growth but also restore immune system function, creating a more favorable environment for cancer treatment. One of the unique properties of our VLPs is that both the targeting moiety and the enzymatic cargo are fully self-assembled within *E. coli*. They are easily purified with high yield and purity, without requiring additional purification methods. These VLPs are highly stable at room temperature and can be stored indefinitely at 4°C. In our research, we evaluate these engineered VLPs in laboratory models as therapeutic tools, investigating their potential as a novel strategy for cancer treatment.

SWRM 2026 SW300

Effect of benzalkonium halide chain length on magnetic cellulose nanocrystal stability

***Thatcher Bentley**, trbentley1000@gmail.com, Juganta K. Roy. Chemistry and Physics, West Texas A&M University, Canyon, Texas, United States*

Biofilm-forming foodborne pathogens such as *Listeria monocytogenes* and *Escherichia coli* are mutable, resisting conventional disinfectants, promoting the development of sustainable antimicrobial materials. Chitosan-functionalized magnetic cellulose nanocrystal (mCNC) composites, used in conjunction with benzalkonium chloride (BKC) or benzalkonium bromide (BKB), are a promising platform to combat these foodborne pathogens. However, the molecular factors governing their stability and interfacial interactions remain poorly explored. In this work, Density Functional Theory (DFT) is used to investigate the effect of benzalkonium-halide alkyl chain length on the interfacial interaction of mCNC@BKC and mCNC@BKB nanocomposites. Leveraging the Van der Waals-corrected functionals, the interfacial phenomenon of the homologous C8, C10, C12, C14, C16, and C18 alkyl chains was investigated to identify energetically favourable configurations. Our results reveal that longer alkyl chains (C18) exhibit greater stability than shorter ones. Trends showed fluctuations in stability with shorter carbon chain lengths, primarily those comprising of 8 to 14 carbons, except BKC, which showed a considerable stability fluctuation at a chain length of 10 carbons. These results identify the most stable alkyl chain being 18 carbons long for both BKB and BKC in terms of binding. Our results demonstrate that the chain length of benzalkonium-halide pivots

the stability of the interfacial binding and the molecular organization of mCNC@BKC/BKB composites. Overall, this study provides a molecular-level guidance to design stable and sustainable cellulose-based nanomaterials and to select candidates for further investigation of antimicrobial and antibiofilm performance.

SWRM 2026 SW301

Synthesis of gallium-based liquid metal nanoparticles

***Benjamin T. Lopez**, lopezben1804@gmail.com, Rahul Meduri, Kate Baumler, Julia Chan. Chemistry/Biochemistry, Baylor University, Waco, Texas, United States*

Gallium-based liquid metal nanoparticles have emerged as an area of research for medicinal applications, including drug delivery, composite materials, and implant coatings owing to their distinctive ability to form an oxide layer on their surface. Previous studies have used metallic gallium (Ga), a soft metal that can be synthesized into a liquid metal nanoparticle via bath ultrasonication, and performed cytotoxicity assays on various human cell lines to assess the viability of Ga-based liquid metal nanoparticles before in vivo implementation. For Ga-based liquid metal nanoparticles, such as Eutectic Gallium-Indium (EGaIn), cytotoxicity assays are only beginning to be explored. While the cytotoxicity of Gallium and EGaIn has already been established, other liquid metals like gallium-zinc (GaZn) and gallium-bismuth (GaBi) have yet to be explored. This study aims to synthesize liquid metal nanoparticles using bath ultrasonication; compare the suspended particles to fully crystalline particles; characterize the Ga-Based nanoparticles through powder X-ray diffraction and energy-dispersive X-ray spectroscopy; establish cytotoxicity assays for GaZn and GaBi; and compare those cytotoxicity profiles against a Ga/EGaIn liquid metal nanoparticle control. Once cytotoxicity assays have been established for GaZn/GaBi and deemed to have negligible cytotoxic effects, the antimicrobial properties of the liquid metal nanoparticles can be assessed for future antibacterial coatings, in vivo drug delivery systems, and cancer treatments.

SWRM 2026 SW302 - Withdrawn

SWRM 2026 SW303

Enzymatic construction of chiral 2D/3D fused heterocyclic ring scaffolds

*Yining Wang, Ru Cui, **Quoc Hoa Ngo**, Benny.Ngo@utdallas.edu, Rudi Fasan. Chemistry and Biochemistry, The University of Texas at Dallas, Richardson, Texas, United States*

Ring systems are ubiquitous structural motifs in small-molecule pharmaceuticals and bioactive natural products, owing to their ability to impart distinct three-dimensional architectures and modulate key physicochemical and biological properties. Among these, two-dimensional (2D) aromatic heterocycles, particularly pyridine, are among the most prevalent scaffolds in medicinal chemistry. Pyridine, in particular, is the most commonly encountered nitrogen-containing heterocycle in FDA-approved small-molecule pharmaceuticals over the past decade, underscoring its broad utility in drug design. In parallel, three-dimensional (3D) aliphatic ring systems have attracted growing interest in medicinal chemistry as strategies to increase molecular complexity and escape the limitations associated with planar aromatic scaffolds due to their relatively low molecular weight, enhanced

solubility, and favorable physicochemical properties. Fusing 2D aromatic and 3D aliphatic ring systems thus provides an appealing strategy to integrate the complementary structural and physicochemical characteristics of both classes of scaffolds within a single molecular framework. Here we report studies toward the development of a biocatalytic method for the construction of chiral 2D/3D fused heterocyclic ring scaffolds via selective carbene transfer reactions. This method can provide access to new, complex molecular scaffolds for medicinal chemistry and other applications.

SWRM 2026 SW304

Establishing a malate dehydrogenase (MDH) drug screening assay for the discovery of MDH selective inhibitors with anticancer potential

***Nicholas A. Furman**, nfurman@student.uiwtx.edu, Zwe Thiha, Rachell E. Booth, Charles Fermaintt. Chemistry and Biochemistry, University of the Incarnate Word, San Antonio, Texas, United States*

The enzyme Malate Dehydrogenase (MDH) reversibly catalyzes the malate-to-oxaloacetate reaction, converting NAD^+ to NADH in the process. Humans express two MDH isoforms involved in distinct biological functions. MDH1 resides in the cytoplasm and is involved in balancing NAD^+ and NADH levels between the cytosol and mitochondrial cavities through the malate-aspartate shuttle pathway. MDH2, on the other hand, is located within the mitochondria and takes part in the Citric Acid Cycle, producing reducing power (NADH) to fuel ATP synthesis. Given the high metabolic importance MDH1 and MDH2 have in meeting energy demand, they are typically overexpressed within most cancers, including breast cancer. Thus, we hypothesized that MDH-selective inhibitors will lead to reduced proliferation in cancerous cells. To do this, we adapted an MDH kinetic protocol into a 96-well plate format that measures the interconversion of NADH and NAD^+ at 340 nm. We found that 1 mM oxaloacetate (OAA) and 10 ng of recombinant MDH produce the most optimal kinetic results in this setting. This assay was then used to screen a series of proposed MDH inhibitors, both from the literature and from an *in silico* screen using the solved 3D structure of each enzyme. To determine which cancer cell line would be the most sensitive to MDH inhibition, we also performed immunoblotting analysis of both human MDH1 and MDH2 in cancer cells representative of the different types of breast cancer. Our data indicate that triple-negative breast cancer (TNBC) cell lines might be optimal candidates to test the anti-proliferative effects of MDH inhibitors.

SWRM 2026 SW305

Biochemical studies of the avocado (*Persea americana*) pit. A potential remedy for the control of diabetes

***Arnulfo Mar**, arnulfo.mar@utrgv.edu. SIBCS, UT Rio Grande Valley, Brownsville, Texas, United States*

Our research program involves the biochemical study of plants that are used as folk remedies in the treatment of diabetes in South Texas. This research focuses on the biochemical analysis of Avocado pits which has been utilized as folk medicine treat diabetes among the Hispanic population in this region. In our studies, we boil the pits and analyze the aqueous solutions for amino acids, proteins and carbohydrates using UV-visible spectrophotometry. Sugar content was determined using the Bennedict Reagent and the sulfuric acid-phenol method, amino acid analysis by means of ninhydrin, protein test using the Biuret reagent. Our results show no evidence for the presence of amino acids or

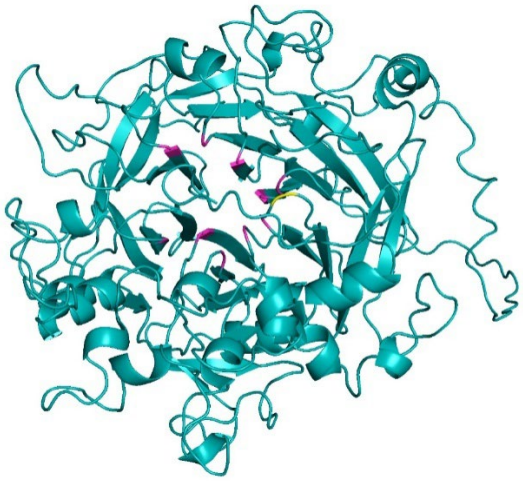
proteins in the extracts. The presence of reducing sugars was detected in the extracts and the concentrations were determined.
We have investigated the presence of quercetin, gallic and ferrulic acids in the pits' extracts since these phenols have been previously proven to regulate clotting patterns and to decrease cellular oxidative stress. We have used preparative column chromatography in the isolation of these compounds and reverse and normal phase high performance liquid chromatography for their identification. Additionally, the presence of these phenols was detected by means of UV-spectrophotometry. Total phenols were detected using Folin-Ciocalteu reagent. The Total anti-oxidant capacity (TAOC) was determined using the FRAP (Ferric reducing antioxidant power) assay. The determination of ascorbic acid is done by using meta-phosphoric acid and 2,4 dinitrophenylhydrazine

SWRM 2026 SW306

Expression and activity profiling of recombinant PhoX from *Shewanella oneidensis* MR-1

***Isabella Ibanez**, iibanez@stedwards.edu. Chemistry, St Edward's University, Austin, Texas, United States*

Shewanella oneidensis MR-1 is known for its ability to use a wide range of electron acceptors, including metal oxides, during respiration. This versatility has made it an important model organism for environmental microbiology and bioremediation research. In iron-rich environments, however, phosphate can become poorly available. Under phosphate-limited conditions, *S. oneidensis* increases extracellular phosphatase activity, allowing the bacterium to recover phosphate from organic sources. PhoX is a predicted extracellular alkaline phosphatase that may contribute to this process. Unlike the well-characterized alkaline phosphatase PhoA, PhoX relies on a complex iron–calcium cofactor for catalysis.
In this study, recombinant PhoX containing a C-terminal hexahistidine tag was expressed in *Escherichia coli* using a pET21-NESG plasmid. The protein was purified by immobilized metal-affinity chromatography and analyzed by SDS-PAGE. A prominent band was observed near 73 kDa, consistent with the expected molecular mass of PhoX. Enzyme activity was measured spectrophotometrically using p-nitrophenyl phosphate (pNPP) as a model substrate. The effects of pH and temperature were also examined. The purified protein hydrolyzed pNPP and exhibited its highest activity under basic conditions within the tested range.
These results demonstrate the successful production of active recombinant PhoX and provide a starting point for future studies of its catalytic properties, metal dependence, and role in phosphorus acquisition by *S. oneidensis.*



AlphaFold-predicted structural model of PhoX from *Shewanella oneidensis* MR-1

SWRM 2026 SW307

Examination of antimicrobial production by a *Pseudomonas donghunesis* strain isolated from Sorcerer's Cave

Amy Osborn[1,3]*, aco21a@acu.edu, Faith Jackson*[1]*,* ***Jessica Leach***[1]*, jel24a@acu.edu, Kathleen Lee*[1]*, Jennifer Huddleston*[2]*. (1) Chemistry & Biochemistry, Abilene Christian University, Abilene, Texas, United States(2) Biology, Abilene Christian University, Abilene, Texas, United States(3) The University of Texas at Dallas, Richardson, Texas, United States*

The rise of antimicrobial-resistant infections is a global healthcare concern, necessitating the search for novel therapeutics from unexamined sources such as caves. A recent exploration of Sorcerer's Cave in Terrell County, Texas, yielded 315 bacterial isolates that were screened for antimicrobial resistance and for antibiotic production. Of these, *Pseudomonas donguensis* strain SC1154 showed the strongest inhibition against eight of the nine tested strains of clinically important bacteria. This study seeks to identify the secondary metabolite excreted by SC1154 that is responsible for the broad-spectrum antibiotic activity. Efforts first focused on determining the optimal time to isolate the antimicrobial from the bacterial culture. The growth profile of SC1154 over a 24-hour period with simultaneous well-diffusion assay of the cultues indicated the antimicrobial production begins one hour into the exponential phase and reaches a maximum at 9 hours. Subsequent efforts focused on isolating and purifying the antibiotic compound. Solid-phase extraction resins separated the secondary metabolites from the liquid cultures, and the crude extracts are submitted to bioactivity-guided fractionation. Finally, triparental mating of the wild type SC1154 strain resulted in two mutants with diminished ability to inhibit *Staphylococcus aureus* and one knockout mutant. Liquid chromatography mass spectrometry-based metabolomics comparison of the wild-type and mutant strains are ongoing.

SWRM 2026 SW308

Genetic modification of designer DNA for glial cell targeting

Yanelisse M. Luiggi Garcia[1,2]*, luiggigarcia.yanelis@stthom.edu, Sai Mallannagari*[2]*, JP McGinnis*[2]*, Benjamin R. Aenkiel*[2]*, Tawana Robinson*[1]*. (1) Department of Chemistry and Biochemistry, University of Saint Thomas, Houston, Texas, United States(2) Molecular and Human Genetics, Baylor College of Medicine, Houston, Texas, United States*

Glial cells are essential components of the central nervous system and play important roles in maintaining neural function and regulating the cellular environment of the brain. Developing effective genetic delivery strategies for glial cells could provide valuable tools for investigating glial biology and advancing therapeutic approaches. Plasmid DNA can be engineered to introduce specific genetic elements into cells for introducing genetically encoded elements into cells; however, generating customized plasmid constructs requires reliable and precise genetic engineering strategies. Nanoparticle-based delivery systems offer a potential approach for targeted genetic delivery to glial cells, but these systems require appropriately engineered plasmid constructs to support future applications. There is therefore a need for reliable plasmid engineering strategies that can generate customized constructs for targeted genetic delivery in glial cell systems. Our goal is to develop a reliable strategy for engineering plasmid DNA that can support future nanoparticle-based genetic delivery applications in glial cells. Our approach involves designing peptide sequences and introducing targeted DNA modifications through recombinant DNA techniques, including PCR and ligation, to generate modified plasmid constructs. Results will demonstrate the recombinant DNA engineering process, including peptide design, PCR amplification, and ligation of targeted DNA sequences to generate customized plasmid constructs. Optimization of plasmid design and cloning is ongoing, with these results establishing a systematic workflow for engineering modified plasmids. This study provides a foundation for future nanoparticle-based genetic delivery studies in glial cells and may enable the development of targeted approaches for genetically manipulating specific glial cell populations.

SWRM 2026 SW309 - Withdrawn

SWRM 2026 SW310

Inhibition of human islet amyloid polypeptide aggregation by the ATP-independent molecular chaperone cpSRP43

Bismah Ahmed*, bnahmed0619@my.msutexas.edu,* ***Aayan Ahmed****, awahmed0619@my.msutexas.edu, Fu Cheng Liang. Chemistry, Midwestern State University, Wichita Falls, Texas, United States*

Type 2 diabetes mellitus (T2D) is a metabolic disorder characterized by insulin resistance and progressive dysfunction and loss of pancreatic β-cells. A major contributor to β-cell dysfunction is the accumulation of amyloid deposits composed primarily of human islet amyloid polypeptide (hIAPP), a 37-residue peptide hormone that is co-secreted with insulin by pancreatic β-cells. Under pathological conditions, hIAPP undergoes conformational changes that promote self-association and amyloid fibril formation, processes associated with β-cell toxicity and dysfunction. Therefore, preventing or disrupting hIAPP misfolding and aggregation may provide a potential strategy for reducing amyloid-associated β-cell damage. Chloroplast signal recognition particle 43 (cpSRP43) is an ATP-independent molecular chaperone that recognizes specific client proteins through molecular interactions and can prevent or reverse protein aggregation. Previous studies have demonstrated that cpSRP43 inhibits the aggregation of several disease-associated amyloid proteins, including amyloid-β

and α-synuclein, suggesting that its chaperone activity may extend to other aggregation-prone proteins and peptides. In this study, we investigate whether cpSRP43 can modulate hIAPP misfolding and aggregation. We hypothesize that cpSRP43 directly interacts with hIAPP and inhibits its conformational transition and self-association, thereby reducing amyloid fibril formation. To test this hypothesis, we examine the effects of cpSRP43 on hIAPP aggregation and characterize changes in amyloid formation in the presence of the chaperone. Understanding the molecular interaction between cpSRP43 and hIAPP may provide new insights into chaperone-mediated regulation of amyloid formation. More broadly, this study explores the potential of molecular chaperones as modulators of hIAPP aggregation and may provide a foundation for developing new strategies to reduce amyloid-associated β-cell dysfunction in T2D.

SWRM 2026 SW311

Comprehensive biochemical analysis of defective high-density lipoprotein (HDL) via cardiovascular-associated oxidative damage

Haylie Tran[2]*, tran.haylie@stthom.edu, Amanda N. Stanley*[1]*, Carlos E. Trujilo*[1]*, Chidera Ugwuanyi*[2]*, Richa Chandra*[2]*, Tawana Robinson*[2]*. (1) Biology Department, University of Saint Thomas, Houston, Texas, United States(2) Chemistry and Biochemistry, University of Saint Thomas, Houston, Texas, United States*

Cardiovascular disease (CVD) remains a leading cause of mortality worldwide, with oxidative stress being one of the potential causes of lipoprotein oxidation. Lipoproteins, a class of biomolecules in lipid transport, are prone to oxidative modifications, which have been linked to atherogenesis. Within this class of lipoproteins, high-density lipoprotein (HDL) is known to demonstrate antioxidant properties that may limit oxidative damage to its counterpart, low-density lipoprotein (LDL). Though HDL exhibits cardioprotective behavior, its potential susceptibility to oxidative damage that leads to modifications in its size and protein structure needs to be further understood. To address this gap, we used a controlled oxidation system to generate hydroxyl radicals using human plasma that contains measured levels of HDL. To determine oxidative stress levels caused through reactive oxygen species (ROS), we utilize a panel of assays to explore the structural modifications in HDL, including Western blot and silver stain, to indicate the degree of protein degradation. For the quantitative assessment of lipid peroxidation and protein carbonylation, we administer a thiobarbituric acid reactive substance (TBARS) and dinitrophenylhydrazine (DNPH), respectively. In summary, we anticipate that ROS generation will disrupt the HDL structure and ultimately impair its antioxidant capacity. We aim that these findings will provide insight into how oxidative modification contributes to the transition from native to dysfunctional HDL in CVD, paving the way for potential therapeutic strategies.

SWRM 2026 SW312 - Withdrawn

SWRM 2026 SW313

Exploring the expression and reactivity of Baeyer-Villiger monooxygenases from *Thermobifida fusca* and *Acinetobacter caloaceticus*

***Daniela Guerrero**, guerrero.dani.01@gmail.com, Sarah Walbridge, Meagan E. Hinze. Chemistry, Sam Houston State University College of Science & Engineering Technology, Huntsville, Texas, United States*

In recent years, the implementation of green chemistry practices has grown and includes the replacement of hazardous chemicals to minimize harm to the environment. To accomplish these changes, biocatalysts are increasingly favored due to their benign byproducts and mild reaction conditions. This study explores Baeyer-Villiger monooxygenases (BVMOs), which are flavin-dependent and catalyze oxidation reactions. While the native reaction transforms ketones into esters, BVMOs have wider potential as biocatalysts. This study will focus on two BVMOs: Phenylacetone monooxygenase (TfPAMO) from *Thermobifida fusca* and cyclohexanone monooxygenase (AcCHMO) from *Acinetobacter caloaceticus*. Preliminary data will detail heterologous expression in *E. coli* and analysis of reactivity.

SWRM 2026 SW314

Comparative investigation of zinc binding in two isomeric peptides using experimental and computational approaches

***Rawan Siddig**, roni.abubakr@gmail.com. East Texas A&M University, Commerce, Texas, United States*

Short zinc-binding peptides have been proposed as potential alternatives to conventional polyhistidine affinity tags for immobilized metal affinity chromatography (IMAC). This study comparatively investigated two isomeric heptapeptides, Ac-CHGPYHC and Ac-CHGPYCH, using ion mobility-mass spectrometry (IM-MS) and semiempirical PM6 molecular modeling. IM-MS was used to identify peptide–zinc complexes and determine experimental collision cross sections (CCS), while PM6-optimized structures were evaluated through comparison of theoretical and experimental CCS values. Distinct peptide–zinc complexes were observed for both peptides, with differences in the predominant species and gas-phase conformations. The selected PM6 models showed excellent agreement with the experimental CCS measurements, supporting the proposed coordination geometries. These results demonstrate that subtle changes in amino acid sequence influence zinc coordination and highlight the value of integrating IM-MS with computational modeling for the structural characterization of zinc-binding peptides.

Experimental Collision Cross Sections (CCS)

Complex	Drift Time	CCS (He Å²)
ZE + Zn	7.45	196 ± 1
ZE + Zn +IDA	8.92	218 ± 1
ZF + Zn	7.61	199 ± 1
ZF + Zn + $IDA_{(ox)}$	8.78	215 ± 1

SWRM 2026 SW315

Synthesis and characterization of dearomatized Cu(I)-C^N^C complexes: Intermediates in catalysis

***Emylie Guthrie**, emylieguthrie@gmail.com, Nick Back, Laleh Tahsini. Chemistry, Oklahoma State University, Stillwater, Oklahoma, United States*

Tridentate pincer transition-metal complexes are predominant in the literature and are capable of catalyzing a variety of chemical reactions. Lutidine-based pincer transition-metal complexes have been shown over the last 20 years to be exceptionally efficient catalysts featuring a distinct dearomatization-aromatization mechanism that forms a dearomatized ligand backbone upon deprotonation of the methylene linker. This dearomatized complex is reactive with a variety of substrates through the methylene carbon, including nucleophilic attack on electrophiles (CO_2, phenylacetylene, etc.) and reactions with deuterated solvents to promote deuterium transfer. Our group has previously reported the synthesis and catalytic activity of pincer Cu(I) complexes bearing 2,6-lutidine-linked bis-NHC ligands in C-C, C-N, C-O cross-coupling reactions. We have also demonstrated the stereoelectronic effects of NHC wingtips on the overall structure of the Cu-CNC complexes bearing aryl wingtips featuring electron-donating/withdrawing substituents. More recently, our group published a report on the tandem carboxylation-esterification of terminal alkynes. A broad substrate scope, including aryl, alkyl, and pyridyl alkynes, was noted, and mechanistic investigations have suggested a mechanism distinct from any other Cu(I)-NHC-catalyzed carboxylation reaction currently reported. My research focuses on the synthesis and characterization of the proposed dearomatized intermediate to provide further insight into the reaction mechanism. This work describes the successful synthesis and complete characterization of dearomatized Cu-CNC complexes bearing Mes, Dipp, and P-CF_3 wingtip substituents.

SWRM 2026 SW316

Data-driven mapping of backbone conformational space across all 400 dipeptides

***Adair Oropeza**, aoropeza@smu.edu, Chuanye Xiong, Peng Tao. Southern Methodist University Dedman College of Humanities and Sciences, Dallas, Texas, United States*

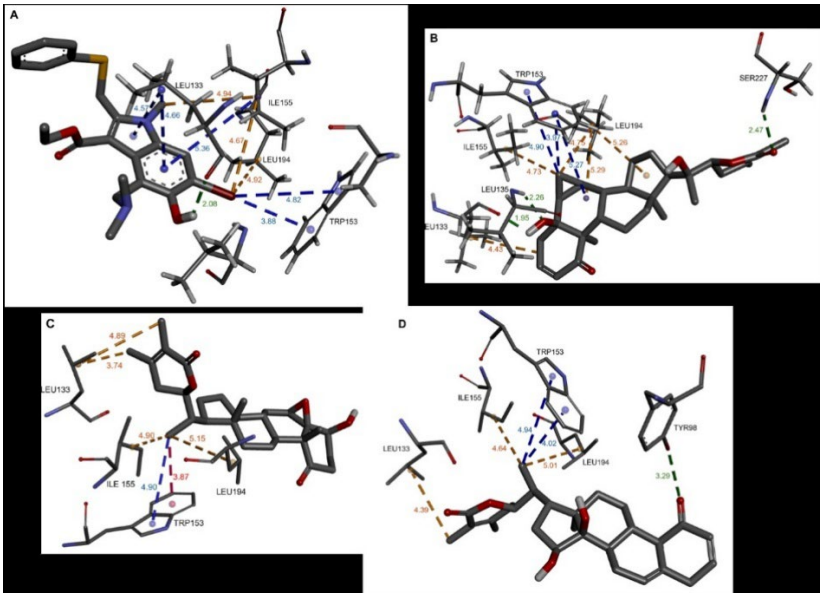
Understanding how amino acid sequence shapes peptide conformational behavior is essential for connecting molecular structure with biomolecular function. Here, we systematically map the conformational space of all 400 canonical dipeptides using molecular dynamics simulations and quantitative analysis of backbone conformational distributions. Despite the simplicity of these systems, the resulting conformational landscapes reveal clear sequence-dependent patterns, with glycine- and proline-containing dipeptides emerging naturally as distinct structural outliers. This work provides a comprehensive benchmark of dipeptide conformational behavior and establishes a foundation for developing sequence-aware generative artificial intelligence (AI) models to predict the structure and dynamics of small peptides.

SWRM 2026 SW317

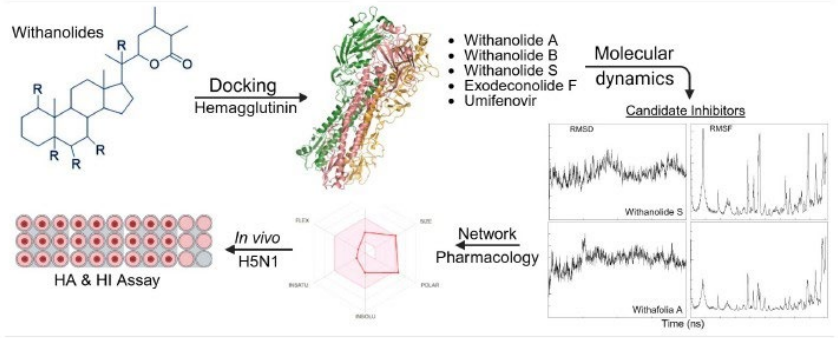
Withanolides targeting H5N1 bird flu: *In silico* screening via pharmacokinetic and molecular dynamics studies

*Nicholas Laroe, Jayendra Chundhuru, **Siwar Kefi**, skefi@ttu.edu, Alejandro Ruiz. Chemistry & Biochemistry, Texas Tech University, Lubbock, Texas, United States*

Influenza A viruses, particularly the highly pathogenic avian strain H5N1, pose substantial risks to human health due to their potential for zoonotic transmission and high human mortality rates. Despite existing antiviral treatments, the emergence of drug-resistant strains necessitates the discovery of novel therapeutics. Withanolides, a class of steroidal lactones, have been shown to exhibit potential antiviral properties. This study employed computational methods, including molecular docking, pharmacokinetics analysis, and molecular dynamics simulations, to evaluate the efficacy of 415 withanolide compounds against the hemagglutinin glycoprotein of H5N1. Molecular docking identified thirteen withanolides with superior binding affinities compared to the control drug umifenovir, with exodeconolide F (**3**) exhibiting the highest binding energy (-6.373 kcal/mol). Pharmacokinetics screening utilizing SwissADME confirmed that all selected compounds met Lipinski's rule, indicating favorable drug-likeness profiles. Molecular dynamics simulations further revealed that **1** demonstrated the most stable interaction with hemagglutinin, maintaining structural compactness and minimal atomic fluctuation throughout a 100 ns simulation. These findings suggest that **1** is a promising lead candidate for development as a new antiviral agent targeting H5N1. Future *in vitro* experimental validation, though challenging due to biosafety concerns, is warranted to confirm these *in silico* predictions.



Withanolides complexed with target protein showing various chemical interactions from AutoDock using Discovery. **A**: **RC1**, **B**: **1**, **C**: **2**, **D**: **3**. With conventional hydrogen bonding (green) and hydrophobic interactions: alkyl-alkyl (gold), pi-alkyl (blue), pi-sigma (red).



Overview of H5N1 screening workflow.

SWRM 2026 SW318

Anti-fouling strategy using triple pulse amperometry for electrochemical detection of xylazine at modified electrodes

***Ella Saltstein**, esaltstein@gmail.com, **Sarah Leiva**, sarah.leiva@richmond.edu. University of Richmond School of Arts & Sciences, Richmond, Virginia, United States*

In conjunction with the United States' widespread opioid crisis, use of Xylazine (XYL), an FDA-approved veterinary tranquilizer, as an opioid adulterant and date-rape drug also continues to increase. XYL, better known as "Tranq-dope" or "Zombie", is unresponsive to Naloxone and not approved by the FDA for human use, but when mixed with fentanyl-based opioids, allows for more efficient opioid production while maintaining the desired euphoric response. With this in mind, an electrochemical approach to XYL sensing offers an opportunity for efficient, cost-effective, and portable detection, ultimately accelerating pre-hospital treatment and increasing protection for healthcare workers. Prior work in our lab employed a nanomaterial-enhanced layer-by-layer sensing scheme on glassy carbon electrodes, utilizing amperometric and voltammetric measurements of XYL oxidation to quantify in beverage and street drug media, respectively. However, such long-term application of high oxidative potentials significantly accelerates surface fouling, diminishing the electrochemical signal. In this work, triple pulse amperometry (TPA), an electrochemical technique traditionally used to clean or "refresh" the surface of a bare electrode, is applied to the modified electrode system, fundamentally mimicking a stripping analysis while minimizing detrimental fouling that was previously observed. While the first pulse stabilizes the electrode under potential control, the second pulse oxidizes XYL into the system and the third pulse reduces a portion of the XYL oxidation product, allowing for their diffusional exist and a resulting cathodic signal directly proportional to XYL concentration. The use of TPA analysis results in an average sensitivity of 0.131(±0.01) μA/μM, a 25-fold increase from the same electrode system used in constant potential amperometry I-t measurements, as well as a limit of detection of ~50 μM that decreases with testing on subsequent days, likely due to initial and slight passivation of the electrode surface. Essentially, utilization of TPA offers an additional avenue for quick and accurate XYL detection which continually proves to be vital amid its nearly ubiquitous use throughout the nation.

SWRM 2026 SW319

Synthesis and study of PDI derivatives for organic semiconductor applications

***Paula A. Sanchez Rendon**, sanchezpaula811@gmail.com, David Mancilla, Nicole Stasek, Alexa Moore, Erica Salinas, Stephen Starnes. Chemistry, East Texas A&M University, Commerce, Texas, United States*

Perylene diimide (PDI) derivatives are organic molecules with semiconducting properties and potential applications as organic photovoltaic materials. Their use could aid in the development of more versatile solar energy devices. Unfortunately, many PDI derivatives exhibit limited solubility because the perylene core promotes strong π-π stacking interactions and intermolecular aggregation. This limitation hinders purification, characterization and potential applications. To investigate the solubility of PDI derivatives, this research focused on functionalizing the imide positions of PDI derivatives. This approach used 3,4,9,10-perylenetetracarboxylic dianhydride (PTCDA), an organic dye which contains the perylene core. Primary amines with varied substituents were reacted with PTCDA through imidization. The primary amines contained a variety of structural features such as branching, bulky substituents, and polar functional groups. The results suggest that using amines

containing a combination of these characteristics can introduce steric hindrance that disturbs π-π stacking and improves PDI solubility. These findings identified structural features in PDIs that can enhance solubility and allow for more processable materials. PDI derivatives were also investigated for their ability to form aggregates using Polarizing Light Microscopy. Further, PDI derivatives were investigated using computational chemistry to examine correlations between structure, solubility and aggregate formation.

SWRM 2026 SW320

Stepwise chemical construction of functional interfaces on mica through covalent surface modification

***Abigail Bellucci**, bellucci@student.uiwtx.edu, Ashok Khanal. Chemistry and Biochemistry, University of the Incarnate Word School of Mathematics Science and Engineering, San Antonio, Texas, United States*

Controlled surface functionalization provides an effective approach for constructing molecular interfaces with tailored chemical properties for applications in biosensing, nanomaterials, and surface chemistry. Here, we report a stepwise strategy for covalent functionalization of freshly cleaved mica through sequential surface reactions. The process begins with silanization using (3-aminopropyl)triethoxysilane (APTES) to introduce an amine-functionalized surface, followed by covalent attachment of an alkyne-PEG_3-maleimide linker. The resulting alkyne-terminated interface was subsequently modified through copper(I)-catalyzed azide–alkyne cycloaddition (CuAAC) with an azide-functionalized alcohol to generate a triazole-linked, alcohol-terminated surface. Each synthetic step was performed under controlled conditions with extensive washing to minimize the presence of unbound reagents and surface-associated impurities. Surface transformations were monitored using Fourier transform infrared spectroscopy coupled with a Harrick VariGATR grazing-angle attenuated total reflection accessory (FTIR-GATR). Characteristic vibrational signals associated with $–CH_2$, –NH, C≡C, C=O, and –OH functionalities provided evidence for the sequential progression of surface modification. In particular, disappearance of the alkyne vibration following CuAAC supported successful conversion of the terminal alkyne functionality. This study demonstrates a practical route for the stepwise construction of functionalized mica interfaces and establishes a versatile platform for future applications in surface chemistry, biosensing, and nanomaterials research.

SWRM 2026 SW321

Uncovering the factors directing the mechanochemical degradation of polythiophenes

***Andrea Mena**, amena7@miners.utep.edu, Robert M. Pankow. The University of Texas at El Paso, El Paso, Texas, United States*

Polythiophenes are conjugated polymers that are ubiquitous in organic electronics with notable applications in organic photovoltaics, field-effect and electrochemical transistors, and electrochromic devices. Recently, we have reported the synthesis of polythiophenes using mechanochemical oxidative polymerization. This polymerization method does not require the use of toxic, hazardous solvents or the application of externally heating, but, instead, it harnesses mechanical energy for covalent C-C bond formation. However, it is known that polymers can mechanochemically degrade through chain-scission or sidechain cleavage, and for non-conjugated polymers this is well-studied

with established mechanisms. However, for conjugated polymers, mechanochemical degradation is not well-studied and it remains relatively unknown what factors influence polymer chain-scission. It is hypothesized that the glass-transition temperature (*T*g), which describes polymer chain mobility, could be an influential parameter governing the mechanochemical degradation of polymers. To probe this hypothesis, the mechanochemical degradation of four polythiophene analogs will be investigated: poly(3-hexylthiophene) (P3HT), poly(3-hexylester thiophene) (P3HET), poly(3-(2-ethylhexyl)ester thiophene) (P3EHET), and poly(3-triethyleneglycol monomethyl ether thiophene) (P3EGET). The polymers will be synthesized with a proximal molecular weight distribution, and the different polymer sidechains will afford varied *T*gs. The mechanochemical degradation will then be monitored via 1H-NMR spectroscopy, gel-permeation chromatography, FT-IR spectroscopy, and optical absorption spectroscopy to analyze changes in the polymer structure and molecular weight distribution. These findings will allow for elucidating the mechanistic pathway and uncovering the key structure-property relationships that govern the mechanochemical degradation of conjugated polymers.

SWRM 2026 SW322

Tracking stepwise mica surface functionalization using FTIR-GATR: A rapid and accessible characterization strategy

***Scarlett Deluna**, sgdeluna@student.uiwtx.edu, Ashok Khanal. Chemistry and Biochemistry, University of the Incarnate Word School of Mathematics Science and Engineering, San Antonio, Texas, United States*

Reliable characterization of surface chemistry is essential for evaluating the formation and progression of functional molecular interfaces. In this study, Fourier transform infrared spectroscopy equipped with a Harrick VariGATR grazing-angle attenuated total reflection accessory (FTIR-GATR) was used to monitor the sequential functionalization of freshly cleaved mica. Surface modification was performed through three consecutive chemical transformations: APTES silanization, coupling of an alkyne-PEG_3-maleimide linker, and copper(I)-catalyzed azide–alkyne cycloaddition (CuAAC) with an azide-functionalized alcohol. Blank mica and modified substrates were analyzed under comparable FTIR-GATR conditions to identify characteristic spectral changes associated with each modification. APTES functionalization produced detectable $–CH_2$ and –NH stretching bands, confirming introduction of the aminosilane layer. Subsequent linker attachment was indicated by the appearance of C≡C and C=O stretching vibrations. Following the CuAAC reaction, the characteristic alkyne absorption decreased or disappeared, accompanied by the emergence of hydroxyl-associated absorption, consistent with formation of the triazole-linked, alcohol-terminated interface. The sequential changes in diagnostic vibrational bands demonstrate the utility of FTIR-GATR for monitoring surface chemical transformations. Compared with more resource-intensive techniques commonly used for surface analysis, FTIR-GATR provides a rapid, nondestructive, and accessible approach for evaluating functionalized surfaces. This methodology is particularly attractive for undergraduate research and laboratories seeking practical approaches to surface-chemistry characterization.

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Synthesis of amino and hydroxyl-group modified polymers using ring-opening metathesis polymerization (ROMP)

***Monique F. Boodram**, faithmicrobiometech@gmail.com, Christopher E. Hobbs. Chemistry, Sam Houston State University College of Science & Engineering Technology, Huntsville, Texas, United States*

This poster describes our recent efforts toward the preparation of amino and hydroxyl group-decorated polymers using ring opening metathesis polymerization (ROMP). The utilization of nitroso Diels-Alder reactions between N-Boc hydroxylamine, 1,3-cyclopentadiene, cyclohexadiene, cycloheptadiene, and cyclooctadiene, in the presence of sodium periodate, allowed us to prepare functional isoxazolidine monomers that could undergo polymerization followed by hydrogenation and post-polymerization ring opening to provide amino and hydroxyl-decorated polymers. Following reductive cleavage of the N-O bonds, the resulting polymer exhibited deliquescence after acidification. To address this, an in-situ crosslinking strategy using acyl chloride is proposed to establish a hydrogel network that prevents liquefaction while maintaining high moisture uptake for applications in atmospheric water harvesting.

SWRM 2026 SW324

Sustainable and chromatography-free synthesis of trityl ether tosylates from glycols and diols

***Khanh Nguyen**, knnguye2@student.uiwtx.edu, Ashok Khanal. Chemistry and Biochemistry, University of the Incarnate Word School of Mathematics Science and Engineering, San Antonio, Texas, United States*

The development of sustainable, economical, and operationally simple protecting-group strategies is important for advancing modern organic and solid-phase synthesis. The trityl (triphenylmethyl) group is an effective hydroxyl-protecting group because of its steric properties, preferential protection of less hindered alcohols, stability under basic, oxidative, and reductive conditions, and facile cleavage under acidic conditions. These characteristics have made trityl protection valuable in the synthesis of DNA, RNA, and peptides. Similarly, tosylation provides a convenient means of converting hydroxyl groups into reactive sulfonate esters, enabling subsequent functional-group transformations. In this study, we present a mild, sustainable, and chromatography-free approach for the preparation of trityl ether tosylates from glycols and diols. Selective mono-tritylation was accomplished under controlled reaction conditions using trityl chloride, with reaction completion monitored by thin-layer chromatography (TLC). Unreacted starting materials and pyridinium salts were removed through aqueous extraction, while di-tritylated impurities and residual pyridine were efficiently separated by selective precipitation. This purification strategy substantially reduces solvent consumption and eliminates the need for conventional column chromatography. The resulting mono-tritylated intermediates were subsequently converted to the corresponding tosylates using sodium hydroxide, providing the desired trityl ether tosylates in high overall yields. Product formation and identity were confirmed by TLC and electrospray ionization mass spectrometry (ESI-MS). Overall, this methodology offers a practical, scalable, and cost-effective alternative to chromatography-dependent synthesis, while minimizing solvent use and purification requirements. The resulting trityl ether tosylates serve as useful synthetic intermediates for applications in advanced organic and solid-phase synthesis.

SWRM 2026 SW325

Twist to upconvert: Conformational control of DSA governs photon upconversion properties

Parker Jia[1,2]*, parkerjia265@gmail.com, Lea Nienhaus*[1]*. (1) Chemistry, Rice University, Houston, Texas, United States(2) Physics, Rice University, Houston, Texas, United States*

To further understand solid-state triplet-triplet annihilation upconversion (TTA-UC), we investigate 9,10-distyrylanthracene, an aggregation-induced emission (AIE)-active molecule, in solution and solid phases. We compare the photophysical properties of DSA in solution, nanocrystals, and crystalline thin films and similarly investigate the corresponding palladium (II) meso-tetraphenyltetrabenzoporphyrin (PdTPTBP)/DSA sensitizer/annihilator pair to clarify the singlet and triplet state properties influencing TTA-UC. We demonstrate that the lack of TTA-UC in DSA solutions is not simply due to a reduced fluorescence quantum yield, but instead due to conformational flexibility that allows for planarization of the vinyl groups, bringing the triplet energy below the 2E(T1) > E(S1) requirement for efficient upconversion. Conversely, in the solid state, the vinyl groups are frozen with a dihedral angle of approximately 75°, preserving the higher triplet energy required for successful TTA-UC, which is visible in the nanocrystal and thin film samples. Our results establish the restriction of dihedral angles as an important molecular design principle for managing excited-state energetics and creating efficient, structurally rigid, solid-state TTA-UC materials.

SWRM 2026 SW326

Automatic matching of excited states through orbital overlap

Mollie Hamman*, mhamman@smu.edu, Devin Matthews. Chemistry, Southern Methodist University, Dallas, Texas, United States*

Excited states are a key component in many chemical processes such as natural and artificial light-harvesting, photocatalysis, and ultrafast probes of electronic and nuclear dynamics. In computational applications, carefully matching up molecules' excited states between calculations under differing computational or physical conditions is important, for example in performing large-scale benchmarking over several excited states, for measuring the effect of chemical environment on local excitations, or with matching free monomer excitations to cluster or ensemble models under highly non-uniform solvatochromic shifts. In order to automatically match excited states from different calculations, we first extract excitation vectors (in the equation-of-motion coupled cluster formalism) and parse a Molden format file to get the molecular orbitals. Then the cross-basis overlap is computed from the molecular and atomic orbitals and is used to transform the excitation vectors to a common basis. This provides a robust yet computationally tractable alternative to full non-orthogonal configuration interaction (NOCI), and can be further simplified by considering only the most significant portions of the excitation vectors. We apply this method to re-analyze excited state data from our previous benchmark of the transition-potential coupled cluster (TPCC) method for core-excited (soft X-ray) states. We find that the correct state matchings can be robustly and automatically obtained, replacing tedious and error-prone hand assignment, especially in the presence of factors such as highly sensitive doubly excited states. As this technique only requires simple excitation vectors and Molden files, it is applicable to a wide range of computer programs and potential applications.

SWRM 2026 SW327

Deep unrolling AI model for compressed sensing reconstruction in GDOES snapshot multi-elemental mapping

***HYUNMO GOO**, hgoo@ttu.edu, Shamika P. Hewage, Rajendra Joshi, Gerardo Gamez. Department of Chemistry and Biochemistry, Texas Tech University, Lubbock, Texas, United States*

Elemental mapping reveals chemical and structural mechanisms that are otherwise difficult to observe. Many high-resolution mapping methods, however, require prolonged acquisition times to build a complete elemental map. Glow discharge optical emission spectroscopy (GDOES) offers a faster alternative. It generates emission by sputtering the sample surface, and the progressive sputtering also provides depth resolution. Turning this speed into high-resolution elemental mapping, however, requires spatial and spectral information to be acquired efficiently. When hyperspectral data are collected sequentially in space or wavelength, the sample consumption over time can compromise depth resolution. This limitation is especially important for three-dimensional mapping of nanoscale materials.

Compressive coded-aperture platforms, such as glow discharge optical emission coded aperture elemental mapping (GOCAM) and glow discharge optical emission coded aperture spectroscopy (GOCAS), address this challenge by encoding spatial and/or spectral information into compressed detector measurements to enable acquisition of the full hyperspectral data cube in a single snapshot, followed by recovery with compressed-sensing algorithms. These iterative reconstructions require careful parameter tuning and can be computationally intensive.

This work investigates deep learning model as an alternative reconstruction strategy for coded-aperture GDOES imaging. A neural network is trained to reconstruct the hyperspectral data cube from coded-aperture measurements. The network incorporates gradient-descent steps derived from the imaging forward model together with a learned image prior and is trained end-to-end without explicit total-variation regularization. The goal is faster, more automated reconstruction while maintaining, or even improving, image fidelity relative to established iterative methods. Quantitative comparisons with coded-aperture reconstruction algorithms, including reconstruction fidelity and processing time, will be presented.

SWRM 2026 SW328

Compositional and morphological effects on phase stability and the shock response of AlCoCrFeNi high-entropy alloys

***Luke Radich**[1], lukeradich26@gmail.com, Garritt Tucker[2,3]. (1) Chemistry & Biochemistry, Baylor University, Waco, Texas, United States(2) Physics and Astronomy, Baylor University, Waco, Texas, United States(3) Materials Science and Engineering Program, Baylor University, Waco, Texas, United States*

High-Entropy Alloys (HEAs) have become a primary focus of materials science research in recent years, owing to their unique thermodynamic properties and impressive mechanical behavior. As such, characterizing the loading responses and deformation mechanisms in these alloys at the atomic level under extreme environments, such as shock loading, has been a key interest for potential application in high-impact industries such as aerospace, technology, and defense. In this study, the shock response of nanocrystalline $Al_x(CoCrFeNi)_{1-x}$ HEA was analyzed using molecular dynamics simulation to determine the effects of chemical composition and defect morphology on the stability of crystal phases and the propensity of deformation mechanisms. We aim to characterize the role of aluminum as a beta-stabilizer for entropy-driven systems and establish a relationship between the thermodynamic nature of metastable microstructures and descriptors of strength in shock-induced deformation.

SWRM 2026 SW329

Training machine learning models with experimental NMR and quantum chemical descriptors to predict Hammett σ constants

***Isabel McLeod**, imcleod@udallas.edu, Prajay Patel. Chemistry, University of Dallas, Irving, Texas, United States*

Efficiently predicting how substituents influence chemical reactivity remains a fundamental challenge in physical organic chemistry. Hammett substituent constants (σ) provide a quantitative measure of these electronic effects and are widely used to relate molecular structure to chemical reactivity. However, using experimentation to determine these constants can expend time and resources. This paper explores a machine learning approach for predicting Hammett σ values of substituted benzoic acids using computational and spectroscopic quantum chemical descriptors. Density functional theory calculations produced a set of theoretical chemical shifts, which were compared to experimental values to select the functional that provided the closest match. A sample set of molecules were used to evaluate relationships between Hammett σ values and quantum descriptors, including Hirshfeld atomic charges, ^{1}H and ^{13}C NMR chemical shifts, frontier molecular orbital energies and Wiberg bond indices. Descriptors showing the strongest relationships were then used to test the full set of 180 molecules for machine learning models to evaluate. Hirshfeld charges, ^{1}H NMR chemical shifts, HOMO–LUMO descriptors, and Wiberg bond indices exhibited strong relationships with Hammett σ values, with correlation coefficients of approximately 0.6 in the descriptor analysis. Among the machine learning models evaluated, LassoLars regression provided the strongest predictive performance, achieving an r^2 value of 0.958. These results demonstrate that quantum descriptors associated with proton electronic environments and atomic charge distributions can provide useful predictors of Hammett σ values and support the development of computational approaches for a more efficient estimation of substituent electronic effects.

SWRM 2026 SW330

Exploring single-site heterogeneity with Universal Models for Atoms

***Marcus Alphonse Broussard**, marcusambroussard@gmail.com, Prajay Patel. Chemistry, University of Dallas, Irving, Texas, United States*

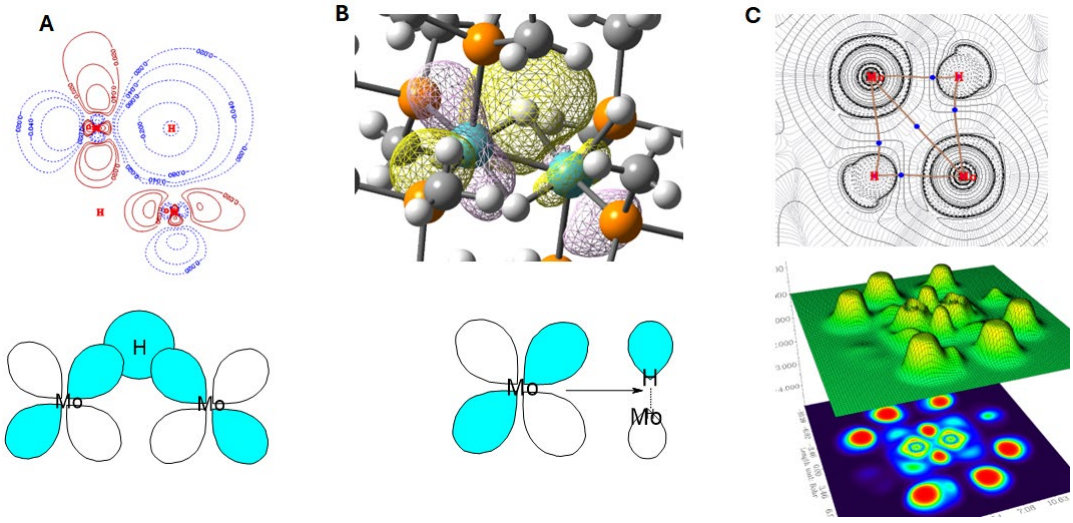
In the organic polymer recycling industry, homogeneous catalysts are traditionally used because of their high selectivity. Single-site heterogeneous catalysis offers a promising alternative because it combines the selectivity of homogeneous catalysis with the stability of heterogeneous catalysts. However, these catalysts are often supported on amorphous surfaces, making their structures and active sites difficult to analyze using traditional experimental methods. This study uses computational methods to investigate amorphous silica as a support for single-site heterogeneous catalysts. The Universal Models for Atoms (UMA) machine-learning interatomic potential was first evaluated as a lower-cost alternative to Density Functional Theory (DFT), a widely used computational method. UMA was used to recalculate properties of amorphous silica structures that had previously been studied using DFT, and the results were compared to determine how well UMA reproduced the DFT results. Metadynamics simulations were then performed using UMA to study the condensation of silanol groups on amorphous silica and the resulting dehydroxylation of the surface. Together, these calculations provide a computational approach for studying how the structure of amorphous silica changes during catalyst preparation and for evaluating whether UMA can be used to study these systems at a lower computational cost.

SWRM 2026 SW331

18 electron rule and metal-metal bonding

*Eamonn Healy, **Andrea Joglar**, ajolgar@stedwards.edu, **Jimena Martinez-Olivares**, jmart199@stedwards.edu. Chemistry, St. Edward's University, Austin, Texas, United States*

Understanding the bonding between main group elements involves the use of the qualitative rules of valence and Lewis' octet rule, supplemented by theoretical calculations. For transition metal complexes the now applicable 18 electron rule is complicated by the variable nature of metal valences. As such determining metal-metal bonding can be significantly more problematic regardless of the sophistication of the computational results. This work shows how a novel electron counting protocol combined with both molecular orbital and topological analyses of the electron density can be used to analyze metal-metal interactions in dimolybdenum complexes.



SWRM 2026 SW332

Machine learning-guided prediction of optical properties in naphthopyran photochromic dyes for next-generation photovoltaics

Ruben Nunez[1]*, rnunez@wtamu.edu, Juganta K. Roy*[2]*. (1) Engineering, West Texas A&M University, Canyon, Texas, United States(2) Chemistry & Physics, West Texas A&M University, Canyon, Texas, United States*

The development of efficient photovoltaics (PV) requires photoactive materials with optical properties capable of effectively absorbing photons from sunlight. Photoactive materials, such as photochromic dyes, are a special class of dyes that respond to light, reversibly controlling the amount of light transmitted or absorbed depending on the intensity of light stemming from the reversible behavior of their open and closed form structure. However, photochromic dye-based PVs are not efficient due to the trade-off limits optimization of transparency and light harvesting. To overcome this limitation, the excited-state properties of this class of dye need to be explored to identify the properties that are

most important. In this work, we implement a machine learning (ML) framework to evaluate and predict the maximum absorption wavelength (λ_{max}) of the closed and open forms of the photochromic dyes. A dataset of 296 molecular structures comprising naphthopyran-based dyes, including their closed- and open-form structures, was considered in this study. We generated a library of 3,700 molecular descriptors using density functional theory (DFT), time-dependent DFT (TDDFT), Morgan fingerprints, and RDKit fingerprints. The models performed well in predicting λ_{max}, with AdaBoost achieving the highest R^2 of 0.876, followed by XGBRegressor with an R^2 of 0.825 and ExtraTree with an R^2 of 0.701. LUMO+1 was the most important descriptor for both AdaBoost and XGBRegressor, with importance values of about 0.31 and 0.34, respectively, while oscillator strength was the most important descriptor for ExtraTree, with an importance value of about 0.40. Our results suggest that photophysics-driven descriptors properties can predict λ_{max} efficiently to screen photochromic dyes for next-generation PV. Finally, this study establishes a chemically interpretable ML framework that connects excited-state descriptors to the optical properties of open and closed naphthopyran forms.

SWRM 2026 SW333

Predicting pK_a of drug-like molecules in aqueous solution via thermodynamic conformers and explicit solvation

Alphonsus Nguyen*, anguyen10@udallas.edu, Prajay Patel. Chemistry, University of Dallas, Irving, Texas, United States*

An understanding of the acidity of molecules is crucial within the field of pharmacology. In this project, the pK_a values of 35 sample drug-like molecules were evaluated computationally. Each molecule had a varying number of conformers that provided a static representation of the molecule's geometry and configuration. Single point energy calculations were performed for all conformers at a specific phase (gas or solution) and state (protonated or deprotonated). Electronic energies were extracted for each phase and state for each molecule and were converted to pK_a via the thermodynamic cycle and Gibbs free energy equations. The purpose of this paper was to examine the change in error as a specific number of explicit water molecules were added. As the number of water molecules increased from 0 to 1 or 2, the error was reduced, but at 5 and 10 water molecules, the error was greater than that under the implicit solvation method. At the same time, the average predicted pK_a value continued to decrease as more water molecules were added. Based on these results, modeling 1 or 2 explicit water molecules was the most effective approach to pK_a prediction across the functionals evaluated, with the lowest root mean square error obtained being 1.30 pK_a units.

SWRM 2026 SW334

Catalytic activity of Kuratowski-type clusters in hydrogenation reactions

Giovanni A. Bartolozzi*, giobart2003@gmail.com, Nikolay V. Tkachenko. Chemistry & Biochemistry, The University of Oklahoma, Norman, Oklahoma, United States*

The use of the pentanuclear MFU-4 type coordination compound $[Zn_5H_4(L_6)]$ utilizing 1,2,3-benzotriazolate as the μ_3-bridging N-donor ligand shows promise in decreasing the activation energy for the hydrogenation of unsaturated hydrocarbons. A reduction in the activation energy of hydrogenation reactions could enhance catalytic efficiency in processes relevant to hydrocarbon

conversion and fuel refinement, both of which are important for industrial applications. We investigated how modifications of both the peripheral and central metal sites affect the catalytic efficiency of the cluster using ethene and itaconic acid as substrates. The peripheral Zn atoms were replaced with Cd, Ag, Ni, Cu, and Pd, and the effect of varying the central metal atom was also examined. The effect of ligand functionalization on catalytic activity was also investigated by introducing electron-withdrawing and electron-donating groups on the benzene ring of 1,2,3-benzotriazolate. Density functional theory (DFT) and the nudged elastic band (NEB) method were employed in ORCA to locate transition-state geometries and determine their corresponding enthalpies and Gibbs free energies.

SWRM 2026 SW335

Redox-controlled reactivity of dinitrosyl cobalt complexes

***Krish Pudu**, kpudu@smu.edu, Esther O. Mosebolatan, Pokhraj Ghosh. Chemistry, Southern Methodist University, Dallas, Texas, United States*

Nitric Oxide (NO) is a biologically important diatomic molecule with diverse physiological functions, acting as both a signaling molecule and, under certain conditions, a cytotoxic species. The reductive coupling of two NO molecules to form Nitrous oxide (N_2O) is an important pathway in NO metabolism and a key transformation in the global nitrogen cycle. In biological systems, this chemistry is mediated by metalloenzymes, highlighting the role of metal centers in controlling NO activation and reduction. Dinitrosyl cobalt complexes (DNCCs), which can be viewed as one-electron congeners of biologically relevant dinitrosyl iron complexes (DNICs), provide useful platforms for examining NO reactivity at cobalt. These complexes can access different $\{Co(NO)_2\}^n$ electronic states, including the $\{Co(NO)_2\}^{10}$ and $\{Co(NO)_2\}^{11}$ states described by the Enemark-Feltham notation. While the $\{Co(NO)_2\}^{10}$ state is resistant to the reductive N-N coupling required for N_2O formation, reduction to the $\{Co(NO)_2\}^{11}$ state is expected to increase electron density at the nitrosyl ligands and facilitate their protonation, providing a potential route to HNO.
To investigate how the ligand environment influences access to these reduced states, we synthesized a series of $\{Co(NO)_2\}^{10}$ complexes supported by two monoanionic formazanate ligands bearing cyano and tolyl backbones. The corresponding dinitrosyl cobalt complexes were characterized by single-crystal X-ray diffraction, FTIR spectroscopy, UV-visible spectroscopy, and electrospray ionization mass spectrometry. The two complexes exhibit distinct ν(NO) stretching frequencies, with representative values of 1834 and 1766 cm^{-1} for the cyano derivative, 1822 and 1752 cm^{-1} for the p-tolyl derivative. Cyclic voltammetry was used to evaluate the reduction chemistry of the complexes and identify the potentials required to access the $\{Co(NO)_2\}^{11}$ state. Initial reactivity studies showed that reduction of the $\{Co(NO)_2\}^{10}$ complex with $NaBH_4$ produces HNO, which can be trapped by phosphines, as shown by ^{31}P NMR and ESIMS, or it can undergo dimerization to form N_2O, as shown by FTIR. These results provide a basis for examining how changes in the formazanate ligand affect the electronic structure and reduction chemistry of dinitrosyl cobalt complexes and their subsequent NO/HNO reactivity.

SWRM 2026 SW336

Understanding the role of S-nitrosothiols as NO carriers at iron

***Kalkidan Abebe**, kabebe@mail.smu.edu, Esther O. Mosebolatan, Pokhraj Ghosh. Chemistry, Southern Methodist University Dedman College of Humanities and Sciences, Dallas, Texas, United States*

S-Nitrosothiols (RSNOs) are biologically important derivatives of nitric oxide (NO) that participate in cellular signaling and nitrosative stress pathways. Yet, the moelcular mechanisms governing their formation and transformation at iron sites remain poorly understood. The labile iron pool has been proposed as an important source of iron-nitrosyl species and may provide a pathway for NO storage and transfer through reactions with thiols and RSNOs. Here, we investigate a redox-active formazanate-supported iron platform, $[LFe(SAd)_2]^-$, to examine the reactivity of NO and RSNO at a well-defined iron complex. The corresponding iron dichloride complex, $[LFeCl_2]^-$, was synthesized and characterized, and its reaction with sodium nitrite results in the formation of a dinitrosyl iron complex (DNIC). The corresponding iron dithiolate complex, $[LFe(SAd)_2]^-$, was subsequently synthesized and characterized by X-ray crystallography and examined in reactions with NO and RSNOs. Density functional theory calculations show that RSNO can bind to the iron center in several distinct orientations, including k^1-S-syn, k^1-N-syn, and k^2-(S, N)-syn geometrics. The three-coordinate Fe-RSNO structures are not stable and rearrange to four-coordinate species in the caculated structures. Experimentally, the reaction of the iron dithiolate with NO/NO^+ and RSNO precursors gives four-coordinate Fe-NO species, with spectroscopic data and X-ray supporting their formation. Reaction with *tert*-butyl nitrite also gives a low-temperature intermediate with an absorption maximum near 670nm that remains observable up to -35 ^{0}C. DFT caculations identify a nitroxyl disulfide formation as an energetically accessible RSNO-derived intermediate, suggesting that rearranagment of the coordinated RSNO may occur during the recation. These results show that this iron system can access both DNIC and Fe-RSNO chemistry and provide a molecular view of how RSNO coordination and rearranagment can lead to changes in iron-nitrosyl speciation.

SWRM 2026 SW337

Synthesis of Ni-Co catalysts for dry reforming of methane

***Ben Jang**, ben.jang@etamu.edu, Boston Walker, Jonathan Quarm, Edmond Duah. Chemistry and Biochemistry, East Texas A&M University, Commerce, Texas, United States*

Dry Reforming of Methane (DRM) is a promising method for converting carbon dioxide (CO2) and methane (CH4) into synthesis gas, which can be used to produce fuels and chemicals. However, DRM is limited by catalyst deactivation caused by carbon deposition and metal sintering. This research focuses on the synthesis of Ni–Co bimetallic catalysts supported on ceria (CeO2) and alumina (Al2O3) to investigate how catalyst support, the order of metal incipient impregnation, and intermediate calcination temperature affect catalytic performance. The catalysts are prepared using sequential incipient impregnation with different drying/calcination temperatures in between impregnation, followed by characterization techniques, such as BET, SEM, TPR, etc. Catalytic performance of the catalysts is evaluated using a CO2/CH4 ratio of 1:1 and a total flow rate of 30 cc/min over 10-100mg of catalysts at 600-800 °C. The goal of this study is to identify catalyst preparation conditions that improve stability, reduce deactivation, and support more efficient syngas production through DRM.

SWRM 2026 SW338

Development of a colorimetric portable sensor for heavy metals

***Andrew Do**, Doaa@jacks.sfasu.edu, Rashid Mia. Department of Chemistry and Biochemistry, Stephen F Austin State University, Nacogdoches, Texas, United States*

A molecular cleft shaped ligand, aniosolbis(imine-hydroxyanisole) (ABIHA) has been designed and synthesized to enhance sensitivity for metal recognition via optical spectroscopy. Molecular cleft ABIHA was synthesized by coupling 3,4-diaminoanisole and 2-hydroxy-m-anisaldehyde in methanol. Incorporating imine moiety adjacent to phenolic hydroxyl group allows cleft shaped probe to form two new six-membered ring system through resonance-assisted hydrogen bonding (RAHB). In contrast, the purpose of incorporating electron donating methoxy group (- OCH_3) in each benzene ring is to build up positive inductive effect on imine-N and phenolic-H atoms to destabilize (weaken) the hydrogen bonding so that a minute amount of metal can disrupt the RAHB and metals can easily coordinate, hence sensitivity increases. In DMSO, the solution produced a blue color with a weak shoulder at 280 nm and a broad absorption band at 350 nm and emission at 474 nm (λ_{ex} = 345 nm). Upon addition of CH_3COO^- anion, no optical response observed both in UV-vis and fluorescence, suggest that there is no hydrogen bonding between imine and phenolic group or RAHB is extremely weak. Upon the addition of various metals, Zn^{2+}, Cd^{2+}, Hg^{2+}, Co^{2+}, and Cu^{2+} ions show optical response, absorption spectra 280 and 350 nm disappeared by red-shifting to three major area 305-325 nm, 359-369 nm, and 406-439 nm. The emission spectra at 474 nm ratiometrically shifted to 435 nm for Zn^{2+}, to 383 nm for Hg^{2+}, to 494 nm for Cd^{2+} and quenched for Cu^{2+} and Co^{2+} ions due to metal ligand charge transfer (MLCT) and chelation quenched fluorescence (CHQF) mechanism. Moreover, portable paper strip also constructed using filter paper (90 mm pore size) by dipping in ABIHA solution, and found that paper strip produced distinct colorimetric responses for Zn^{2+}, Cd^{2+}, Hg^{2+}, Co^{2+}, and Cu^{2+} ions which are observed under UV-lamp (365 nm).

SWRM 2026 SW339

Evaluation of dopant retention in carbothermally synthesized ZnO tetrapods

***Joshua Humphrey**, jchumphrey2004@gmail.com, John H. Brannon, Yuri Strzhemechny. Physics and Astronomy, Texas Christian University, Fort Worth, Texas, United States*

Metal oxide nanomaterials have received significant attention because their structural characteristics can be readily manipulated to produce desirable properties for a broad range of applications. Among the factors that influence their performance, morphology is particularly important, as changes in particle structure can affect properties such as surface area, reactivity, optical behavior, and electrical characteristics. Synthesis conditions therefore play an important role in determining the final structure and functionality of these materials. In addition to controlling morphology through synthesis, the properties of metal oxides can be further modified through doping. Zinc oxide (ZnO) is a well-studied material due to its versatility and the variety of structures that can be produced through different synthesis techniques. Among these structures, tetrapodal ZnO has attracted interest because of its distinctive three-dimensional geometry and potential applications in sensing, optoelectronics, and photocatalysis. The tetrapod structure can be produced using relatively straightforward vapor-phase synthesis techniques. In one established approach, zinc is heated to generate vapor, which subsequently reacts with oxygen to form ZnO. Another approach replaces metallic zinc with ZnO powder and introduces a carbon-based reducing agent, such as graphite, to promote the volatilization of zinc-containing species. These species can then react with oxygen during cooling and crystallization, resulting in the formation of ZnO tetrapods. Although carbothermal methods have been demonstrated for producing ZnO tetrapods, the starting material is generally an undoped ZnO. This

raises the question of whether dopants present in the ZnO precursor can survive the synthesis process and become incorporated into the resulting tetrapod structures. If successful, this approach could provide an alternative to post-synthesis doping, potentially simplifying the production of doped ZnO tetrapods while allowing the dopant to be introduced before morphological development occurs. Our objective is to investigate the feasibility of producing doped ZnO tetrapods through a carbothermal synthesis route using as the precursor doped ZnO powders synthesized hydrothermally. We characterize the resulting materials using several experimental techniques to establish whether precursor doping represents a practical alternative to conventional post-synthesis doping for ZnO tetrapods.

SWRM 2026 SW340

Host-guest complexation of pillar[6]arenes towards PFAS

***Gavin D. Harman**, gavindharmanb1@gmail.com, Xuxian He. Chemistry and Physical Sciences, Nicholls State University, Thibodaux, Louisiana, United States*

Per- and polyfluoroalkyl substances (PFAS) represent a rapidly growing global environmental concern due to their widespread use, extreme chemical stability, and persistence in water systems, where they are associated with adverse health effects. Supramolecular chemistry offers a promising strategy for the selective capture and removal of PFAS from contaminated water. In this study, sulfated pillar[6]arene—a macrocyclic host molecule with a robust multigram synthesis, well-defined cavity size, and electron-rich property—is investigated as a potential receptor for PFAS. Host–guest interactions between sulfated pillar[6]arene and various perfluoroalkyl acids are evaluated by determining binding constants using nuclear magnetic resonance (NMR) spectroscopy and isothermal titration calorimetry (ITC), while formation of well-defined complexes is further confirmed by single-crystal X-ray diffraction when possible. This work aims to establish a fundamental understanding of PFAS recognition by pillar[6]arene and to provide a foundation for the development of new materials for PFAS capture and water remediation.

SWRM 2026 SW341

pH-dependence of reduced graphene oxide membrane-based osmotic batteries

***Rayyah Shah**, rwshah@ualr.edu, Krishna Subedi, Wei Zhao. University of Arkansas at Little Rock, Little Rock, Arkansas, United States*

There is a global need for clean, renewable and sustainable energy. By using a semipermeable membrane in the salinity gradient interface, osmotic energy, also called blue energy, can be harvested as electricity, leading to an osmotic battery, a bioinspired mimic of electric eels. It can be utilized using sources of fresh and salt water, like captured rainwater over the ocean. We have recently developed NaCl-based osmotic batteries using reduced graphene oxide (RGO) forward osmosis membranes, operating at a neutral pH level. In this work, we have further studied how different pH levels of salt solutions would affect the performance of the osmotic batteries. Here, nanoporous RGO is synthesized by chemical oxidation of graphene oxide sheets with hydrogen peroxide, followed by hydrothermal reactions for tuning sheet pore sizes and sheet charge density. RGO membranes are prepared by vacuum filtration and are further thermally treated for controlled interlayer spacing for ion selectivity. A saturated NaCl solution is paired with a 100 mM NaCl solution

separated by a RGO membrane. The pH of the solutions is adjusted at different levels of 4-10. The ion transport properties and the osmotic energy generation efficiency of the osmotic battery devices at different pH levels are evaluated by current-voltage measurements under different loading resistances using two types of electrodes, Ag/AgCl and carbon cloth fiber. The relationships between output power density of the devices and solution pH levels will be presented and discussed in detail.

SWRM 2026 SW342

Electrophoretic deposition of barium titanate on carbon electrodes

***Meggan A. Collicelli**, meggancollicelli@my.unt.edu, Riju Suguna Robin, Saeed Hemmati, Teresa Golden. Chemistry, University of North Texas College of Science, Denton, Texas, United States*

The aim of this study is to determine the impact of polarization on the electrochemical interface of the front side carbon electrode when the backside surface has been coated with barium titanate ($BaTiO_3$) through electrophoretic deposition. $BaTiO_3$ was selected due to its ferroelectric properties, which allows the polarization to remain after the electric field has been removed. Initial multiphysics electrostatic simulations were conducted using COMSOL. The simulation demonstrated an increase in $BaTiO_3$ layer thickness leading to an increase in the induced potential. The simulation likewise showed that an increase in carbon electrode thickness reduces the electrostatic coupling from the back to the front of the electrode. $BaTiO_3$ coatings were deposited using both constant direct current (DC) potential and pulsed-DC potentials using a custom pulsing system. This system consists of a DC power supply, Transistor-Transistor Logic (TTL) interface, signal generator, and Metal Oxide Semiconductor Field Effect Transistor (MOSFET) switching board designed to control the frequency, voltage, and duty cycle of the deposition. Scanning electron microscopy was conducted prior to and after deposition. These results showed that electrophoretic deposition of $BaTiO_3$ under constant-DC potentials lack uniformity despite allowing for a thicker deposition. In comparison, electrophoretic deposition of $BaTiO_3$ under pulsed-DC potentials results in a thinner layer of deposition that is more uniform.

SWRM 2026 SW343

Investigation of pH-dependent static quenching of fluorescein by graphene oxide (GO) using steady-state and time-resolved techniques

***Daniel Kim**, kimdaniel124@gmail.com, Evan Cappucio, Alyson Trumbo, Rajesh Nayak. Chemistry, Physics & Engineering, Cameron University, Lawton, Oklahoma, United States*

Understanding the mechanisms governing fluorescence quenching in graphene oxide (GO)–fluorophore systems is essential for the rational design of fluorescence-based sensing, bioanalytical, and optoelectronic applications. Here, the pH-dependent fluorescence quenching of fluorescein by graphene oxide was systematically investigated using an integrated approach combining UV–Visible absorption spectroscopy, steady-state fluorescence spectroscopy, time-correlated single-photon counting (TCSPC), sphere-of-action modeling, and model-derived thermodynamic analysis. Fluorescence quenching was examined over the pH range of 3–11 using graphene oxide concentrations from 4 to 120 μg mL^{-1}. The highest quenching efficiency was observed at pH 3, with progressively lower quenching at pH 6, 7, and 11, demonstrating that solution pH strongly influences fluorescein–graphene oxide interactions.

SWRM 2026 SW344

Development of chemoselective reactions for amino acid sidechain for applications in protein sequencing

***Cannon Casey**, cannonball331@gmail.com, Calvin Heyl, Joseph A. Buonomo. Department of Chemistry, The University of Texas at Arlington, Arlington, Texas, United States*

A cell's proteome reflects its current functional state and shifts continuously in response to a range of different influences. A sensitive and quantitative characterization of this proteome would open a new window into cellular status that would offer a real value for discovering biomarkers and advancing molecular diagnostics, since reliable quantification is essential when protein levels change dynamically in complex diseases. Mass spectrometry remains the main approach today, but it comes with notable limitations. An alternative strategy tags amino acid residues with fluorescent tags and then applies successive Edman degradation steps to produce a fluorescence signal, but this approach suffers from poor stability and incomplete amino acid coverage. In response, our laboratory is developing a new approach to protein sequencing built on nanopore-based detection, which will involve designing amino acid-specific reactions to chemically barcode individual sidechains. For arginine, selectivity is achieved through a dicarbonyl group that forms a five-membered ring with the guanidinium group, yielding an imidazolone. Adding a "click" handle to this carbonyl-based probe further enables straightforward, arginine-specific barcoding.

SWRM 2026 SW345

Investigation of an alternative zinc binding affinity tag by experimental and computational methods

***Jessica Dall**[1], jtdall4@gmail.com, Rawan Siddig[1,2], Laurence A. Angel[1]. (1) Chemistry and Biochemistry, East Texas A&M University, Commerce, Texas, United States(2) The University of Texas at Dallas School of Natural Sciences and Mathematics, Richardson, Texas, United States*

To enhance our understanding of alternative metal binding affinity tags, a study was performed on a zinc binding peptide; acetyl-Cys_1-His_2-Gly_3-Pro_4-Tyr_5-His_6-Cys_7. Experimental methods such as ion mobility - mass spectrometry, HPLC, and UV-Vis spectrophotometry were used to evaluate its binding and elution from zinc chelating resins, used in the protein purification process of Immobilized Metal Affinity Chromatography (IMAC). The binding behavior was similar to the commonly used His-tag with the alternative affinity tag showing superior elution properties. This study also evaluated the alternative affinity tag's performance to two other isomeric peptides. A computational investigation of the peptides geometric structure, using a mix of semi-empirical and density functional theory methods, was applied to facilitate in understanding the architecture of the peptide and how that affects the peptide's zinc binding performance in relation to its isomers and the His-tag.

SWRM 2026 SW346

Molecular docking and microwave-assisted synthesis of imidazole derivatives as potential CYP51B inhibitors in *Aspergillus fumigatus*

***Mollie F. Wheeler**, mw958106@cameron.edu, Elizabeth A. Nalley. Chemistry, Cameron University, Lawton, Oklahoma, United States*

Imidazoles are a class of organic heterocyclic compounds containing a five-membered diazole ring ($C_3H_4N_2$), known for their critical role in biochemistry and extensive use in pharmacology. They serve as the foundational scaffold for numerous antifungal treatments. *Aspergillus fumigatus* is responsible for invasive aspergillosis, a severe infection affecting immunocompromised patients. Current azole drugs target sterol 14-α-demethylase (CYP51). However, increasing antifungal resistance has created the need for more effctive CYP51 inhibitors. This study investigated a series of substituted imidazole derivatives as protentional CYP51B inhibitors using microwave-assisted synthesis using a CEM reactor and molecular docking. Lophine and para-substituted methoxy, chloro and nitro derivatives were synthesized in yields ranging from 43.8 - 63.0% and characterized by infrared spectroscopy. Additional triphenyl and dimethyl imidazole derivatives were evaluated using AutoDock 4.2 against the, A. fumigatus CYP51B crystal structure (PDB ID: 5FRB). Binding energies, predicted inhibition constants (Ki), and Fe–N coordination distances were compared with the reference antifungal fluconazole. Triphenyl imidazole derivatives generally exhibited stronger predicted binding than the corresponding dimethyl imidazole's. The 4-chloro triphenyl derivative produced the most favorable binding energy, while the 4-methoxy derivative also demonstrated strong binding affinity. Nitro, methoxy, fluoro, hydroxy, and lophine derivatives all exhibited predicted nanomolar K_i values. Whereas the dimethyl imidazole's displayed weaker binding energies and micromolar Ki values. Successful synthesis and computation evaluation identified promising results for several substituted triphenyl imidazole's for further synthesis and biological evaluation as potential CYP51B inhibitors.

SWRM 2026 SW347

Development and protection of functionalized aminophenols for oxazaborole-based macrocycle synthesis

***Carlos Rea**, car207@shsu.edu, Dustin Gross, Bernard Mensah. Chemistry, Sam Houston State University, Huntsville, Texas, United States*

Dynamic covalent chemistry uses reversible covalent bonds to form stable molecular structures. Our group studies boron-containing dynamic covalent systems, including benzoxazaboroles, and their use in forming macrocycles and other molecular structures. Benzoxazaboroles are especially interesting because they undergo rapid exchange similar to dioxaborole systems, but have been studied less extensively.
Our current research focuses on developing aminophenol-based monomers for the exploration of benzoxazaborole oligomers and macrocycles. The synthesis of these aminophenol-based monomers would benefit from the use of a protecting group. Therefore, methods are being investigated to protect the neighboring amino and hydroxyl groups using simultaneously using 2,2-dimethoxypropane and acetone. Once the synthesis of the aminophenol monomers achieved, oxazaborole-based macrocycle synthesis will be pursued.

SWRM 2026 SW348

Development of a SPE-UPLC-MS/MS method for detection of steroid sex hormones in wastewater samples from wastewater treatment plants

*Kefa K. Onchoke, **Ben Lewis**, lewisbs2@jacks.sfasu.edu, Ken Fiffick, Jamie Humphries, Jack Weeks. Chemistry & Biochemistry, Stephen F Austin State University, Nacogdoches, Texas, United States*

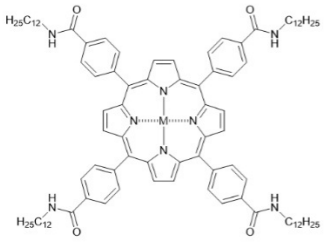
Seventeen commonly used sex hormones were quantified by using solid-phase extraction (SPE) technique and ultra-performance liquid chromatography with mass spectrometry detection (UPLC/MS/MS) in wastewater treatment plants. After solid-phase extraction, separation and quantification were done using a C_{18} analytical column, and gradient mobile phase consisting of ethylacetate/water at a flow rate of 0.5 mL/min. Analyte concentrations were detected simultaneously within 8 minutes with LOD and LOQ values of 0.2 and 0.5 ng/mL, respectively. Calibration curves based on integrated peak area counts gave satisfactory linearity ($R^2 \geq 0.9995$). The developed and validated method is useful for the detection of these emerging pollutants using triple quadrupole mass spectrometry. and is suitable for routine quantitative and qualitative analysis in wastewater and environmental samples.

SWRM 2026 SW349

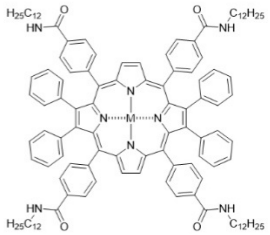
Synthesis and characterization of β-functionalized porphyrin liquid crystals

***Imad Al Naqeeb**[1,2], imad.alnaqeeb@gmail.com, Joshua Martinez[1], Prabha Sharma[1], Hong Wang[1], Xiaowei Wang[2], Akhila Joy[2], Xiao Li[2]. (1) Chemistry, University of North Texas College of Science, Denton, Texas, United States(2) Materials Science and Engineering, University of North Texas College of Engineering, Denton, Texas, United States*

Porphyrin liquid crystals (PLCs) are unique classes of functional materials, merging the photoactive, macrocyclic core of porphyrin with highly organized molecular ordering, with applications in optoelectronics, photovoltaics, and advanced functional materials. Despite their potential, PLCs struggle with macroscopic alignment and molecular aggregation, which reduces solubility. Most PLCs are based on *meso*-functionalized porphyrins, which have D_{4h} symmetry and possess rigid planar geometry, leading to limited packing diversity and severe aggregation. To address these issues, this project will introduce *β*-functionalized *π*-extended porphyrin into PLCs and compare them with *β*-unfunctionalized PLCs. Previous work in our group indicates *β*-functionalization and *π*-extension in porphyrins can introduce non-planar conformations and influences the electronic and photophysical properties. This work will include the synthesis of PLC1 bearing long aliphatic chains. These PLCs derived from *meso*-functionalized, *β*-unfunctionalized porphyrins will serve as the control PLCs. Then, PLC2 will be synthesized, and its liquid crystal characteristics will be evaluated. The molecular structures of the compounds will be determined using ^{1}H and ^{13}C NMR spectroscopy and single crystal X-ray diffraction. Photophysical properties will be studied through UV-vis and fluorescence spectroscopy. LC phases and phase transition temperatures will be identified through differential scanning calorimetry (DSC). Finally, liquid crystal morphology and defect topology will be studied through polarized optical microscopy (POM) and atomic force microscopy (AFM).



PLC1
M = 2H, Ni



PLC2
M = 2H, Ni

SWRM 2026 SW350

Synthesis of β-ketoester substrates and biocatalytic oxidations to access to α-acyloxy ketone scaffolds through biocatalytic Baeyer-Villiger oxidation

***Samantha Shannon**, sts033@shsu.edu, Natalie Salmeron, Claire Martinez, Meagan E. Hinze. Chemistry, Sam Houston State University College of Science & Engineering Technology, Huntsville, Texas, United States*

Selective oxidation at or proximal to carbonyl-containing compounds remains an important challenge in synthetic chemistry. A transformation of particular interest to our lab is the Baeyer-Villiger (BV) reaction, which converts ketones into esters or lactones. However, the process typically relies on harsh reagents such as peroxides or peracids which can present safety limitations and produce unwanted environmentally hazardous by-products. We have investigated an alternative, greener biocatalysis approach to the BV reaction by utilizing a family of enzymes known as Baeyer-Villiger Monooxygenases (BVMOs) to enable selective transformations under milder reaction conditions. We report the synthesis of a library of β-ketoester substrates with varied aromatic substituents and the potential of these scaffolds to access α-acyloxy carbonyl motifs. Authentic standards of the putative oxidation products will be generated through orthogonal routes when necessary. Additionally, initial studies comparing chemical and enzymatic oxidation outcomes will be disclosed.

SWRM 2026 SW351

Analysis and extraction of pesticides from biosolids

***Kefa K. Onchoke**, kefaon@yahoo.com, **Joe Kinnear-Meza**, kinnearmjo@jacks.sfasu.edu. Chemistry & Biochemistry, Stephen F Austin State University, Nacogdoches, Texas, United States*

Ten commonly used pesticides (atrazine, chlorothalonil, malathion, metolachlor, chlorpyrifos, permethrin, coumophos, 4,4'-DDT, paraquat, carbaryl) were quantified by using QuEChERS method (Quick, Easy, Cheap, Effective, Rugged, Safe extraction) technique and gas chromatography-quadrupole mass spectrometry in biosolids collected from wastewater treatment plants. After extraction, separation and quantification were done using a C_{18} analytical column, and a gradient temperature programming at a flow rate of 1 mL/min, and column oven ramped from 110 °C to at 300 °C. All analyte concentrations were detected within 45 minutes and gave LOD and LOQ values between 0.1 ng/g - 2 ng/g, and 0.39 ng/g to 1.5 ng/g, for most pesticides, respectively Calibration curves based on integrated peak area counts gave satisfactory linearity ($R^2 \geq 0.9998$). This method

provides low detection and sensitivity for pesticides and is deemed best suited for analysis in wastewater treatment plants (WWTPs). The developed and validated method is useful for low concentration levels with mass spectrometry, and is suitable for quantitative and qualitative analysis of pesticides in wastewater and environmental samples.

SWRM 2026 SW352

Varying linear solvation energy relationship descriptors using fentanyl surrogates and analogs for supercritical fluid chromatography

***Elijah D. Almanza**, elijah.almanzamacias03@gmail.com, Richard McCrary, Teresa D. Golden. Chemistry, University of North Texas System, Denton, Texas, United States*

The surge of fentanyl use along with its' analogs have persisted over the past decade, resulting in many casualties caused by overdosages in the United States. Such is the case for markets that procure fentanyl analogs that differ slightly in chemical structure, with each configuration of the parent structure influencing unique physiochemical properties, pharmacological activity, and chromatographic behavior. Supercritical fluid chromatography (SFC) is known for its efficient separations and is becoming increasingly favored in pharmaceutical applications. However, basic drugs prove difficult to separate in SFC and analogs provide an even greater challenge. Many of these fentanyl analogs share a structural framework but differ slightly in their composition. These minute differences present a significant analytical challenge when attempting to achieve chromatographic separation. This emphasizes the need for a reliable and efficient model to characterize interactions to predict the retentions of each compound. This study uses SFC with an isocratic mobile phase and the Abraham solvation model to describe and characterize fentanyl analogs. The chromatographic conditions employed are a CO_2 and methanol mixture without an additive and five different stationary phases, including silica, pentafluorophenyl, cyano, amine, and C18. Under the chromatographic conditions of the method, fentanyl and several of its analogs were characterized revealing a mechanistic understanding of retention in SFC and helps to establish LSER modeling as a tool for reducing empirical method development in the separation of closely related fentanyl analogs.

SWRM 2026 SW353

Total phenolic content and antioxidant capacity of white teas from different geographic origins

***Graciela Gonzalez**, graciela.gonzalez@cameron.edu, Kandalama Priyasantha. Chemistry, Physics and Engineering, Cameron University, Lawton, Oklahoma, United States*

White tea is a minimally processed tea containing naturally occurring phenolic compounds that may contribute to its antioxidant properties. Although white teas are produced in several regions of the world, variations in growing environment, cultivar, and processing may result in differences in their chemical composition and antioxidant activity. This study evaluates and compares the total phenolic content and antioxidant capacity of white teas originating from different geographic regions.
White tea samples were prepared using a standardized hot-water extraction procedure. Total phenolic content (TPC) was determined using the Folin–Ciocalteu assay, while antioxidant capacity was evaluated using the ferric reducing antioxidant power (FRAP) assay. Calibration standards were

used for quantitative analysis, and replicate measurements were performed to assess experimental variability. Results from both assays were compared across the different white tea samples, and the relationship between total phenolic content and antioxidant capacity was evaluated.
Variations in TPC and FRAP responses among the samples demonstrate differences in the chemical and antioxidant properties of white teas from different geographic origins. Correlation of TPC with FRAP measurements provides additional insight into the contribution of phenolic compounds to the overall reducing capacity of the tea extracts. This study provides a comparative assessment of global white teas and establishes a foundation for identifying individual compounds responsible for differences in antioxidant activity.

SWRM 2026 SW354

Influence of growing environment on the phenolic profile of Sri Lankan tea: An HPLC study

***Felicity Gomez**, felicity.godwins@cameron.edu, Kandalama Priyasantha. Chemistry, Physics and Engineering, Cameron University, Lawton, Oklahoma, United States*

Tea (*Camellia sinensis*) contains a complex mixture of phenolic compounds that contribute to its chemical characteristics and potential biological properties. The composition of these compounds can be influenced by environmental factors such as elevation, temperature, rainfall, and growing conditions. Sri Lankan tea is cultivated across geographically diverse regions, ranging from warm, low-elevation areas to cooler, high-elevation regions traditionally associated with tea production. This study investigates whether these contrasting growing environments influence the phenolic composition of Sri Lankan tea.
Tea samples representing lowland and highland growing regions of Sri Lanka were extracted using a standardized hot-water extraction procedure and analyzed by high-performance liquid chromatography with photodiode array detection (HPLC-PDA). Reference phenolic standards were analyzed under the same chromatographic conditions to establish retention times and calibration curves for identification and quantification of selected compounds. Chromatographic profiles of the tea extracts were compared to evaluate differences in the occurrence and abundance of phenolic compounds between growing regions.
Differences observed among the chromatographic profiles indicate chemical variation among Sri Lankan teas grown under contrasting environmental conditions. Quantitative analysis of selected phenolic compounds provides an opportunity to determine whether these differences are associated with growing region and elevation. This research contributes to understanding how environmental growing conditions may influence the chemical composition of Sri Lankan tea and provides a foundation for identifying teas with distinctive phenolic profiles.

SWRM 2026 SW355

Comparative HPLC analysis of phenolic compounds in white teas from different geographic origins

***Lydia Park**, lydia.park@cameron.edu, Felicity Gomez, Kandalama Priyasantha. Chemistry, Physics and Engineering, Cameron University, Lawton, Oklahoma, United States*

White tea, produced from the young leaves and buds of *Camellia sinensis*, undergoes relatively limited processing compared with many other tea types. This minimal processing may preserve

naturally occurring phenolic compounds; however, differences in geographic origin, environmental growing conditions, cultivar, and processing practices may contribute to variation in chemical composition. This study compares the phenolic profiles of white teas originating from different regions of the world using high-performance liquid chromatography (HPLC).
White tea samples representing different geographic origins were extracted using a standardized hot-water extraction procedure. Following filtration, the extracts were analyzed by reversed-phase HPLC with photodiode array (PDA) detection. Phenolic reference standards were used to establish retention times and calibration curves for the identification and quantification of selected compounds. In addition to targeted analysis, chromatographic fingerprints were compared among samples to evaluate broader differences in phenolic composition.
Variation in chromatographic profiles among the white tea samples demonstrates that teas classified as the same general type can exhibit distinct chemical compositions. Differences in the presence and relative abundance of individual phenolic compounds may reflect geographic, environmental, or processing-related factors. This study provides insight into the chemical diversity of white teas from different regions and establishes a foundation for investigating relationships between specific phenolic compounds and the antioxidant properties of white tea.

SWRM 2026 SW356

Harnessing microalgal functionality in cellulose nanofiber films for sustainable functional materials

*Balasubramanian Rukmanikrishnan[1], Kaden Teague[2], **Ning Zhang**[1], ning_zhang@baylor.edu. (1) Mechanical Engineering, Baylor University, Waco, Texas, United States(2) Biology, Baylor University, Waco, Texas, United States*

Nature produces chemically complex biological systems with intrinsic optical, antioxidant, and interfacial functionalities that are difficult to reproduce using conventional synthetic materials. Harnessing these naturally encoded functions offers an intriguing strategy for engineering sustainable materials that provide functionality beyond structural performance. Here, we integrate cellulose nanofibers (CNFs) with whole *Chlorella* microalgal biomass to create renewable, multifunctional biocomposite films through a simple aqueous casting process. CNFs provide a mechanically robust, high-aspect-ratio fibrillar framework, while *Chlorella* introduces a chemically diverse biological phase containing proteins, polysaccharides, pigments, and other naturally occurring functional components. The resulting CNF–*Chlorella* composites form self-standing films whose morphology, mechanical behavior, moisture response, thermal stability, and optical properties can be systematically tuned through microalgae incorporation. Notably, incorporation of *Chlorella* introduces strong UV-shielding functionality while preserving the structural integrity of the CNF network, demonstrating that the intrinsic biochemical complexity of whole microalgal biomass can be directly translated into macroscopic material functionality. The relationships among *Chlorella* content, CNF–microalgae interactions, mechanical performance, UV shielding, antioxidant activity, barrier behavior, and biodegradability are further investigated. These findings establish a simple strategy for transforming photosynthetic biomass into functional components of engineered nanocellulose materials, opening opportunities for sustainable UV-protective interfaces, optical and chemical sensors, wearable and biointegrated devices, and other light-responsive functional materials.

SWRM 2026 SW357

Determination of phosphate in soil extracts in Lower Barnett Shale: A green chemistry enzymatic method

***Elsie Kambili Okoye**, eko2205@hsutx.edu, Sabrina Nelson, Michelle Dose, Steven Rosscoe. Midwestern State University, Wichita Falls, Texas, United States*

A project is currently being undertaken to study the lithological and faunal elements of the Lower Barnett Shale Unit at San Saba, TX and the Upper Salesville Shale Unit at Mineral Wells, TX. The lower Barnett Shale is known to contain natural gas deposits and it is our hope that we will be able to find one or more easily measured lithological and/or faunal features that correlate to the viability of certain formations for gas exploration. Several studies have already been completed on the Lower Barnett Shale, including total organic carbon by loss on ignition, total number of conodont elements, and gamma ray detection. In this project we describe the analysis of the phosphate content of the outcrop, following the procedure of Campbell and Warsko. This procedure utilizes a portable enzymatic method for the determination of phosphate in soil extracts using a low-volume reagent system designed according to principles of green chemistry. This method requires less than 1 mL of total reagent per analysis and generates substantially less chemical waste. These results demonstrate the potential of an enzyme-based colorimetric approach as a rapid, low-waste method for phosphate screening directly in the field.

SWRM 2026 SW358

Metal-ion-mediated assembly of ambient-dried cellulose nanofiber–spirulina biofoams

*Balasubramanian Rukmanikrishnan[2], **Isabelle Maki**[3], Isabelle_Maki1@baylor.edu, Ning Zhang[1]. (2) Mechanical Engineering, Baylor University, Waco, Texas, United States(3) Chemistry, Baylor University, Waco, Texas, United States*

The convergence of sustainability and biology is creating new opportunities to transform renewable biological building blocks into high-performance functional materials. However, constructing lightweight and mechanically robust porous materials from biomass remains challenging because nanofibrillar networks are susceptible to aggregation, shrinkage, and structural collapse during drying. Here, we report a rapid and scalable strategy to fabricate cellulose nanofiber (CNF)–microalgae biofoams through metal-ion-mediated crosslinking followed by ambient drying. CNFs provide a high-aspect-ratio fibrillar framework with abundant surface functionality, while protein-rich *Spirulina* introduces a chemically diverse renewable biomass phase with strong adhesive characteristics. Metal-ion interactions reinforce the hybrid network, enabling the formation of lightweight, self-supporting porous architectures under ambient conditions without the energy-intensive drying processes commonly required for nanocellulose foams. Remarkably, the resulting CNF–Spirulina biofoams simultaneously exhibit low density, high compressive strength, excellent water stability, and resistance to direct flame exposure while retaining structural integrity. Systematic variation of composition and metal-ion interactions reveals their important roles in regulating network stability and macroscopic performance. This work demonstrates how chemical interactions between complementary biological building blocks can be harnessed to engineer robust hierarchical porous materials through energy-efficient processing, providing a versatile platform for sustainable functional materials with potential applications spanning thermal management, environmental technologies, energy devices, and biointegrated systems.

SWRM 2026 SW359

Synthesis, characterization, and cytotoxic assessment of dinuclear copper(II) complexes targeting triple-negative breast cancer

Isaac Borrego[1]*, iborrego@student.uiwtx.edu, Hadi D Arman*[2]*, Rafael A. Adrian*[1]*. (1) Department of Chemistry and Biochemistry, University of the Incarnate Word, San Antonio, Texas, United States(2) Department of Chemistry, The University of Texas at San Antonio, San Antonio, Texas, United States*

Triple-negative breast cancer (TNBC) lacks estrogen, progesterone, and HER2 receptors, leaving it without access to hormonal or HER2-targeted therapies and among the most difficult breast cancer subtypes to treat. Platinum-based chemotherapeutics such as cisplatin remain widely used but are limited by severe, non-specific toxicity, including nephrotoxicity, ototoxicity, and myelosuppression. Copper(II) complexes offer a promising alternative, exhibiting anticancer activity through DNA intercalation, redox cycling, and reactive oxygen species (ROS) generation, and dinuclear copper species bridged by phenanthroline- or bipyrimidine-type ligands are of particular interest, since cooperative action between two proximal copper centers can strengthen DNA binding and amplify oxidative DNA damage. In this work, a library of six dinuclear copper(II) complexes incorporating substituted phenanthroline and bipyridine ligands—including 1,10-phenanthroline, 1,10-phenanthroline-5,6-dione, 4,4′-dimethoxy-2,2′-bipyridine, 5-chloro-1,10-phenanthroline, 2,2′-bipyridine, and 4,4′-di-tert-butyl-2,2′-bipyridine—was synthesized in moderate to good yields (38–89%). FT-IR spectroscopy confirmed ligand coordination for all complexes through characteristic C=N and C=C stretching frequencies, and single crystals of complexes 1 and 3, grown by vapor diffusion of diethyl ether into acetonitrile solutions, were analyzed by X-ray diffraction to establish their solid-state structures. These results provide a synthetic and structural foundation for evaluating the potential as chemotherapeutic agents of dinuclear copper(II) complexes.

SWRM 2026 SW360

Synthesis and characterization of palladium(II) complexes with phenanthroline and bipyridine ligands for selective cytotoxicity against triple-negative breast cancer

Natalia Aguilar[1]*, naaguil1@student.uiwtx.edu, Hadi D Arman*[2]*, Rafael A. Adrian*[1]*. (1) Department of Chemistry and Biochemistry, University of the Incarnate Word, San Antonio, Texas, United States(2) Department of Chemistry, The University of Texas at San Antonio, San Antonio, Texas, United States*

Triple-negative breast cancer (TNBC) is an aggressive subtype lacking estrogen, progesterone, and HER2 receptors, leaving few targeted treatment options; metastatic cases carry a median survival of only 8–13 months. Platinum-based chemotherapeutics such as cisplatin remain central to cancer treatment but are limited by significant toxicities, including nephrotoxicity, ototoxicity, and myelosuppression. Palladium(II) complexes offer a structurally analogous but potentially safer alternative, and nitrogen-donor phenanthroline and bipyridine ligands—whose planar aromatic frameworks enhance metal complex stability, cellular uptake, and DNA interaction—were incorporated to improve the selectivity and potency of palladium-based agents against TNBC. A series of six palladium(II) complexes bearing substituted phenanthroline and bipyridine ligands, including 4,4′-di-tert-butyl-2,2′-bipyridine, 1,10-phenanthroline, 4,7-dimethoxy-1,10-phenanthroline, 5-chloro-1,10-phenanthroline, 4,4′-dimethoxy-2,2′-bipyridine, and 2,2′-bipyridine, was synthesized in moderate to excellent yields (48–95%). Infrared spectroscopy confirmed ligand coordination through characteristic shifts in C=N and C=C stretching frequencies, and single-crystal X-ray diffraction of complex 4 confirmed a distorted square-planar Pd(II) geometry, with two bidentate nitrogen-donor

ligands occupying all inner coordination sites. These complexes are proposed to interact with DNA and induce redox-mediated oxidative stress, and are being evaluated for cytotoxicity against HCC1806 TNBC cells to assess their potential as selective, targeted chemotherapeutic candidates.

SWRM 2026 SW361

Design and characterization of heteroleptic copper complexes for enhanced antitumor activity with reduced side effects

Stefina M. Cortese[1]*, cortese@student.uiwtx.edu, Hadi D Arman*[2]*, Rafael A. Adrian*[1]*. (1) Department of Chemistry and Biochemistry, University of the Incarnate Word, San Antonio, Texas, United States(2) Department of Chemistry, The University of Texas at San Antonio, San Antonio, Texas, United States*

Cisplatin and related platinum drugs such as oxaliplatin remain mainstays of chemotherapy but are limited by toxicity, resistance, and poor selectivity. Copper(II) complexes offer a promising alternative given their biological relevance, redox activity, and potential for lower systemic toxicity, and bipyridine-based ligands allow precise tuning of the structural and electronic properties of these complexes. In this work, a series of heteroleptic copper(II) complexes was synthesized incorporating 4,4′-dimethyl-2,2′-bipyridine as an ancillary ligand alongside systematically substituted bipyridine ligands—2,2′-bipyridine, 4,4′-dimethoxy-2,2′-bipyridine, and 4,4′-di-tert-butyl-2,2′-bipyridine—with the hypothesis that this ligand design would enhance complex stability, cellular uptake, and redox activity relative to cisplatin. Four complexes were obtained in good to excellent yield (28–86%) and characterized by infrared spectroscopy and elemental analysis; IR spectra confirmed ligand coordination through comparison of C=N and C=C stretching frequencies between the free ligands and their corresponding complexes. Single-crystal X-ray diffraction of complex 1 revealed a five-coordinate Cu(II) center in a distorted square-pyramidal geometry, with two triflate counterions occupying elongated axial positions. Crystal packing and Hirshfeld surface analysis further characterized the intermolecular contacts governing the solid-state structure. Together, these results establish a structurally diverse series of heteroleptic copper complexes as candidates for evaluating structure–activity relationships and anticancer potential relative to cisplatin.

SWRM 2026 SW362

Preparation of very pure osajin and pomiferin for testing against cultured pancreatic cancer cells

Garrett Heimann*, garrett.heimann@go.tarleton.edu,* ***Jacob Rasmussen****, jacob.rasmussen@go.tarleton.edu, Joseph Dulaney, Timyee Leung, Rajani Srinivasan, William L. Whaley. Chemistry, Tarleton State University, Stephenville, Texas, United States*

Osajin and pomiferin are two prenylated isoflavones produced in the fruit of Osage orange, a species that is native to central Texas. At micromolar concentrations, both isoflavones kill cultured pancreatic cancer cells (PANC-1) and lung cancer cells (A549) within a 48-hour period. When these agents are grafted onto carbohydrate polymers obtained from fenugreek, the delivery to cultured cancer cells is dramatically improved. A protocol using deactivated silica was developed for an efficient separation and recovery of osajin and pomiferin, each at 95% purity or greater. An Alumina B miniature column was used to remove traces of pomiferin from samples of osajin. A silica miniature column was used to

remove traces of osajin from samples of pomiferin. The cleanup columns provided very high purity isoflavones for testing the anti-tumor activities. Pomiferin exhibited an IC_{50} value of about 5 micromolar while osajin exhibited a higher IC_{50} value of about 25 micromolar. When pomiferin was grafted to galactomannan polymer (isolated from fenugreek), and the IC50 value was used in PANC-1 cultures, a 98% kill rate was obtained. Osajin has been reported to promote apoptosis while pomiferin was reported to be an inducer of autophagy. It has been reported that osajin and pomiferin have a synergistic activity against cultured neuroblastoma cells. Osajin and pomiferin are now being tested for synergistic activity against PANC-1 cells which are known to develop resistance to many anti-cancer agents including doxorubicin. (This research was sponsored by the 2025 Tarleton PERS Program and by the Welch Foundation Departmental Research Grant Program AS-0012).

SWRM 2026 SW363

Extraction, isolation, and cytotoxic evaluation of gaillardin from West Texas *Gaillardia pulchella*

***Sophia Peltier**, peltier.sophia@mcm.edu. McMurry University, Abilene, Texas, United States*

Gaillardin is a naturally occurring sesquiterpene lactone isolated from the flowering plant Gaillardia pulchella; it is known to exhibit antibiotic and cytotoxic activity. Gaillardia pulchella is commonly known as “Indian blanket” and grows natively in West Texas. The principal goals of this project include (1) developing an updated method for the extraction, isolation, and purification of gaillardin from the plant source, and (2) assaying for cytotoxic effects against various human cancer cell lines. Former methods to extract gaillardin from the plant involve the use of dichloromethane and/or chloroform. In this project, plant material was soaked in hexane and ethyl acetate, and further purification was achieved using column chromatography. Collected fractions were characterized using gas chromatography - mass spectrometry (GC-MS), infrared spectroscopy (IR), and proton nuclear magnetic resonance spectroscopy (1H NMR). Chromatographic separation produced a gaillardin-enriched fraction comprising >80%, as determined by GC-MS chromatographic area, and a second fraction indicated a second compound with similar chromatographic behavior. Cytotoxicity of fractions was measured using resazurin-based cell viability assays against human cancer cell lines MDA-MB-231, MCF-7, A375, and G361. Both compounds demonstrated cytotoxic activity, with the gaillardin-enriched fraction displaying greater potency. Half-maximal cytotoxic concentration (CC50) values for the gaillardin-containing fraction suggest values as low as 25 μM. Future experiments include obtaining improved isolation of the compounds, structural characterization of the second compound, and better-defined CC50 values for both.

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Fluorescence quenching dynamics and photophysics of rhodamine 6G dyes in confined reverse micelle environment in graphene oxide nanocolloid (GOnc) using steady state and time-resolved fluorescence techniques

***Evan Capuccio**, evan.capuccio@cameron.edu, Rajesh Nayak. Chemistry, Physics and Engineering, Cameron University, Lawton, Oklahoma, United States*

Fluorescence quenching and photophysical dynamics of Rhodamine 6G (R6G) were investigated using steady-state UV-Vis and fluorescence as well as Time-resolved photoluminescence (TRPL)

streak camera tracking and Dynamic Light Scattering (DLS) in both aqueous and reverse micelle environment. Our results show that Upon titration with GOnc, open bulk water exhibits unhindered ground-state dimerization, severe hypochromic band broadening, a continuous red-shift in aggregate emission, and rapid, quantitative fluorescence quenching below 60 ug/mL. Conversely, encapsulation within micellar droplets provides robust macroscale shielding that prevents complete emission deactivation even at 132 ug/mL. Time-resolved photoluminescence (TRPL) streak camera tracking result show that the R6G dye undergoes predominantly static quenching where as in reverse micelles, the R6G dyes undergo both static and dynamic quenching.

SWRM 2026 SW365

Stereochemically defined cyclohexylamide scaffolds as chiral peptidomimetics for mimicking α-helical surfaces

***Julia Floyd**, dal578045@utdallas.edu. Chemistry, The University of Texas at Dallas, Richardson, Texas, United States*

α-Helix–mediated protein-protein interactions are difficult to inhibit because they require exact replication of native side-chain orientation and spacing. Current helix mimetics provide rigidity but lack predictable stereochemical control and adjustable side chain positioning. However, we've developed chiral cyclohexylamide scaffolds that uniquely combine structural rigidity with precise placement of side chains, enabling accurate imitation of α-helical patterns. These scaffolds, composed of stereodefined tri-substituted cyclohexanecarboxylic acids, are modular and span the i, i+4, i+7, and i+11 positions of three helical turns. Through regio- and stereoselective bromo-lactonization, eight different cyclohexane stereoisomers were synthesized and assembled into oligomers, cyclohexylamide oligomers, capable of selectively disrupting protein-protein interactions. These scaffolds were used to mirror the BH3 domains of pro-apoptotic Bcl-2 proteins and induce apoptosis. They were made to engage the 3-4 helical turn hydrophobic pocket in anti-apoptotic Bcl-2 proteins like Bcl-xL, where extended scaffolds can maximize molecular contacts, strengthening both binding affinity and biological activity.

SWRM 2026 SW366

Optimization of ZnO electrodeposition on stainless steel mesh for photoelectrochemical applications

***Charles Bonagura**, cbonagura@udallas.edu, Ellen Steinmiller. Chemistry, University of Dallas, Irving, Texas, United States*

Zinc oxide is a wide-bandgap semiconductor with applications in photoelectrochemical and photocatalytic systems. In this study, ZnO was electrochemically deposited onto stainless steel mesh electrodes, and the effects of deposition conditions on the photoelectrochemical response of the resulting electrodes were investigated. Electrodeposition parameters, including deposition time, applied potential, and precursor concentration, were systematically varied to evaluate their influence on ZnO formation and photocurrent response. Photocurrent measurements using a Xe arc lamp were used to evaluate the photoactivity of the deposited ZnO films and compare the performance of electrodes prepared under different deposition conditions.

SWRM 2026 SW367

Unlocking edge-site activity in MNenes for green electrochemical ammonia production

***Joshua Ferguson**, joshua.ferguson@tamu.edu. Artie McFerrin Department of Chemical Engineering, Texas A&M University, College Station, Texas, United States*

The electrochemical Nitrogen Reduction Reaction (NRR) is a promising pathway towards the sustainable production of ammonia utilizing atmospheric nitrogen and water under mild conditions. However, low yield and selectivity of current catalysts resulting from the thermodynamic stability of Nitrogen and competition with the parasitic Hydrogen Evolution Reaction (HER) limit the widespread implementation of this technology. An emerging class of 2D materials, Nitride MXenes (MNenes), have attracted considerable interest as electrocatalysts due to their ability to facilitate NRR through a Lattice Nitrogen Mediated Pathway. While the lattice nitrogen-mediated pathway has been established as a mechanism for ammonia production on MNenes, the influence of particle size and the resulting density of exposed edge sites on NRR performance has yet to be systematically investigated. This work seeks to address this gap by examining the relationship between particle size, edge-site availability, and catalytic activity. To investigate this relationship Ti2NTx, Ti4N3Tx, and Ti3CNTx MNenes were bath-sonicated for varying durations to modify particle size distribution and expose edge sites. Resulting samples were then characterized using laser diffraction and electrochemically tested for NRR.

SWRM 2026 SW368

Evaluation of a Cu(II) salophen complex for Chan-Lam C-N coupling

***Ansh Chugh**, anchugh@ttu.edu, Xander Duke, Anne E. Gorden. Department of Chemistry & Biochemistry, Texas Tech University, Lubbock, Texas, United States*

Carbon–nitrogen bond formation through cross-coupling is a foundational transformation in organic synthesis, with broad importance in pharmaceutical and materials chemistry. Although simple copper salts are commonly employed in Chan–Lam coupling, well-defined ligand-supported copper complexes offer opportunities to control the coordination environment and tune the reactivity of the metal center. This project investigates whether a Cu(II) salophen complex can serve as an effective catalyst for the oxidative coupling of amines with arylboronic acids. The rigid, tetradentate salophen framework provides a well-defined coordination environment and represents a potentially robust and tunable platform for Chan–Lam catalysis. Using aniline and phenylboronic acid as model substrates, GC-MS analysis indicated moderate-to-high conversion to diphenylamine under relatively mild conditions using acetonitrile as the solvent, one equivalent of triethylamine as the base, and heating at 60 °C for 24 h. Ongoing work focuses on optimizing the base, solvent, catalyst loading, temperature, reaction time, reactant stoichiometry, and atmospheric conditions. The optimized system will then be evaluated with additional amines and arylboronic acids to investigate substrate scope, functional group tolerance, and selectivity. This work seeks to establish a new catalytic application for the Cu(II) salophen scaffold and expand the range of well-defined copper complexes used for Chan–Lam C–N bond formation.

SWRM 2026 SW369

Towards the synthesis of Zn-Oxy-DPA-Diiodo-BODIPY photosensitizer for intracellular photodynamic therapy

***Michael P.**, michaelpuste@gmail.com, Emily Osborn, Miguel Gaspar, Jeremiah J. Gassensmith. School of Natural Science and Mathematics, The University of Texas at Dallas, Richardson, Texas, United States*

Many bacterial pathogens exploit niches in host cells to evade their immune system and proliferate. Among these bacteria, uropathogenic Escherichia coli (UPEC) is the most common culprit for urinary tract infections (UTIs). Equipped with an array of virulence factors, UPEC can successfully invade, persist, and multiply inside bladder epithelial cells. In an era of escalating antibiotic resistance, there is an urgent need for novel treatments that can access intracellular niches. Boron-dipyrromethene (BODIPY) derivatives are well-studied compounds for photodynamic therapy (PDT). Those which incorporate heavy atoms like iodine shift the excited-state relaxation pathway toward nonradiative intersystem crossing. This triplet-state population allows the photosensitizer to generate reactive oxygen species (ROS) upon irradiation. Zinc(II) 2,2′-dipicolylamine (Zn-DPA) complexes exhibit a strong affinity for the negatively charged membranes of both Gram-positive and Gram-negative bacteria. However, Zn-DPA complexes cannot permeate intact mammalian cell membranes, limiting their usage. Modifying this scaffold with an oxygen bridge yields Zn-Oxy-DPA, which readily permeates the membrane while strongly targeting bacteria through distinct coordination and electrostatic interactions. Previously, researchers coordinated diiodo-BODIPY with Zn-DPA to synthesize an efficient antimicrobial photosensitizer. Because the probe could not enter infected host cells, we designed a synthesis which incorporates Zn-Oxy-DPA to explore its efficacy as an intracellular bacterial PDT treatment. Herein, we report the successful completion of the initial synthetic steps establishing the separate BODIPY core and Zn-Oxy-DPA targeting unit. Future work includes the conjugation of these components to assemble the complete probe, followed by in vitro PDT assays to evaluate its efficiency in eliminating intracellular UPEC.

SWRM 2026 SW370

Bridging the gap: Ligand-directed assembly of dinuclear palladium phenanthroline complexes

***Muqtadir Musharaf**[1], musharaf@student.uiwtx.edu, Hadi D Arman[2], Rafael A. Adrian[1]. (1) Department of Chemistry and Biochemistry, University of the Incarnate Word, San Antonio, Texas, United States(2) Department of Chemistry, The University of Texas at San Antonio, San Antonio, Texas, United States*

Platinum-based chemotherapeutics such as cisplatin remain among the most widely used anticancer agents, but their clinical utility is limited by dose-dependent toxicity and acquired resistance. Palladium(II) complexes offer a structurally versatile and highly tunable alternative platform, and dinuclear architectures—in which two metal centers may act cooperatively—are of particular interest for their potential to enhance biological activity relative to mononuclear analogs. In this work, a series of phenanthroline-based palladium(II) complexes was synthesized using 1,10-phenanthroline and its 4,7-dichloro, 4,7-dimethoxy, and 5,6-dimethyl derivatives, together with ethylenediamine, as ancillary ligands, with 2,2′-bipyrimidine employed as a bridging ligand to direct assembly of well-defined dinuclear Pd(II) cores. The complexes were isolated in modest yields (11–25%) and characterized by infrared spectroscopy, elemental analysis, and single-crystal X-ray diffraction. Infrared spectra showed characteristic shifts in C=N and C=C stretching modes consistent with coordination of the

bipyrimidine bridge to the metal centers, and the crystal structure obtained for one complex confirmed a dinuclear, tetraanionic architecture in which each palladium center adopts the expected square-planar geometry, symmetrically bridged by 2,2′-bipyrimidine. Hirshfeld surface analysis and crystal packing studies were used to further probe the intermolecular interactions governing solid-state assembly. Together, these results establish a synthetic and structural foundation for evaluating this class of dinuclear palladium complexes as potential anticancer agents.

SWRM 2026 SW371

Photopolymerization, characterization and aquatic toxicity of PEDOT

***Neetika Sainju**, sainju.neetika@mcm.edu, Edward G. Donnay, Terrence Boyle. Biology and Biochemistry, McMurry University, Abilene, Texas, United States*

PEDOT (poly(3,4-ethylenedioxythiophene) is a commercially available conductive polymer used in electronic and biomedical applications. A “cradle to grave” appraisal of the environmental effects of the polymer was undertaken. A green synthesis of PEDOT was evaluated by attempting both traditional chemical oxidation and a photopolymerization method. Different light conditions for the photopolymerization were attempted including daylight, blue, yellow, and red light and compared to a no-light control. The obtained materials were characterized using FTIR, UV-Visible spectroscopy, steady state emission spectroscopy, ^{1}H NMR, and SEM and then compared with the literature. Furthermore, the potential effects of PEDOT on aquatic organisms have not been fully explored. Preliminary toxicity was studied using the estuarine crab *Rhithropanopeus harrisii*, the white fingered mud crab, as they are known bioindicators for toxicity. The crabs were exposed to 1:1 mixture of commercial PEDOT:PSS (poly(styrenesulfonate)) and saline solution which resulted in rapid mortality. Preliminary findings suggest that exposure to concentrated PEDOT may pose risks to aquatic organisms if there is an accidental environmental release.

SWRM 2026 SW372

Synthesis of porphyrin-based receptors for perfluoroalkyl substances (PFAS)

***Kharese Alexander**, kharesealexander@gmail.com, Stephen Starnes. Chemistry, East Texas A&M University, Commerce, Texas, United States*

This project describes the synthesis and analysis of porphyrin-based sensors for perfluoroalkyl substances (PFAS). The sensing apparatus utilizes supramolecular host- guest chemistry, wherein porphyrins (the hosts) are modified to selectively bind to a PFAS (guest). Porphyrin is used as the structural base due to its ease of modification and strong absorbance in UV-Vis. Upon complexation, a spectral shift is observed, allowing for the determination of efficacy and selectivity of the host-guest interaction. The host design includes a fluorinated arm derived from perfluorooctanoic acid (PFOA)– which is intended to promote host-guest interaction by catering to PFAS fluorophilicity. As fluorocarbon chains exhibit hydro- and lipophobicity, the fluorinated arm further serves to reduce binding interactions between host and hydrocarbon-based guests. The center cavity of the porphyrin was metalated with zinc to improve coordination with the PFAS guests, where the guest is bound via non-covalent hydrogen bonding, metal-coordination and fluorophilic interactions. Characterization of hosts was achieved via ^{1}H-NMR and ^{19}F-NMR, and Electrospray Ionization Mass Spectrometry (ESI-MS). Selectivity of the synthesized hosts was determined through the comparison of association

constants (K_a) with tetrabutylammonium salts of perfluorooctanoic acid (PFOA) and octanoic acid using UV-Vis spectrophotometric titration. The hosts exhibited association constants averaging 2-3 times larger when titrated with the fluorinated anion as compared to the non-fluorinated anion. The 2-3 fold increase in binding favoring the perfluoro guest indicates perfluoro selectivity, considering that octanoate anion is recognized as a significantly stronger base and would be expected to more readily hydrogen bond and coordinate the metal. Such findings support the host design and demonstrate the potential for effective porphyrin-based PFAS detection.

SWRM 2026 SW373

Synthesis of square planar pincer ligand transition metal complexes

***Alexander Jimenez**, alex.j.rdrgz@gmail.com, **Leah Autry**, lautry@stedwards.edu, Jackson Reyna. Chemistry, Saint Edward's University Munday Library, Austin, Texas, United States*

Pincer ligands are tridentate molecules that bind to a transition metal atom, forming a rigid complex. These pincer structures are favorable for applications in catalysis due to their stability and selectivity under harsh conditions. The focus of this research is to investigate the use of a t-bu substituted tripyrrane ligand in forming square planar pincer ligand transition metal complexes. Cobalt was used as the central transition metal. The ligand went through a process of synthesis, deprotonation, and metalation that occurred under an air-free environment. Color changes were observed throughout the metallation process, with strong indication that the product had been successfully formed and metalated. NMR analysis was conducted on the products synthesized as well as the starting materials to observe any chemical shifts that were attributed to reactivity and potential product formation. Future works include full characterization of the synthesized materials.

SWRM 2026 SW374

To condense the diffused light of a page

***Emily R. Carrizales**, emilycarrizales@my.unt.edu, Donald C. Ballew, Teresa Golden. Chemistry, University of North Texas College of Science, Denton, Texas, United States*

Documents exposed to high levels of heat due to fires result in the loss of text and loss of structural integrity of the paper material. Clear identification of text from charred documents offers forensic investigations further applications for recovering evidence. The aim of this project is to develop an approach to decipher text from charred documents with different preservation techniques through captured digital photographs using infrared and ultraviolet light. The images of the charred documents are obtained in an LED apparatus with UV and IR wavelengths. Then post-processed with Photoshop is done to enhance and quantitate text in the digital images. The sample images were collected with a modified DSLR camera. The camera and samples of various levels of blackened charring were placed in an enclosed environment to retrieve images taken under wavelengths ranging from 395 nm and 940 nm. The data from graphite pencil writing on paper is dependent on the incident angle of the LED circuit at 395 nm. The text from ink-based writing instruments shows no absorption in the 940 nm wavelength but absorption in the 395 nm wavelength region. The visible contrast recovered hidden text from the damaged documents showing the charred document as a lighter background and the text as a darker color. With this research we offer a non-destructive method to decipher and recover text in damaged documents.

SWRM 2026 SW375

Design and synthesis of self-assembling peptides for the formation of coacervates

*Debdatta Das[1], Jenny Nguyen[1], Navneet Sahoo[1], Chuanye Xiong[2], Haritha Asokan-Sheeja[1], Yan Chang[3], **Raniyah Ali**[1], aliraniyah1126@gmail.com, Eleanor D. Smith[2], Chad A. Brautigam[4], Yi Hong[5], Zui Pan[3], Peng Tao[2], He Dong[1]. (1) Department of Chemistry and Biochemistry, The University of Texas at Arlington, Arlington, Texas, United States(2) Department of Chemistry, Southern Methodist University, Dallas, Texas, United States(3) College of Nursing and Health Innovation, The University of Texas at Arlington, Arlington, Texas, United States(4) Department of Biophysics, The University of Texas Southwestern Medical Center, Dallas, Texas, United States(5) Department of Bioengineering, The University of Texas at Arlington, Arlington, Texas, United States*

Peptides are versatile molecules that can be engineered to form a variety of nanostructures, which can subsequently be used to construct hydrogels and nanoparticles. In addition, the recent discovery of biomolecular condensates has attracted significant interest for applications in cellular engineering and biological systems. While most current studies on biomolecular condensates primarily focus on intrinsically disordered structures, the role of molecular ordering has received comparatively little attention. However, understanding this aspect is crucial for improving mechanistic insight and expanding the design space of synthetic peptides for constructing functional condensates. Multidomain peptides (MDPs) have emerged as promising candidates in this field because their amino acid composition, sequence length, assembly and disassembly domains, and secondary structural propensity can be tuned to generate partially ordered structures that promote condensate formation. These peptides typically contain amphiphilic regions that facilitate self-assembly into secondary structures, along with arginine residues that play a key role in promoting interactions during coacervate formation. The peptides were synthesized using a solid-phase peptide synthesizer and purified by high-performance liquid chromatography (HPLC). Circular dichroism (CD) spectroscopy was used to analyze the partial secondary structures of the peptides, while matrix-assisted laser desorption/ionization (MALDI) mass spectrometry confirmed successful peptide synthesis. These peptides were further utilized to generate enzyme-triggered condensation, enabling the formation of complex materials suitable for a wide range of biological applications.

SWRM 2026 SW376

Cajun Country POGIL: Supporting student success and college preparedness in general chemistry

Nelson Eguizabal[2], *neguizabal@nicholls.edu, Mylea Riggle[1], Bella Bourgeois[1], **Theodore E. Alivio**[1], theodore.alivio@nicholls.edu. (1) Department of Chemistry & Physical Sciences, Nicholls State University, Thibodaux, Louisiana, United States(2) Department of Biological Sciences, Nicholls State University, Thibodaux, Louisiana, United States*

Owing to its “math-heavy” nature, two-semester General Chemistry has been regarded as a “gatekeeper” course for most first-year STEM students. High DFW and attrition rates create a major hurdle for these students, preventing them from continuing with their degree plans across science, engineering, healthcare, and other related fields. This challenge is particularly acute at Nicholls State University, a public, primarily undergraduate institution that serves many first-generation (and non-traditional) students with varying levels of mathematical literacy and college preparedness. In Fall

2025, the Process Oriented Guided Inquiry Learning (POGIL) pedagogy was introduced into the General Chemistry lecture curriculum at Nicholls. Preliminary results suggest that POGIL effectively scaffolds learning for students with low and average arithmetic fluency while cultivating important workforce process skills such as teamwork, critical thinking, and problem solving. Our study evaluates how POGIL fosters student success and persistence as a function of their arithmetic fluency and logical reasoning, as measured by diagnostic tools such as the Math-Up Skills Test (MUST) and the Test of Logical Thinking (TOLT). These findings offer a roadmap for instructors at peer institutions to design targeted interventions and strategies that narrow the college preparedness gap in General Chemistry.

SWRM 2026 SW377

Nanospace engineering for sustainability

***Shengqian Ma**, shengqian.ma@unt.edu. University of North Texas, Denton, Texas, United States*

The space within nanoporous materials provides virtually unlimited room for imagination, allowing designed incorporation of different functionalities for numerous potential applications. This is particularly the case for advanced porous materials such as porous organic polymers (POPs), which feature robust covalent framework structures with high water and chemical stability as well as high surface areas and tunable pore sizes. We will demonstrate how to engineer the nanospace of POPs via task-specifically designing and functionalizing them as nanotraps for applications in sustainability including water decontamination, precious metal recovery, and metal source extraction.

SWRM 2026 SW378

Guest binding in cyclobenzoin derivatives

***Ognjen Miljanic**, miljanic@uh.edu. University of Houston System, Houston, Texas, United States*

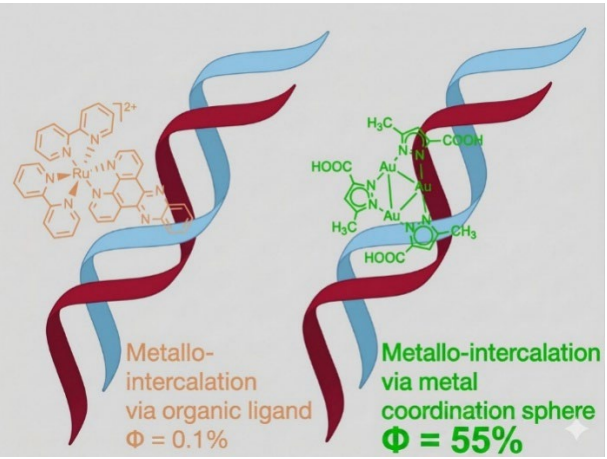
Cyclobenzoins are organic macrocyclic molecules easily prepared by the benzoin condensation of aromatic dialdehydes. Their rigid, shape-persistent cavities are lined with aromatic surfaces, allowing favorable interactions with electric-rich linear guests within the cavity, including environmentally relevant species such as carbon dioxide and C3 hydrocarbons. Their electrochemically addressable nature also means that they are competent organic electrode materials for use in lithium-ion batteries. Very recently, we have discovered that threefold symmetric cyclobenzoins can also complex anions on the outside, using a combination of aromatic and aliphatic C-H bonds to establish convergent anion binding interactions.

SWRM 2026 SW379

"Genuine" vs "fake news" DNA metallointercalation via planar coordination spheres in green aqua systems

***Mohammad A. Omary**, omary@unt.edu, Bisola Adeyemi, Nur Rabah, Gabriel Re Calderon, Omar Valsson, Elizabeth Skellam. Department of Chemistry, University of North Texas, Denton, Texas, United States*

This project describes "green chemistry" approaches to the sensitization the photoluminescence quantum yield (PLQY) of novel “light-switching complexes” *vs* state-of-the-art predecessors in purely aqueous environments under physiological conditions. DNA intercalation in predecessors is manifest *via* pendant ORGANIC ligands (*i.e.*, distant-dppz in $[Ru(bpy/phen)_2dppz]^{2+}$ away from metal centers) *vs* INORGANIC-coordination-sphere genuine metallo-intercalation herein (*e.g.*, triangular gold(I)-9-membered-ring cyclic-trinuclear complexes; oligomeric-chain platinum(II)-bis(pyridyltriazolates)). Phosphorescence sensitization for $[Ru(bpy)_2dppz]^{2+}$-type conventional metallo-intercalators entails PLQY increases from merely 10^{-4} (0.01%) levels in buffer solutions without DNA to merely 10^{-3} (0.1%) levels in buffered-aqueous DNA or organic solvents. Novel complexes herein can attain drastically higher sensitization to reach PLQY = 0.5-1.0 (50-100%) “on” state levels in aqueous media of micellar biocompatible polymers nanoparticle; indeed, even the “off” level herein is higher than the “on” level of conventional metallo-intercalators (0.5% *vs* 0.1%)! The light-switching “on” state herein, therefore, amounts to 100x > its “off” state and > 500x or > 5000% the “on” state of Ru(II)-dppz complexes! Furthermore, DFT computations reveal > 50% higher binding energy to DNA base pairs by representative planar phosphors *vs* conventional organic intercalators. The combination of extremely high PLQYs in aqueous buffer environments and high binding energies of the novel metallo-intercalators are promising toward alternative dyes in standard agarose gel electrophoresis kits used for DNA bioimaging (*e.g.*, ethidium bromide; ellipticine; cyber-safe series) upon further developments of different classes of d^{10} and d^8 bright/fast phosphors (> 50% PLQY/100 ns lifetime range) under investigation.



SWRM 2026 SW380

Real-world digital chemistry: Putting quantum simulation, machine learning, AI, and big data into practicing chemists’ hands

***Benjamin G. Janesko**, bjanesko@gmail.com. Texas Christian University, Fort Worth, Texas, United States*

Quantum simulation, machine learning, AI, chemical databases, and related tools are emerging as chemistry’s “new NMR”, capable of dramatically accelerating innovation across the chemical enterprise. A key remaining obstacle is to ensure that these new tools can be used effectively by real chemists. I present a series of endeavors at Texas Christian University designed to address this

obstacle. Our “Computational Chemistry for Experimentalists” program builds on the core chemical principles taught to every chemist: bonding, hybridization, orbital overlap, electronic excitation, and more. In this approach, chemical databases are presented in terms of R-group substitutions, electronic structure theory is presented in terms of MO diagrams, machine learning and feature extraction are discussed in terms of kinetics experiments, and so on. Training is intentionally nonspecialized, with a focus on using established computational workflows, leveraging chemical intuition, putting predictions into context, and communicating effectively with computational specialists. This is a proven approach: few organic chemists are experts in nuclear spin dynamics, but all of them use NMR to solve real chemical problems. I discuss detailed training modalities, successes and failures, and offer suggestions for extending this approach to regional stakeholders and the broader chemical enterprise.

SWRM 2026 SW381

From C-H bonds to functionalities: Toward more practical and sustainable catalysis

Xin Cui[1]*, xin.cui@unt.edu, Xue Xu*[2]*, Deb Mlsna*[3]*. (1) Chemistry, University of North Texas, Denton, Texas, United States(2) Chemistry, The University of Texas at Arlington, Arlington, Texas, United States(3) Chemistry, Mississippi State University College of Arts & Sciences, Mississippi State University, Mississippi, United States*

Developing efficient strategies to transform simple molecules into functional and structurally complex compounds is a central goal of sustainable synthetic chemistry. Catalysis provides powerful opportunities to improve step and atom economy while enabling new patterns of reactivity and selectivity. In this presentation, I will highlight our efforts to develop practical catalytic approaches for converting simple C–H and alkene frameworks into valuable molecular functionalities.
Our research explores complementary catalytic strategies, ranging from ruthenium(II)-catalyzed C–H functionalization to tandem Lewis acid catalysis. Mechanistically guided Ru(II) catalysis enables selective and stereoselective functionalization of C–H bonds in arenes and alkenes, providing efficient access to chiral building blocks and molecular structures relevant to synthetic and medicinal chemistry. In parallel, Fe-catalyzed tandem amidomethylation transforms simple alkenes through sequential bond-forming events to rapidly generate structurally complex nitrogen-containing molecules. Together, these approaches demonstrate how catalyst design and mechanistic understanding can uncover new reactivity while reducing synthetic steps, materials, and waste.
The tandem catalytic chemistry was further translated into an undergraduate organic chemistry laboratory, where students explored catalytic cycles and reaction mechanisms through TLC and 1H NMR analysis. This integration of research and teaching illustrates how contemporary catalytic chemistry can provide both practical synthetic solutions and meaningful opportunities for chemistry education. Overall, these efforts aim to advance efficient, selective, and more sustainable approaches to molecular synthesis.

SWRM 2026 SW382

Development of an intrinsic tryptophan FRET platform for studying GAG-protein interactions

Nneoma James, Francis N. Eze, ***Daniel K. Afosah****, daniel.afosah@unt.edu. Chemistry, University of North Texas, Denton, Texas, United States*

Glycosaminoglycans (GAGs) are anionic biomacromolecules that interact with multiple proteins and modulate biological processes such as coagulation, growth, inflammation and infection. Elucidation of GAG-protein interactions therefore has broad implications for understanding disease mechanisms and identifying novel therapeutic targets. However, relatively few specific GAG-protein interactions have been identified and characterized to date. A major limitation is the lack of accessible, high-throughput methods for screening and characterizing GAG-protein interactions.
In recent years, microarrays have gained prominence as tools for studying macromolecular interactions; however, their application to glycosaminoglycans (GAGs) remains limited. Major challenges include the limited availability of well-defined GAG oligosaccharide sequences and difficulties with the detection of GAG-protein interactions. Most current GAG microarray platforms require fluorescently labeled proteins or antibody-based detection, which limits the range and number of proteins that can be evaluated. In addition, these platforms require specialized instrumentation, such as microarray printers and scanners, which may not be readily accessible to many research groups. Collectively, these requirements increase cost and limit the broader use of GAG microarrays. To address these limitations, we explored the use of intrinsic tryptophan FRET technology for the study of GAG-protein interactions. This approach has the potential to enable direct detection of GAG binding to a broad range of proteins without the need for protein labeling or secondary antibodies. Here, we describe the synthesis of iFRET-compatible probes, their conjugation to GAGs, characterization of the resulting GAG probes, and their application to the detection and analysis of GAG-protein interactions. These studies provide proof of concept for the development of a cost-effective, scalable, multi-well platform for higher-throughput and quantitative analysis of GAG-protein interactions.

SWRM 2026 SW383

Sustainably enabling computational chemistry in the condensed phases by combining the SeA high-throughput hybrid DFT engine and Deep Potential molecular dynamics

Bharatha Kaushalya Gunawardana, Deepa Ranabhat, Kriti Alam, Priya Limbu, Yizhi Song, ***Hsin-Yu Ko****, hsin-yu.ko@unt.edu. Department of Chemistry, University of North Texas, Denton, Texas, United States*

Hybrid density functional theory (DFT) represents the fourth rung of the five-rung Jacob's ladder of DFT exchange-correlation approximations and is known to provide semiquantitative chemical accuracy. However, the necessary Hartree-Fock (exact) exchange in hybrid DFT is typically subject to 100x–1000x higher computational cost compared with other semilocal ingredients in the condensed-phase environment, therefore leading to unsustainable consumption of electricity in the routine application of hybrid DFT for solids, liquids, solutions, and interfaces. In this work, we address this challenge by combining (1) a recently developed SeA high-throughput hybrid DFT engine that harnesses three levels of computational savings from the natural sparsity of the exchange interaction in a localized orbital representation and (2) a deep potential machine-learning force field (MLFF) training ecosystem. In doing so, we sustainably reduce the overall cost of direct hybrid DFT by 10x–100x with SeA and achieve an additional $>10^6$x speedup in MLFF-based ab initio molecular dynamics, extending the simulation length and time scales accessible for modeling condensed-phase chemistry. We will present proof-of-principle case studies covering large-turnover radical and ionic polymerization reactions under experimental conditions.

SWRM 2026 SW384

Degradation behavior of polyethylene of different densities under reactive extrusion process

MASUD MONWAR[3]*, monwam@cpchem.com, Miguel Gonzalez Borja*[1]*, Lily Cui*[1]*, Margaret Sobkowicz*[2]*, Patrick Masembe*[2]*. (1) Chevron Phillips Chemical Co LP Kingwood Technology Center, Kingwood, Texas, United States(2) Plastics Engineering Department, University of Massachusetts Lowell, Lowell, Massachusetts, United States(3) Bartlesville R&T Center, Chevron Phillips Chemical Co, Bartlesville, Oklahoma, United States*

In recent years, recycling and upcycling of post-consumer polyethylene (PE) have attracted significant academic and industrial interest due to growing environmental concerns and regulatory requirements. Although chemical, mechanical, and thermal recycling technologies have been extensively studied, the development of an economically viable commercial upcycling process remains a challenge.
Reactive extrusion offers a promising route for PE upcycling, especially when combined with chemical methods in the subsequent step, by inducing polymer degradation under high-temperature and high-shear conditions. The use of catalysts during extrusion may further enhance chain scission and facilitate subsequent chemical conversion processes.
In this study, commercial polyethylene grades with varying densities were subjected to reactive extrusion in the presence and absence of catalysts. Changes in polymer microstructure and degradation behavior were investigated using several polymer characterization techniques. The influence of polymer density, additive, extrusion conditions, and catalyst addition on PE degradation mechanisms is discussed.

SWRM 2026 SW385

Data-driven insights into machine learning–accelerated density functional theory for catalytic materials discovery

Sara Castillo, Sofia Bernstein, Lauren Orozco, ***Shiru Lin****, slin6@twu.edu. Texas Woman's University, Denton, Texas, United States*

Density Functional Theory (DFT) is a cornerstone of computational catalysis, yet its high computational cost and intrinsic approximations limit its scalability for large chemical spaces. Machine learning (ML) has recently emerged as a powerful strategy to accelerate DFT workflows and enhance predictive performance in catalyst discovery. In this work, we present a comprehensive data-driven analysis of over 100 ML-assisted DFT studies published within the past five years. We systematically compare widely used algorithms, including kernel ridge regression, random forests, Gaussian process regression, and neural networks, with respect to dataset size, feature engineering strategies, target properties, and reported error metrics. Our analysis summarizes relationships between model performance, descriptor design, algorithm selection, and dataset size across the collected studies. We also compare how uncertainty quantification and model generalizability are reported under different machine learning frameworks and data scales. In addition, we compile reported error types and value ranges to provide a consistent overview of model accuracy in ML-assisted DFT studies. Finally, we briefly discuss current challenges, including data consistency, benchmark availability, and model transferability, as well as potential directions such as physics-informed approaches and applications to more complex catalytic systems.

SWRM 2026 SW386

Incorporating responsible chemistry and sustainability across the curriculum: Transforming teaching, research, and student engagement

***Manal Rawashdeh-Omary**, momary@twu.edu, Nasrin Mirsaleh-Kohan. Chemistry and Biochemistry, Texas Woman's University College of Arts & Sciences, Denton, Texas, United States*

The Division of Chemistry and Biochemistry at Texas Woman's University is transforming the way we teach and practice chemistry by integrating sustainability, green chemistry, responsible chemistry, and real-world applications across our curriculum, laboratory experiences, research, and student activities. Rather than treating sustainability as a stand-alone topic, we embed these concepts throughout courses and research to help students understand both the power of chemistry to address global challenges and the responsibility that comes with practicing it.
Through curriculum development and laboratory instruction, students explore safer chemical practices, waste reduction, sustainable materials, energy efficiency, and the environmental and societal impacts of chemical processes. Our research similarly connects chemistry with challenges in environmental remediation, sustainable materials, chemical recycling, and human health.
These efforts extend beyond the classroom through initiatives such as our Zero Impact Project, which encourages more sustainable approaches to departmental activities, and public research presentations that help students communicate the broader impact of their work.
In this presentation, we will share examples of how we are embedding sustainability and responsible chemistry across teaching, research, and student engagement, and how these experiences help prepare students to consider the environmental, ethical, and societal impacts of the chemistry they practice.

SWRM 2026 SW387

Interactions of hydroxylamines and aldoximes with synthetic metalloporphyrins

***George B. Richter-Addo**, grichteraddo@ou.edu, Tsitsi Kapfunde, Jennifer Londoño-Salazar, Nobuyuki Yamamoto. Chemistry, The University of Oklahoma, Norman, Oklahoma, United States*

Heme enzymes are involved in the binding and metabolism of various RNHxOy compounds such as alky/arylhydroxylamines and oximes. The simplest hydroxylamine (NH_2OH) has been identified as an intermediate in enzymatic nitrite reduction and in hydrazine biosynthesis, and is a substrate for the multiheme enzyme hydroxylamine oxidoreductase. Alkylhydroxylamines and arylhydroxylamines are biologically relevant species that have been shown to engage with heme Fe centers in various heme proteins. However, atomic level structural information of their binding to heme has to a large degree remained elusive.
Aldoximes (RCH=NOH) play important biological roles in the regulation of plant growth and defence, and in plant communication with the environment. The role of heme in oxime metabolism is gaining increased attention. In particular, a relatively new class of heme enzymes has been reported that catalyses the dehydration of aldoximes to nitriles.
We previously reported the X-ray structural characterization of *N*-hydroxyamphetamine adducts of Fe(II) and Co(II) porphyrins, and determined that the AmphNHOH ligand displayed the expected *N*-binding mode to the metal centers. What was unexpected was the observation of an unprecedented intramolecular H-bond between the hydroxylamine-O*H* proton and a porphyrin N-atom. We determined, using a natural bond order (NBO) analysis, that the intramolecular H-bond comprises a donor pi N=C (porphyrin) to acceptor sigma* O–H (hydroxylamine) interaction.
Interestingly, we now also show by X-ray crystallography and DFT calculations that the intramolecular

H-bond may be present in some oxime adducts of cobalt metalloporphyrins. The relevance of these observations to the metabolism of RNHxOy compounds by heme active sites will be discussed.

SWRM 2026 SW388

Tuning product selectivity in nonheme iron-catalyzed nitrogen oxyanion reduction

Alison R. Fout*, fout@tamu.edu, Hsien-Liang Cho, Daoyang Zhang. Chemistry, Texas A&M University System, College Station, Texas, United States*

Bio-inspired nonheme iron complexes offer a versatile platform for challenging multi-electron/multi-proton transformations of diverse chemical feedstocks. This work demonstrates how secondary coordination sphere interactions in non-heme iron complexes direct mechanistic branching across distinct chemical and electrochemical redox reactions. For nitrogen oxyanion reduction ([endif]--> and [endif]-->), tuning reaction conditions either chemically through choice of reductant or electrochemically unlocks selective conversion to either [endif]--> or [endif]-->. Detailed mechanistic studies, supported by isotopic labeling, spectroscopy, and computations, aid in understanding how electron transfer rates and secondary coordination sphere interactions influence product outcomes.

SWRM 2026 SW389

Low oxidation state metallocorroles: Bioinspired motifs with applications in catalysis and energy

Zachary J. Tonzetich*, zachary.tonzetich@utsa.edu. Chemistry, The University of Texas at San Antonio, San Antonio, Texas, United States*

Metallocorrole chemistry is dominated by complexes featuring metal centers in formal oxidation states of 3+ or greater. This preference stems in large measure from the trianionic nature of the corrole macrocycle, which better supports high oxidation state species as compared to related porphyrins. While such metallocorroles have proven effective for a variety of purposes, the reactivity of their lower oxidation state counterparts remains much less explored. This fact is surprising given the potential advantages associated with the more electron-rich nature of the corrole ligand. This presentation will focus on the synthesis and reactivity of several metallocorrole complexes containing metal centers in formal oxidation states less than 3+. Such compounds are accessed via alkali metal reduction of standard precursors leading to isolable examples of new anionic metallocorrolates. In the case of iron and cobalt, these species exist as unsaddled square-planar complexes that demonstrate a reluctance to coordinate additional axial ligands. Computational studies reveal that the corrole ligands in these compounds are redox innocent, consistent with reduction occurring at the metal center. The reactivity of the low oxidation state complexes has been shown to include NO-binding, superoxide generation, and oxidative addition of alkyl electrophiles. Several compounds undergo further reduction to produce dianionic species. Features of the reduced corrolate species relevant to catalysis and energy applications will be discussed and compared with their porphyrin counterparts.

SWRM 2026 SW390

Multifunctional antioxidant macrocycles as small-molecule mimics of endogenous defense systems

***Kayla N. Green**, kayla.green@tcu.edu. Chemistry & Biochemistry, Texas Christian University, Fort Worth, Texas, United States*

Oxidative stress is implicated in aging and numerous pathological conditions, including neurodegenerative disorders. While endogenous antioxidant enzymes such as catalase and superoxide dismutase (SOD) provide critical protection against reactive oxygen species (ROS), the development of small-molecule therapeutics capable of reproducing multiple antioxidant functions remains a significant challenge. Our research program focuses on the design of tetra-aza macrocyclic ligands and transition metal complexes that operate as multifunctional antioxidant systems.
A library of antioxidant-active macrocycles and metal complexes was synthesized and evaluated for their ability to modulate oxidative stress through complementary mechanisms. These compounds exhibit catalase-like hydrogen peroxide disproportionation, superoxide scavenging activity, metal ion coordination, and direct protection against ROS-induced cellular damage. Systematic modification of ligand architecture and metal coordination environments enabled identification of key structural features governing antioxidant performance. Studies revealed that incorporation of pyridine-containing donor groups and strategic tuning of the macrocyclic scaffold significantly influence redox properties, catalytic activity, and biological efficacy. Several compounds demonstrated the ability to address multiple oxidative pathways simultaneously, exceeding the capabilities of traditional single-function antioxidants.
These findings establish macrocyclic antioxidant platforms as versatile, multifunctional agents that mimic the cooperative action of endogenous antioxidant defenses. By integrating ROS detoxification, metal regulation, and catalytic antioxidant activity within a single molecular framework, this work provides design principles for next-generation therapeutics targeting oxidative stress-associated disease.

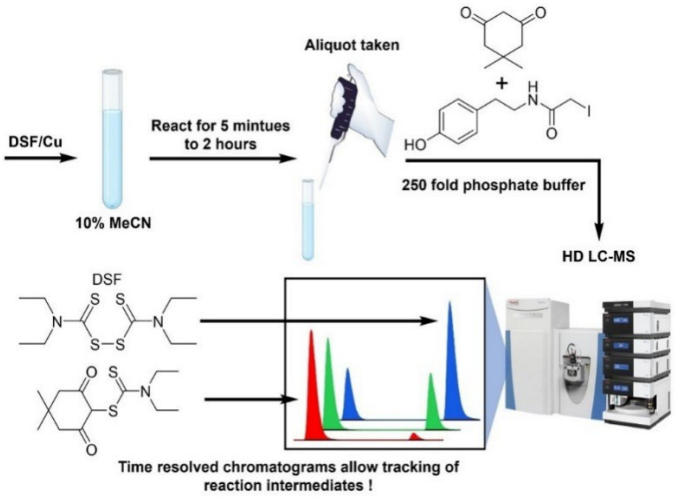
SWRM 2026 SW391

Investigation of the DSF/Cu reaction using LC HDMS and reactivity studies

***Patrick J. Farmer**[1,2], patrick_farmer@baylor.edu, Jordan Lyons[1]. (1) Chemistry & Biochemistry, Baylor University, Waco, Texas, United States(2) School of Earth and Environmental Studies, Baylor University, Waco, Texas, United States*

Cuprotosis is a unique mode of cell death being explored in many new therapeutic anticancer studies. A widely used approach is the combination of Cu(II) salts with diethyldithiocarbamate disulfide, disulfiram (DSF), an alcohol-sensitizing drug Antabuse, which generates the toxic Cu(II)bis(diethyldithiocarbamate), Cu(deDTC)$_2$, in a complex redox reaction. The mechanism for the generation of Cu(DTC)$_2$ in this reaction, which we term the DSF/Cu reaction, has been examined using high-resolution liquid chromatography-mass spectroscopy (HR LCMS) by monitoring the reaction at different sampling times to determine sequential speciation of reaction intermediates. Other intermediates of this reaction are characterized by the addition of adduct-forming "traps" used to characterize thiol and sulfenic acid species generated throughout the reaction. The time-resolved spectra reveal that one initial reaction is a 2-electron oxidation of a thione moiety in DSF to a sulfine (DSF-O), which implies a concurrent reduction of Cu(II) to Cu(0). Other results suggest the involvement of Cu(I) in the titled reaction, most likely formed by comproportionation of Cu(0) with Cu(II) in the MeCN/H_2O solutions used. Additional intermediate products indicate a variety of sulfur oxidation, hydrolysis and insertion/extrusion reactions forming species that also feed into pathways

generating $Cu(DTC)_2$. We intend this work to help inform new strategies for medicinal applications of cuprotosis.

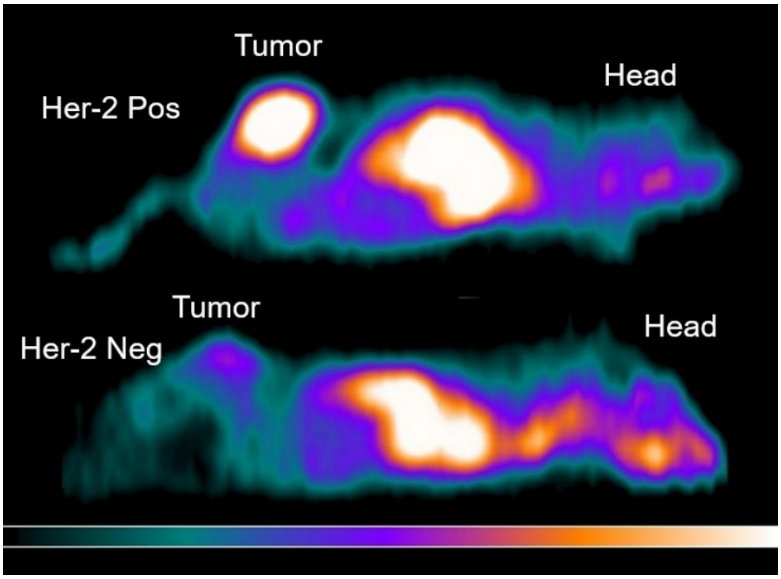


SWRM 2026 SW392

Configurational isomers with a CB-TE2A core

Paul Jurek[1]*, pauljurek@hotmail.com, Slade Lee*[1]*, Cara Ferreira*[2]*, Donald Yapp*[3]*, Gary George*[4]*, Fernando Avecilla*[5]*, Pedro Cruz*[6]*, Carlos Geraldes*[6]*. (1) Macrocyclics, Inc., Plano, Texas, United States(2) Lumina Pharmaceuticals, Boston, Massachusetts, United States(3) British Columbia Cancer Agency, Vancouver, British Columbia, Canada(4) Triclinic Labs Inc, Lafayette, Indiana, United States(5) Universidade da Coruna, A Coruña, Spain(6) Universidade de Coimbra, Coimbra, Portugal*

Configurational isomers, each with a distinct cross-bridged cyclam CB-TE2A core, were prepared and structurally characterized by single crystal X-ray diffraction (SCXRD). The p-NO_2-phenylbutyric acid arm of one configuration, (4)-G, is in the gauche conformation while it is antiperiplanar in the other (4)-AP. The latter binds Cu-64 at a rate that is acceptable for radiolabeling applications. NMR analysis and potentiometry were obtained to help characterize the isomers in solution. Despite similar CB-TE2A cores, they have significant differences in basicity. The pKa values are > 11.5, 8.46, 2.74, and 1.99 versus > 11.5, 10.55, 3.32, and 2.26. The copper complexes of both configurations were also characterized by SCXRD. Upon complexation, (4)-AP undergoes an inversion of the bowl-shaped CB-TE2A core. In contrast, (4)-G does not undergo an inversion of the CB-TE2A core. Both form copper complexes with an almost identical coordination geometry around the copper ion. Lower basicity and a ring inversion complexation mechanism results in advantageous Cu-64 complexation kinetics of (4)-AP over (4)-G.



SWRM 2026 SW393

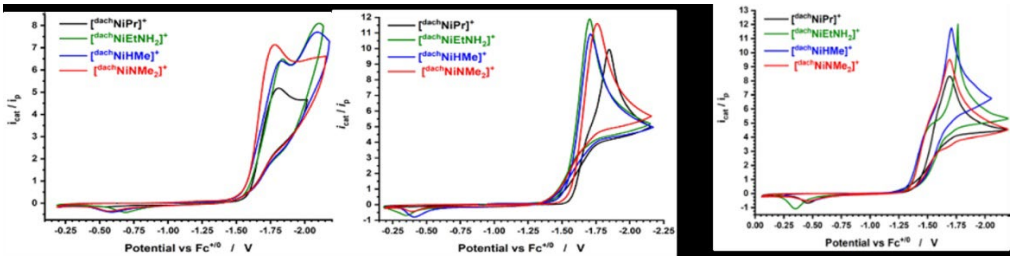
Control of secondary coordination spheres of nickel(II) dithiolate complexes through sulfur functionalization: Effects on electrochemistry and the HER

Marcetta Y. Darensbourg*, marcetta@chem.tamu.edu, Kyle Burns, Sourav Deb. Chemistry, Texas A&M University, College Station, Texas, United States*

Secondary coordination sphere interactions in metalloenzyme active sites are acknowledged to facilitate bond-forming and -breaking steps, stabilize reactive intermediates, act as proton shuttles, and mediate outer-sphere electron transfer. Secondary sphere effects have been explored throughout synthetic transition-metal chemistry as well, where the introduction of pendant motifs have expanded structure-function relationships within small molecule catalysts. The hydrogenase active sites are exemplars of how secondary coordination sphere (SCS) environments modulate properties, such as redox potentials and Lewis acidities of metal centers. Synthons with capability to install a functionality are valued in mechanistic studies; the preparation of diiron complexes outfitted with an azodithiolate bridge as [FeFe]-H_2ase active site models is a prime example.

The Ni(II)-N_2S_2 metallodithiolate class of complexes has been studied within H_2-ase biomimetic catalysis, producing H_2 at ca. -2.0 V vs $Fc^{+/0}$, and facilitating the HER reaction in combination with metal-bearing synthons that create Ni(μ-$SR)_2$M' heterobimetallics.[3] Here we present results of sulfur alkylation in a series of cationic $[NiN_2SS^R]^{n+}$ complexes (R = Pr, $EtNH_2$, MePy, etc.); these modifications cathodically shift the nickel-based reduction potentials by ca. 500 mV. Some of the motifs also introduce steric effects that result in interesting physical properties.

A subset of these complexes containing pendant amine motifs, established the S-modified nickel metallodithiolates as active proton reduction/H_2 evolving catalysts in the presence of a wide range of organic acids; from acetic acid ($pK_{a,\,MeCN}$ = 23.51) to salicylic acid ($pK_{a,\,MeCN}$ = 16.6). The catalysis occurs at a relatively low onset potential (ca. -1.6 V vs. $Fc^{+/0}$) with measured turnover frequencies ca. 10^5 s^{-1} in the high acid concentration regime. The role of these pendant bases during catalysis has been explored in both low and high substrate concentration; with computational support, the function of the pendant amine is suggested to shift the catalytic mechanism based on acid pK_a. This comparative study demonstrates nuances between thiolate sulfur-derived pendant amine functionality as proton shuttle and enhancements of the HER electrochemical activity.



SWRM 2026 SW394

Lamellar hybrid metal chlorides A_2MCl_4 for thermal energy management: Alkyl cation engineering of 2D and 0D hybrids

***Kyle McCall**, kylemccall2014@u.northwestern.edu. The University of Texas at Dallas Erik Jonsson School of Engineering and Computer Science, Richardson, Texas, United States*

The recent surge in low-dimensional metal halides with efficient luminescence and long-chain cations has delivered new 2D and 0D hybrids with applications including LED phosphors, luminescent solar concentrators, and solid-solid phase-change materials for barocaloric and thermal energy storage. The latter application is especially promising, as the precision of organic cations can tune the thermal behavior based on the solid-solid transition corresponding to “chain melting” disordering of the vdW-based organic layers. The vast array of potential counter-cations offers wide potential for design of these compounds, but poses a challenge to predicting the resulting crystal structure. Here, we explore the role of alkyl chain length and the impact of cation head shape amongst the family of 2D and 0D manganese and copper chlorides, aiming to provide design rules for maximizing transition enthalpy and tunability of phase transition temperature. This presentation summarizes the recent findings of our work on A_2MCl_4 hybrids, where A is an ammonium-based cation with a long alkyl chain (C_{10} or more) and M = Mn^{2+} or Cu^{2+}. For the series of simple alkylammonium cations (denoted C_n-Am), these compounds adopt Ruddlesden-Popper 2D perovskite crystal structures, with each inorganic octahedral slab hosting dual layers of cations above/below it. In contrast, larger trimethyl-(C_n-TMA) and benzyldimethyl-ammonium (C_n-BDA) cations induce the formation of 0D crystal structures, as trimethyl-terminated $(C_{14}\text{-TMA})_2MnCl_4$ and $(C_{18}\text{-TMA})_2MnCl_4$ crystallize in a novel 0D structure with isolated $MnCl_4$ tetrahedra that pack in layers with the larger TMA chain heads; these layers are separated by the nonpolar carbon chains. Crucially, the interlayer chains in such phase are partially (C_n-BDA) or fully (C_n-TMA) interdigitated, and we report on the implications for this using differential scanning calorimetry coupled with variable-temperature powder X-ray diffraction, tracking the chain melting transitions in real time. This presentation illustrates the role of cation shape in directing the structure of these hybrid halides, with implications for development of novel halide semiconductors. This work will elucidate the structural features that dictate the melting temperature and enthalpy of long-chain hybrid phase change materials, providing solid-solid phase-change materials for application in thermal energy management in power electronics and batteries.

SWRM 2026 SW395

Surface sp^2 carbon elimination and hydroxylation of polycrystalline diamond

***Renuka Rathnayake Mudiyanselage**[1], nilminirathnayakemudiyanselage@my.unt.edu, Mahesh Dungana[1], Donald C. Ballew[1], Abdullah Ali Maruf[1], Stella C. Amagbor[1], Chisom Ifeobu[2], Teresa*

Golden[1], Nigel Shepherd[2], Jeffry Kelber[1]. (1) Chemistry, University of North Texas College of Science, Denton, Texas, United States(2) Materials Science and Engineering, University of North Texas College of Engineering, Denton, Texas, United States

Diamond is a promising ultra-wide bandgap semiconductor for high-power electronics and quantum information applications. However, the presence of sp^2 carbon (C) on a diamond surface, even after the standard triacid etch cleaning procedure, degrades device performance by creating conductive pathways and interface instabilities while also inhibiting the chemical modification of carbon atoms at the diamond surface for subsequent thin-film deposition. One such modification is surface hydroxylation for enhanced nucleation during atomic layer deposition (ALD) of gate dielectrics. Herein, we report an effective strategy for sp^2 C elimination and subsequent surface hydroxylation of polycrystalline diamond (PCD) using a sequence of triacid etching, then ultra-high vacuum (UHV) annealing to 900 K, and then water vapor exposure at room temperature under controlled vacuum conditions. *In situ* characterization using take-off angle-resolved X-ray photoelectron spectroscopy (XPS) has been applied to track surface changes after each treatment step. While triacid etching showed significant but incomplete removal of sp^2 C, further UHV annealing at 900 K resulted in the total elimination of sp^2 C, as well as reduction of surface and near-surface C-O-C and C=O species. Subsequent exposures to water vapor at room temperature (RT) promoted the formation of C-OH species. C-OH functional groups were stable at 473 K. These results provide a novel but practical approach to the cleaning and modification of diamond surfaces for high-quality ALD growth of gate insulators in microelectronics and quantum information processing.

SWRM 2026 SW396

Synthesis, characterization, and photothermal effect of CuS nanoparticles deposited on MXene

*Rupesh L. Karn[2], **Gururaj Neelgund**[1], gmneelgund@pvamu.edu. (1) Chemistry, Prairie View A&M University, Prairie View, Texas, United States(2) Mechanical Engineering, Prairie View A&M University, Prairie View, Texas, United States*

The photothermal effect of CuS nanoparticles was enhanced by combining with MXene. The NIR (Near-Infrared)-responsive MXene-CuS nanocomposite is prepared by deposition of CuS nanoparticles over the surface of MXene. Prior to the deposition of CuS nanoparticles, the MAX-phased MXene was treated with acid and delaminated using dimethyl sulfoxide. The deposition of CuS nanoparticles on the surface of delaminated MXene was achieved by the hydrothermal process. The FESEM images of MXene-CuS revealed its hybrid nanoarchitecture, with uniform deposition of CuS nanoparticles across the entire MXene surface. The powder XRD, XPS, and EDS of MXene-CuS confirmed the formation of right-structured CuS nanoparticles and their co-existence with MXene. The TGA demonstrated that the thermal stability of MXene and CuS was improved when combined in MXene-CuS. The BET analysis showed a higher surface area for MXene-CuS than for MXene and CuS. The formation of MXene-CuS was further confirmed by FTIR and Raman. The photothermal effect of MXene-CuS was estimated by illuminating the aqueous dispersion of MXene-CuS with an NIR laser. The photothermal effect of MXene-CuS was significantly higher than that of MXene and CuS. It was found that the photothermal effect of MXene-CuS was dependent on its concentration, and the wavelength, and the power density of the NIR laser.

SWRM 2026 SW397

Bismuth vanadate-based photoanodes for photoelectrosynthetic biomass conversion

***Ben Sherman**, bdsherma@gmail.com. Chemistry and Biochemistry, Texas Christian University, Fort Worth, Texas, United States*

Biomass valorization (i.e., lignin depolymerization) and upgrading of biomass derived chemical feedstocks such as HMF (5-hydroxymethylfurfural) presents an emerging area of study for photoelectrosynthetic solar cells that complements the traditional focus on solar fuels. This presentation will highlight recent work from the Sherman Group at TCU and collaborators at UT-RGV and SUNY-ESF using $BiVO_4$-based photoanodes to drive chemical conversions related to biomass utilization. Examples of cell chemistries include benzyl alcohol dehydrogenation, controlled HMF oxidation to DFF (2.5-diformyfuran), and lignin depolymerization. In each case, a mediated photoelectrochemial approach is used whereby an N-oxyl species (e.g., TEMPO) is used to couple light driven heterogeneous oxidation to catalysis in solution. Examples with different mediator species and how the design and composition of the photoanode surface impact the photoelectrosynthetic activity, among other topics, will be presented.

SWRM 2026 SW398

Electrocatalytic and magnetic properties of porous iron phosphide nanorods

***Yolanda Vasquez**, yolanda.vasquez@okstate.edu, Shubham Sharma. Chemistry, Oklahoma State University, Stillwater, Oklahoma, United States*

Nanoscale transition metal phosphide systems hold significant technological potential due to their distinctive optoelectronic properties, high catalytic activity, superparamagnetism, and high diffusion coefficient of Na/Li ions. However, attempts to synthesize phase-pure FeP, a promising electrocatalyst, have utilized expensive and/or highly reactive phosphide precursors such as tri-*n*-octylphosphine (TOP), white phosphorus, tris(trimethylsilyl) phosphine, and tri-*n*-butylphosphine. These methods often require high temperatures and/or multistep reaction processes. Here, to address these limitations, we present a solution-based synthesis method to produce phase-pure FeP nanoparticles. In this synthesis, we react iron oxyhydroxide as a cost-effective, environmentally friendly, and air-stable source of iron with tris(diethylamino) phosphine as a phosphorus source at 280 °C. The resulting FeP is formed in a porous nanorod morphology. The particles were characterized by TEM and XPS. Magnetic measurements of the phase-pure FeP nanoparticles indicate paramagnetic behavior, contrasting the antiferromagnetic behavior observed in bulk FeP. In addition to their unique magnetic properties, these porous FeP nanorods demonstrate promising HER performance, achieving an overpotential of 267 mV at a geometric current density of −10 mA cm^{-2} in acidic media, with stable electrocatalytic activity maintained for up to 12 h at −50 mA cm^{-2}. This study represents the first documented low-temperature, time-efficient, solution-based thermal decomposition method for synthesizing phase-pure FeP nanoparticles using tris(diethylamino) phosphine and iron oxyhydroxide as sources of phosphorus and iron, respectively, at 280 °C.

SWRM 2026 SW399 – Withdrawn

SWRM 2026 SW400

Synthesis and phase evolution of MAX phases to multimetal MNenes

*Bright Ngozichukwu[1], **Abdoulaye Djire**[1,2], adjire@tamu.edu. (1) Chemical Enginerring, Texas A&M University System, College Station, Texas, United States(2) Materials Science and Engineering, Texas A&M University System, College Station, Texas, United States*

Compositionally complex layered solids are often limited not by elemental availability, but by whether their crystal structures can accommodate the simultaneous redistribution of multiple species across distinct crystallographic sublattices during synthesis. This challenge is particularly pronounced for nitride and carbonitride MAX phases, where multimetal compositions remain far less accessible than their carbide counterparts and are highly sensitive to competing phase formation and structural reconstruction. Here, we investigate solid-state interdiffusion between binary MAX-phase precursors to synthesize multimetal nitride and carbonitride MAX phases through controlled redistribution across the M and X sublattices. Ti-based nitride MAX phases were reacted with V-, Nb-, and Mo-containing carbide MAX phases under controlled high-temperature conditions. In the Ti–V system, interdiffusion produces a multimetal carbonitride MAX phase while preserving the characteristic layered morphology, with elemental mapping confirming homogeneous distributions of Ti, V, Al, C, and N. In contrast, Ti–Mo and 413 MAX systems exhibit composition and temperature-dependent attenuation of characteristic low-angle reflections together with the emergence of new layered-phase signatures, revealing that phase formation can proceed through either lattice homogenization or structural reconstruction depending on constituent chemistry. The resulting multimetal MAX phases subsequently serve as precursors for O_2-assisted molten-salt conversion to multimetal MNenes. These results demonstrate that access to compositionally complex nitride and carbonitride layered materials is governed not simply by nominal composition, but by the solid-state reaction pathways controlling M- and X-sublattice redistribution and phase formation. These findings establish a route to nitride multimetal MAX phases and derived MNenes with composition-dependent electronic, redox, and catalytic properties.

SWRM 2026 SW401

High frequency dynamic nuclear polarization in rotating solids

***Robert G. Griffin**, rgg@mit.edu. Chemistry, Massachusetts Institute of Technology, Cambridge, Massachusetts, United States*

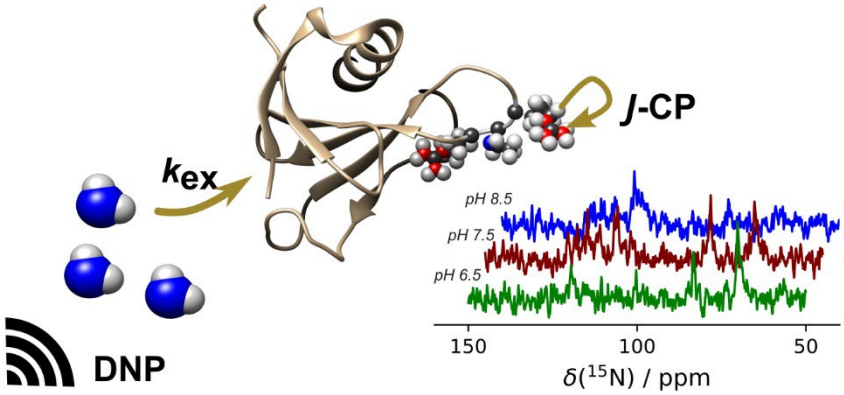
High frequency dynamic nuclear polarization (HFDNP) is now established as a widely applicable approach to enhance the sensitivity of magic angle spinning (MAS) NMR experiments. We briefly review the development of the microwave instrumentation and polarizing agents necessary for DNP and highlight some of the successful applications to structural biology, materials science, and surface chemistry where DNP-enhanced sensitivity has enabled measurements not otherwise feasible.
A current limitation of DNP is the cost of the instrumentation and the fact that gyrotron sources are difficult to employ in time domain experiments. This has stimulated the development of a new generation of solid-state microwave sources which we have employed to perform frequency swept DNP and which have the potential to execute time-domain experiments and address the limitations of continuous-wave methods at high frequencies. In addition, we show that at high frequencies, ZrO_2 rotors exhibit significant microwave losses which can be circumvented with rotors laser machined from diamond. Finally, we discuss our recently discovered DNP mechanism, *resonant mixing*, and its relation to the Overhauser effect and thermal mixing DNP in insulating solids.

SWRM 2026 SW402

Mapping protein hydration and exchange dynamics by cross-polarization from hyperpolarized water

***Olivia Chatterjee**, oliviachatterjee@tamu.edu, Nirmalya Pradhan, Christian Hilty. Chemistry, Texas A&M University System, College Station, Texas, United States*

The intrinsically low sensitivity of ^{15}N remains a limitation for NMR studies of biomolecules at physiologically relevant concentrations. Dissolution dynamic nuclear polarization (D-DNP) can transiently increase nuclear spin polarization by several orders of magnitude, providing a substantial sensitivity gain. Hyperpolarized water acts as a polarizing agent because its abundant ^{1}H spins can transfer magnetization to exchangeable sites in biomolecules through chemical exchange and NOE. Here, hyperpolarized water is demonstrated as a polarization source for exchange-mediated ^{1}H-^{15}N *J*-cross-polarization (CP), enabling direct detection of rapidly exchanging backbone and side-chain ^{15}N sites in RNase Sa. Using 0.4 mM protein, significant ^{15}N signal enhancements were observed, whereas refocused INEPT and NOE produced no detectable signal under similar conditions. Arginine guanidinium NH_2 signal intensities were measured as a function of CP contact time and fitted using a CP-exchange model, yielding an exchange rate in accordance with the theoretically calculated exchange rate. Across the pH range of 6.5-8.5, backbone and side-chain signals exhibited distinct pH-dependent intensity changes, reflecting differences in proton-exchange kinetics. Residue-specific simulations using exchange rates derived from protection factors showed qualitative and quantitative agreement with experimental pH-dependent signal intensities and identified an optimal regime for polarization transfer. Thus, exchange-mediated *J*-CP acts as a dynamic filter, preferentially detecting rapidly exchanging, solvent-accessible protein sites. This technique provides a new window into biomolecular structure and function, enabling exchange-sensitive probing of protein hydration, dynamics, and intermolecular interactions under physiological conditions.



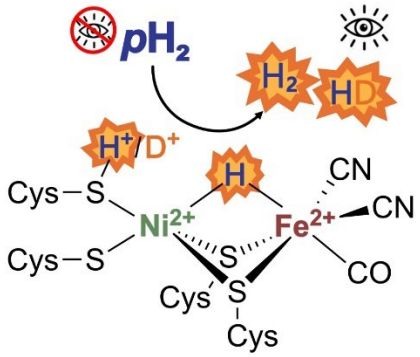
SWRM 2026 SW403

Studying hydrogen-bound states of hydrogenases under turnover conditions by parahydrogen-enhanced NMR

***Julius Frederik F. Matz**[1], julius.matz@mpinat.mpg.de, Lukas Kaltschnee[2], Manuel Gehl[3], Georgi Stoychev[4,5], Christoph Riplinger[4,5], James Birrell[6], Olaf Rudiger[7], Frank Neese[5], Serena DeBeer[7], Wolfgang Lubitz[8], Seigo Shima[3], Christian Griesinger[1], Stefan Gloeggler[9]. (1) NMR-based Structural Biology, Max-Planck-Institut fur Multidisziplinare Naturwissenschaften, Göttingen, NDS, Germany(2)*

Eduard-Zintl-Institute for Inorganic and Physical Chemistry, TU Darmstadt, Darmstadt, Germany(3) Microbial Protein Structure, Max-Planck-Institut fur terrestrische Mikrobiologie, Marburg, HE, Germany(4) FACCTs GmBH, Köln, Cologne, Germany(5) Molecular Theory and Spectroscopy, Max-Planck-Institut fur Kohlenforschung, Mülheim, NRW, Germany(6) School of Life Sciences, University of Essex, Colchester, England, United Kingdom(7) Inorganic Spectroscopy, Max-Planck-Institut fur chemische Energiekonversion, Mülheim, NRW, Germany(8) Biophysical Chemistry, Max-Planck-Institut fur chemische Energiekonversion, Mülheim, NRW, Germany(9) The University of Texas Southwestern Medical Center Department of Biomedical Engineering, Dallas, Texas, United States

Understanding the mechanistic principles of fundamental natural processes, such as hydrogen conversion, can inspire the design of more efficient and selective synthetic catalysts. However, mechanistic pathways often involve low-concentration transient species that are difficult to detect using conventional analytical techniques. This challenge is particularly evident in hydrogenase catalysis, where diamagnetic intermediates – such as hydrogen-bound species at the active site – remain elusive to EPR-based methods. Instead, structural insides into these species typically rely on high-resolution diffraction (XRD) or nuclear resonance vibrational spectroscopy (NRVS) to provide atomic-level information. In principle, ^{1}H NMR spectroscopy is well-suited for studying hydrogenase enzymes, as it can detect both the substrate (H^+/H_2) and product (H_2/H^+). Recently, the sensitivity limitations of NMR were overcome by leveraging parahydrogen, enabling the characterization of diamagnetic enzyme states. Combined with DFT calculations and spin dynamics simulations, this approach revealed two previously undetected on-cycle intermediates in [Fe]-hydrogenase catalysis. Furthermore, we demonstrated that parahydrogen can also be applied to symmetric complexes mimicking nitrogenase reactivity. In this work, we extend this methodology to another class of hydrogenase enzymes, showing that parahydrogen-enhanced NMR can probe hydrogen-bound intermediates with exceptional sensitivity under catalytic turnover conditions.



SWRM 2026 SW404

High-field liquid-state Overhauser DNP: From sub-picosecond dynamics to high-resolution spectroscopy

Tomas Orlando[1,2]*, torlando@magnet.fsu.edu. (1) Electron magnetic Resonance, National High Magnetic Field Laboratory, Tallahassee, Florida, United States(2) Florida State University, Tallahassee, Florida, United States*

Recent progress in Overhauser Dynamic Nuclear Polarization (OE-DNP) has greatly expanded its potential application for high-field liquid-state NMR spectroscopy.
Systematic studies have demonstrated significant signal enhancements for ^{13}C, ^{19}F, and ^{31}P nuclei across magnetic fields ranging from 1.2 T to 14.1 T, [1] primarily driven by electron-nuclear scalar

relaxation.
The theoretical framework for this mechanism identifies sub-picosecond fluctuations of the hyperfine coupling as the primary driver of polarization transfer at high fields. By integrating molecular dynamics, density functional theory, [2] and more recently quantum mechanics/molecular mechanics (QM/MM), research has shown that transient complexes, such as those formed through hydrogen bonding, halogen bonding, or other non-covalent interactions favor large hyperfine couplings. Notably, these complexes do not impede, but rather promote, the fast dynamics necessary for efficient DNP.
Recent instrumental advancements at 9.4 T [3,4] and 14.1 T [5] have enabled the verification of these transient interaction models across a broader range of chemical systems and target nuclei. These improvements provide the resolution and sensitivity required to observe site-specific enhancements in complex molecules, including pharmaceuticals and natural products, while operating under conditions compatible with routine liquid-state NMR spectroscopy.
This mechanistic insight could facilitate the development of novel, chemically versatile polarizing agents designed to selectively target specific molecules, enabling site-directed hyperpolarization within complex mixtures [6].

SWRM 2026 SW405

Characterization of nitroxides multi-radicals and their effects on DNP enhancement

***Emmanuel Ameh**, emmanuel.ameh@utdallas.edu. Physics, The University of Texas at Dallas School of Natural Sciences and Mathematics, Richardson, Texas, United States*

Nitroxides are the most commonly used polarizing agents in DNP due to their affordability and availability. TEMPO and its derivatives are among the most extensively studied nitroxide radicals for DNP. These radicals significantly enhance NMR signals because of their favorable electron-spin properties and efficiently transfer to nearby nuclei. In this study, we characterized 4-Oxo-TEMPO-based polyradicals and evaluated their role in DNP efficiency. Preliminary data suggest promising DNP efficiency using multi-radical polarizing agents. Details of this study will be discussed. The authors would like to acknowledge support for this work by the Robert A. Welch Foundation grant number AT- 2111-20220331 and the Congressionally Directed Medical Research Program (CDMRP) grant numbers HT9425-25-1-0241 and HT9425-24-1-0287.

SWRM 2026 SW406

Developing HP 15N-MRI probes targeting aberrant metabolism for cancers

***Qiu Wang**, qiu.wang@duke.edu. Chemistry, Duke University, Durham, North Carolina, United States*

TBA

SWRM 2026 SW407

Low-field NMR with sensitivity enhancement by parahydrogen and applications in chemistry and biochemistry

Christian Hilty[1], *chilty@tamu.edu, Ashes Roy*[1], *Priyanku Garg*[1], *Zefan Zhang*[1], *Igor Savukov*[2], *Oindrila Biswas*[1], *Pierce Pham*[1], *Ratnamala Mandal*[1]. *(1) Chemistry, Texas A&M University, College Station, Texas, United States(2) Los Alamos National Laboratory, Los Alamos, New Mexico, United States*

Nuclear spin hyperpolarization enables NMR measurements in the physiological concentration regime, at faster time scale and with enhanced selectivity. Parahydrogen based hyperpolarization methods can provide benefits of large signal enhancements at low cost. They extend the magnetic field for sensitive detection to the low or ultralow magnetic field range. Signal enhancements of several hundred-fold at 9.4 T are obtained, resulting in enhancements in the mT field range that are proportionally higher by orders of magnitude. We demonstrate the detection molecular interactions through a spin relaxation measurement, providing a new modality for the application of NMR in the study of biological processes and drug discovery. We further introduce a nano-scale phase separated medium formed by reverse micelles, which allows for the efficient parahydrogen polarization of biological molecules. The ability to measure spin relaxation in a wide magnetic field range unlocks the potential to study the dynamics of molecular processes over the corresponding broad time scales. Multiple nuclei, such as proton and fluorine, can be measured in a single spectrum at low field. We demonstrate the detection of chemical compounds using heteronuclear NMR, by employing heteronuclear polarization transfer and J-coupling resolution in the absence of chemical shift. Overall, parahydrogen polarization provides a sensitive means for identifying chemical compounds and detecting biomolecular interactions. In combination with low-field NMR, it is applicable to molecular characterizations on the benchtop, in the field or in environmental applications.

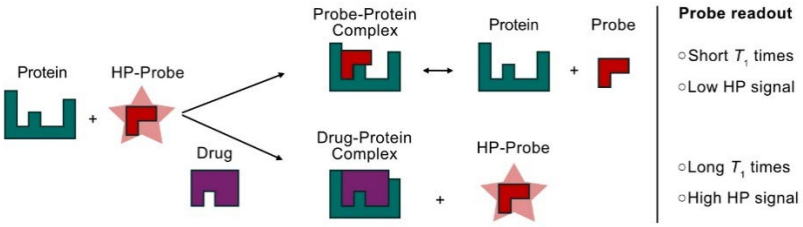
SWRM 2026 SW408

Hyperpolarized magnetic resonance at low magnetic fields enables assessment of drug-protein binding *in vivo*

Charlotte von Petersdorff-Campen[2,1], *charlotte.petersdorff-campen@mpinat.mpg.de, Gonzalo G. Rodriguez*[3,1], *Lisa M. Fries*[2,1], *Ruhuai Mei*[2,1], *Andrea Markus*[4], *Maria D. Santi*[2,1], *Frauke Alves*[4,5,6], *Stefan Gloeggler*[7,8]. *(1) Universitatsmedizin Gottingen Center for Biostructural Imaging of Neurodegeneration, Göttingen, NDS, Germany(2) NMR-based Structural Biology, Max-Planck-Institut fur Multidisziplinare Naturwissenschaften, Göttingen, NDS, Germany(4) Translational Molecular Imaging, Max-Planck-Institut fur Multidisziplinare Naturwissenschaften, Göttingen, NDS, Germany(5) Clinic of Hematology and Medical Oncology, Universitatsmedizin Gottingen, Göttingen, NDS, Germany(6) Institute for Clinical and Interventional Radiology, Universitatsmedizin Gottingen, Göttingen, NDS, Germany(7) Advanced Imaging Research Center, The University of Texas Southwestern Medical Center, Dallas, Texas, United States(8) Department of Biomedical Engineering, The University of Texas Southwestern Medical Center, Dallas, Texas, United States*

The characterization of drug-protein interactions constitutes a fundamental step in pharmaceutical development, directly influencing a drug candidate's pharmacokinetic and pharmacodynamic profile. Given that approximately 90% of drug candidates fail during development, tools capable of assessing these interactions non-invasively and under *in vivo* conditions are of substantial interest. Magnetic resonance represents a powerful platform for such investigations. Here, we demonstrate that hyperpolarization, combined with low field magnetic resonance provides a particularly sensitive readout of drug-protein binding *in vivo*. At low magnetic field strength, protein binding markedly

accelerates the longitudinal relaxation of hyperpolarized probes, in some cases resulting in near-complete signal depletion, an effect that is comparatively negligible at conventional high fields. We exploit this pronounced field dependence to establish a competitive displacement assay using hyperpolarized [2-^{13}C]pyruvate as a model probe and albumin as the target protein. In the absence of a competing ligand, pyruvate binds reversibly to albumin, and the resulting acceleration of T_1 relaxation leads to rapid depletion of the hyperpolarized signal. Upon administration of a ligand, e. g. a possible drug candidate, exhibiting higher binding affinity for the same albumin side, pyruvate is competitively displaced into its free, unbound state, restoring its markedly longer T_1 relaxation time thereby producing a measurable recovery of the hyperpolarized signal. The field-dependent relaxation behavior establishes a direct readout of drug-protein binding events in a living organism.



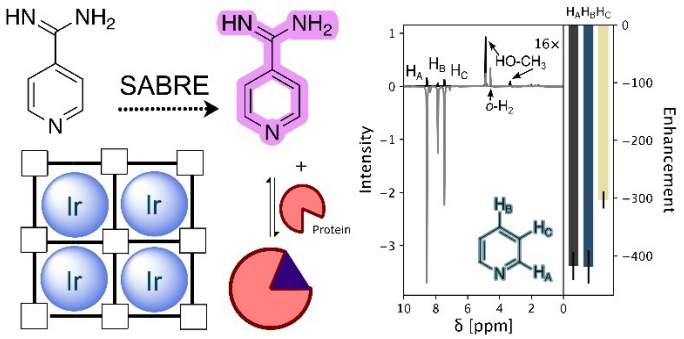
Schematic depiction of the displacement methodology to study drug-protein interactions using hyperpolarized molecules as readout probes presented in this proof-of-principle study.

SWRM 2026 SW409

Parahydrogen hyperpolarization with a reusable MOF catalyst: Applications in ligand binding

***Ashes Roy**, ashes@tamu.edu, Christian Hilty. Chemistry, Texas A&M University, College Station, Texas, United States*

Metal-Organic Frameworks (MOFs) provide tunable platforms for immobilizing molecular catalysts. Here, Chloro(1,5-cyclooctadiene)[4,5-dimethyl-1,3-bis(2,4,6-trimethylphenyl)imidazol-2-ylidene]iridium(I) ([IrCl(cod)(dimes)]) is anchored in the Zr-UiO-67-bpy framework, thereby enabling the production of nuclear spin hyperpolarization via the Signal Amplification by Reversible Exchange (SABRE) mechanism. Strong NMR signal enhancements of 419- and 99-fold were achieved for pyridine and pyrimidine substrates. Catalyst leaching was found to be minimal, as confirmed by SABRE enhancements. The catalyst was recycled for multiple experiments across repeated polarization cycles, and losses were characterized by repeated signal acquisitions. A temperature-dependent study of the signal enhancements confirmed bidentate anchoring of iridium on the MOF, leaving a single remaining ligand coordination site, and attributed the catalyst's stability to this binding mode. The catalyst was found to be selective towards one of the bulkier pyrimidine substrates, N-(pyridin-4-ylmethyl)pyrimidin-2-amine (MPMPA), over 4-amino-2-benzylaminopyrimidine (ABAP). Furthermore, the catalyst's reusability was demonstrated under biocompatible conditions by a change in spin-spin relaxation (R_2) of the ligand binding to protein. The binding of 4-amidinopyridine to the protein trypsin resulted in a significant change in R_2 relaxation in a milli-Tesla magnetic field, which offers an advantage over a high field by eliminating the relaxation due to exchange between the catalyst and ligand. In the future, the heterogeneous polarization catalyst can allow the production of metal-free hyperpolarized product solutions for biochemical and biomedical applications.



SWRM 2026 SW410

Revealing hyperpolarized 2-methylsuccinic acid for dual applications: Anti-bacterial drug discovery and renewable feedstocks

Quy S. Luu[1]*, sonquy.luu@utsouthwestern.edu, Gabriel Rocha*[2]*, Stefan Gloeggler*[1]*. (1) Advanced Imaging Research Center, The University of Texas Southwestern Medical Center, Dallas, Texas, United States(2) Biomedical Engineering, The University of Texas Southwestern Medical Center, Dallas, Texas, United States*

2-methylsuccinic acid (MSA) is a vital C5 branched-chain reagent in polymer industries, including the production of poly(butylene 2-methylsuccinate), a biodegradable polyester used in coatings and cosmetic solvents. In addition, MSA is not only applied in polymer industries but also in biology. In biology, MSA is the product of bacterial detoxification of itaconate, which is an antimicrobial compound produced by macrophages. Hence, the results of this research are toward the goal of understanding the enzymatic pathway for biosynthetic production of renewable feedstocks like methane and developing a novel antibacterial drug through the target bacterial defense mechanisms. Nuclear magnetic resonance (NMR) is one of the useful methods to study the chemical structure of intermediates for enzymatic reactions. NMR, however, has low sensitivity; to overcome this limitation, we applied a hyperpolarization technique via the parahydrogen-induced polarization (PHIP) method. We built a semi-automatic polarizer system with a bubbling, vacuum, and injection function and detected the hyperpolarized NMR signal using a conventional benchtop 1T NMR. The ^{1}H NMR signal of MSA was hyperpolarized well through adiabatic longitudinal transport after dissociation engenders nuclear alignment (ALTADENA), and parahydrogen and synthesis allow dramatically enhanced nuclear alignment (PASADENA) techniques with a high enhancement factor (6000-fold), and the longitudinal (T_1) relaxation time is approximately 5 to 15s. Alongside hyperpolarized ^{1}H of MSA, we also obtained a 3000-fold hyperpolarized ^{13}C NMR signal through the combined ALTADENA and cross-polarization pulse sequence. Ongoing research will investigate the kinetic modeling of enzyme reactions to reveal the metabolism of MSA in bacteria.

SWRM 2026 SW411

Leveraging millitesla SABRE dynamics to hyperpolarize ^{13}C in proximity to quadrupolar ^{14}N

Loren Smith*, loren.smith@duke.edu, Warren S. Warren. Duke University, Durham, North Carolina, United States*

Signal Amplification by Reversible Exchange (SABRE) and its heteronuclear variants (X-SABRE) are beginning to produce clinically usable levels of hyperpolarization on a variety of targets. This report will summarize our recent theoretical, apparatus design, and experimental work to increase polarization levels and technique generality.

SABRE and X-SABRE work through polarization transfer from parahydrogen to one of hundreds of different target ligands, mediated by reversible binding of both species to an iridium catalyst. Most experiments use a constant magnetic field tuned to a specific value (~6.5 mT for ^{1}H-SABRE, ~0.5 μT for X-SHEATH) which permits efficient transfer. While the basic SABRE/X-SABRE principles are now well understood, real applications rely on addressing challenges generally omitted in simple model systems. For example, many biologically interesting molecules contain both carbon and nitrogen in proximity; however, the fast quadrupolar relaxation of ^{14}N quenches build-up on the ^{13}C, forcing reliance on isotopically labeled species in a way that is often impractical.

Our work has focused on two- and three-dimensional tailored fields which can improve efficiency by about an order of magnitude. In exploring the expansive space of possible useful fields, we recognized a new SABRE polarization pathway available to the many ligands which contain both a heteronucleus (^{13}C or ^{15}N) and protons. Here, hyperpolarization proceeds entirely through J couplings rather than relying on the chemical shift between parahydrogen hydrides and the target nucleus. Application of this pathway greatly simplifies the equipment needed for SABRE.

The present work seeks to leverage recent research which uses shaped low-field pulses to tune J couplings in the polarization transfer complex to address this class of molecules which contain a ^{13}C neighboring a quadrupolar ^{14}N. The intuition gained from the field-independent pathway is applied to craft a pulse sequence which operates in the milli-Tesla regime and allows for significant ^{13}C hyperpolarization on ligands in which the ^{13}C is strongly bound to a quadrupolar ^{14}N. We will present both computational and experimental evidence of enhanced polarization of [1-^{13}C]-acetonitrile as a model system and discuss extensions to biological molecules.

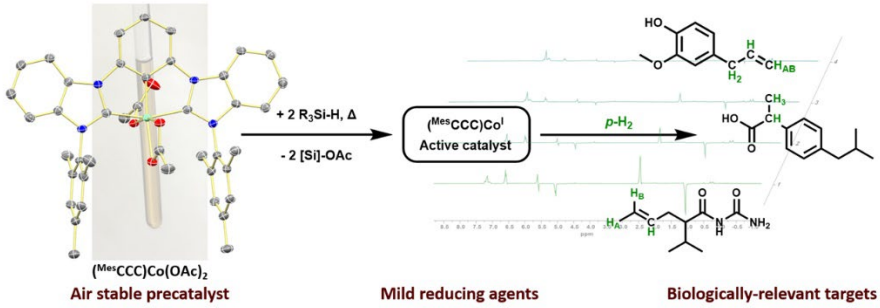
SWRM 2026 SW412

Synthesis and application bench-stable, mildly-reducible cobalt catalysts for PHIP

Brennan M. Vaught*, bvaught3@tamu.edu, Alison R. Fout. Chemistry, Texas A&M University, College Station, Texas, United States*

NMR is used ubiquitously by chemists for structural characterization, reaction monitoring, and kinetic elucidation. However, one problem with the technique concerns its inherent low sensitivity. Thankfully, mechanisms exist to create non-Boltzmann nuclear spin populations, and thus, increasing the signal-to-noise ratio (SNR) for a given NMR-active nucleus (*e.g.* ^{1}H, ^{13}C, ^{15}N, etc.); these approaches are termed “hyperpolarization.” One technique, *para*-hydrogen induced polarization (PHIP) uses the singlet spin isomer of hydrogen gas (*p*-H_2) to transfer its spin-order to a substrate of choice. This strategy significantly reduces the financial burden of hyperpolarization compared to techniques such as dynamic nuclear polarization (DNP) or spin-exchange optical pumping (SEOP), which require costly dedicated systems. PHIP has long been dominated by second- and third-row transition metals due to their ability to avoid unwanted one-electron reactivity and paramagnetic spin states that could quench potential polarization. Another advantage of heavier metal PHIP catalysts pertains to the ambient stability of their precatalyst forms, while requiring rudimentary *in situ* activation conditions (*i.e.* hydrogenation of a dienyl co-ligand). Given a strong enough ligand field, correct oxidation state, and favorable geometry, 3d-metals have been shown to perform PHIP. Yet, pyrophoric reductants (*ex.* $NaHBEt_3$) are needed for *in situ* activation of known bench-stable 3d-PHIP precatalysts. Additionally, the increased cost and scarcity of those heavier metals necessitate the need for lower-cost, more abundant, alternatives. This presentation will focus on the development

and application of a 3d-based PHIP precatalyst that was activated by tertiary silanes and a thermal trigger, as well as the application of a 3d-PHIP catalyst towards the polarization of biologically relevant small molecules.



This image depicts the general application strategy for the activation and use of the (^{Mes}CCC)Co(OAc)$_2$ precatalyst towards polarization of alkenyl substrates.

SWRM 2026 SW413

Holleman, Wiberg, and a textbook of inorganic chemistry that has lasted more than a century

***Christine Hahn**, christine.hahn@tamuk.edu. School of Mathematics and Physical Sciences, Texas A&M University-Kingsville, Kingsville, Texas, United States*

In 1898 the Dutch chemist Arnold Frederik Holleman (1859-1953) founded the textbook Inorganic Chemistry (*Leerboek der anorganische chemie*). He was a professor of chemistry in Groningen and Amsterdam. His textbook was first translated to German by Wilhelm Manchot (1869-1945) and published as the "1st Edition" in 1900. The first 21 editions were authored by A. F. Holleman, although for the 20th and 21st editions (1930 and 1937) he was represented by Ernst Hendrik Büchner (1880-1967), a lecturer at the University of Amsterdam. In 1943 Egon Wiberg (1901-1976) took over the authorship until the 90th edition and substantially revised the textbook. E. Wiberg was a professor of Inorganic Chemistry at the University of Munich. His son Nils Wiberg (1934-2007) has already assisted his father from the 34th edition on and continued the authorship with the 91th edition (1985). As content rapidly has grown on variety of areas of inorganic chemistry, further major revisions were made. N. Wiberg died in 2007 shortly after the 102nd edition of his textbook was published. The *Holleman-Wiberg* has been the most popular and comprehensive textbook for Inorganic Chemistry in Germany over a long period of time, however it is nearly unknown outside the German speaking community. Apart from a few English editions by Wiley in the early 20th century only the 101st German Edition (1995) was finally translated and published in 2001 as the "1st" modern English edition by Academic Press (Elsevier). The 103rd German edition is the latest edition and was published by De Gruyter in 2016 comprising 2600 pages, printed now in two volumes. A new English edition of the thoroughly revised 103rd edition is planned to be published by De Gruyter in near future.

SWRM 2026 SW414

Facts, ideas, and words: Lavoisier's lesson on chemistry communication

***Eszter Trufan**, trufane@uhd.edu, Elene F. Bouhoutsos-Brown. Natural Sciences, University of Houston-Downtown, Houston, Texas, United States*

Antoine Lavoisier is widely recognized for transforming chemical nomenclature and helping establish modern chemistry. Less frequently discussed is the broader philosophy presented in the opening chapters of *Elements of Chemistry* (1787), where he argues that every branch of physical science consists of three inseparable components: the facts that are observed, the ideas that represent those facts, and the words by which those ideas are expressed. For Lavoisier, language was not simply a means of recording scientific discoveries but an essential component of scientific reasoning. The same commitment to precision that characterized his quantitative measurements also guided his reform of chemical nomenclature, reflecting his belief that scientific ideas could only be communicated faithfully through clear, accurate, and unambiguous language. This presentation revisits Lavoisier's philosophy through the lens of contemporary chemistry education. His progression from facts, to ideas, to words provides an enduring model of scientific discovery. Experimental observations become scientific understanding through reasoning, and that understanding is ultimately transformed into knowledge that can be communicated, reproduced, and extended. Scientific communication is therefore not simply the final product of scientific work, but the culmination of the scientific process itself. The enduring lesson from Lavoisier is not merely that scientific language should be precise, but that scientific judgment develops through repeated movement between experimental evidence, conceptual understanding, and their faithful expression in language. Expert chemists learn to move in both directions through this cycle, using scientific communication to identify unanswered questions, recognize gaps in reasoning, and design new experiments. As generative AI increasingly produces scientifically plausible language, Lavoisier's philosophy reminds us that the central challenge of chemistry education is no longer producing words, but developing the discernment to determine whether those words faithfully represent scientific ideas and whether those ideas faithfully represent experimental reality. More than two centuries later, this remains one of chemistry's most enduring lessons and one of its greatest educational responsibilities.

SWRM 2026 SW415

Pioneers of chemical nomenclature: Torbern Bergman, his predecessors, and his followers

***Nicolay V. Tsarevsky**, nvt@smu.edu. Department of Chemistry, Southern Methodist University, Dallas, Texas, United States*

Prior to the publication of the celebrated "*Méthode de Nomenclature Chimique*" by Guyton de Morveau, Lavoisier, Berthollet, and Fourcroy in 1787, various ideas had been disseminated that paved the way to a rational, i.e., composition-based, chemical nomenclature. The most significant proponent of such a naming system was the Swedish scientist Torbern Bergman (1735-1784) who contributed to the development of the language of chemistry in several ways – not only by suggesting new names of (mostly inorganic) compounds, but also by proposing ways to represent chemical reactions, and even by attempting to use simple letter-based chemical formulas. He himself had been influenced by his compatriots Carl Linnaeus (1707-1778) whose name is associated with the binomial nomenclature still used in botany and zoology and Axel Cronstedt (1722-1765) who had worked toward the development of a composition-based classification of minerals. In this talk, the main characters and events that led to the development of systematic chemical nomenclature in the 18th century will be discussed.

SWRM 2026 SW416

Determination of magnesium levels in natural waters by conductometric titration

Linda D. Schultz*, schultz@tarleton.edu, Ayden Thao, Kyndin Breaux, Julianna Nava-Willborn. Division of Chemistry and Physics, Tarleton State University, Stephenville, Texas, United States*

Magnesium is an element of major significance. It is the third most abundant element in seawater and the sixth most abundant metal in the earth's crust. It is also an essential element to living organisms. It has numerous industrial applications but also contributes to water hardness and boiler scale, forming toxic salts. Hence, it has the potential to become a developing pollutant and its levels in water sources should be closely monitored - especially in remote and underdeveloped areas. Water samples were collected from four different sources in central Texas. These included two wells and two rivers. All samples were analyzed by three different techniques. The Hach photometric method is a portable instrument which is EPA approved. The ion chromatograph is a 'gold standard' instrument used by large municipal water facilities and research laboratories, and conductometric titration is an old method dating back to the 1930's which was never widely accepted. All three methods produced similar results, But the conductometric titration required only a fraction of the cost and was much simpler to use. Conductometric titration is worthy of further study as a method of analysis of water. (This research was sponsored by the Welch Foundation Departmental Research Grant #0012.)

SWRM 2026 SW417

From chemistry to iconic scents: The history of perfumes built on aldehydes, lactones, and damascones

Mihaela C. Stefan*, mihaela@utdallas.edu. Department of Chemistry and Biochemistry, University of Texas at Dallas, Richardson, Texas, United States*

The history of modern perfumery is closely linked with the discovery and creative use of aroma chemicals. Among the most influential organic molecules used in perfumery are aldehydes, lactones, and damascones, whose distinctive olfactory properties have transformed the vocabulary of fragrance and enabled perfumers to create effects that were difficult or impossible to achieve with natural materials alone.

This talk traces the development of these three chemical families from their early use in perfumery to their role in some of the most significant fragrances of the twentieth and twenty-first centuries. Aldehydes, particularly aliphatic aldehydes, played a defining role in the emergence of modern abstract perfumery, contributing radiance, diffusion, and a characteristic sparkling quality. Lactones introduced creamy, fruity, milky, and peach-like facets, expanding the possibilities for both floral and gourmand compositions. Later, damascones and related norisoprenoids provided powerful rose, fruity, woody, and tobacco-like nuances and became important tools for reconstructing and enhancing complex natural accords. By examining the chemistry, olfactory character, historical context, and landmark applications of these materials, the presentation explores how advances in organic chemistry repeatedly reshaped artistic practice in perfumery. Ultimately, the story of aldehydes, lactones, and damascones illustrates the continuing dialogue between science, technology, and creativity that has defined the evolution of modern fragrance.

SWRM 2026 SW418

Elemental rhymes and tunes: Using poetry and music to convey chemical ideas

Nicolay V. Tsarevsky*, nvt@smu.edu. Department of Chemistry, Southern Methodist University, Dallas, Texas, United States*

The power of the literary arts – e.g., poetry – in aiding education was recognized more than two millennia ago by Lucretius (ca. 99 – 55 BCE) in whose work *De Rerum Natura*, early atomistic ideas were presented. In the following centuries, several didactic poems dealing with the natural sciences, including alchemy and chemistry, were created. In the 16th century, music also began to be used to depict natural phenomena or the activities of the practitioners of chemistry. For instance, the work of alchemists attempting to make silver was represented by music by Jean-Baptiste Lully (1632-1687); the elements (in the Aristotelian sense) inspired music by several baroque composers, including Pietro (Antonio) Cesti (1623-1669), Michel Richard Delalande (1657-1726), Andre Cardinal Destouches (1672-1749), Jean-Fery Rebel (1666-1747), Antonio de Literes (1673-1747), and others. The book *Atalanta Fugiens* by Michael Maier (1568-1622), consists of descriptions of alchemical procedures by a combination of poems, short musical pieces (cannons), and images. In this talk, examples will be given of (al)chemical verses and musical pieces, and a recent educational Elemental Art project inspired by earlier artists will be presented.

SWRM 2026 SW419

Toward predictive organic chemical physics: From automated quantum chemistry and machine learning to fundamental reactivity

Alistair Sterling*, asterlingchem@gmail.com. Department of Chemistry and Biochemistry, The University of Texas at Dallas, Richardson, Texas, United States*

The ability to predict chemical reactivity remains a central challenge in organic chemistry. In this talk, I will describe recent efforts from our group to develop computational tools and theoretical frameworks that expand the predictive power and physical understanding of organic and organometallic reactivity. First, I will present ChemRefine, an automated computational framework that orchestrates quantum chemical and machine learning methods to enable fast, reproducible, end-to-end studies of chemical reactivity with minimal user intervention. By leveraging recent advances in computational methods, software, and hardware, ChemRefine enables routine investigation of increasingly complex mechanistic problems that would be impractical using traditional quantum chemistry approaches. I will highlight applications developed in collaboration with synthetic organic chemists to elucidate catalytic mechanisms, understand reaction selectivity, and guide experimental reaction development.
I will also discuss our broader efforts to establish a more fundamental understanding of chemical reactivity. Going beyond numerical predictions, we seek to understand the physical origins of activation barriers and bond strengths by relating them directly to the quantum mechanical nature of chemical bonding. These studies aim to identify simple, physically meaningful principles that govern reactivity across diverse classes of organic and organometallic reactions, providing a foundation for new predictive models of catalysis and molecular design.

SWRM 2026 SW420

Integrated platform for experimental discovery and predictive modeling of electron donor–acceptor complexes

***Jacquelyne Read**, jacquelyne.read@utsa.edu. Chemistry, The University of Texas at San Antonio, San Antonio, Texas, United States*

Photochemical methods have grown immensely over recent decades, leading to a diversity of approaches to access radical mechanisms under mild conditions. Instead of employing an exogenous photocatalyst, however, visible light can also be harnessed through the *in situ* formation of electron donor–acceptor (EDA) complexes that are held together by weak intermolecular forces. Despite the evolution of strategies to exploit EDAs for use in chemical transformations, identification of new EDA complexes continues to be limited by trial-and-error empiricism. We present a combined experimental and computational approach to aid the discovery of new EDA complexes and predict pairs likely to form. An experimental platform was developed to screen for EDA complex formation in a parallelized fashion, collecting 3,711 data points that not only revealed new EDA complexes but could also be used to train a machine learning model to predict EDA formation more generally. The random forest model was able to predict EDA complexes published in the literature in 2025 and 2026 with high accuracy. Applications to reaction development will be discussed, highlighting the design of our integrated platform to predict hits and guide screening for reactions of interest involving EDA complexes.

SWRM 2026 SW421

Mechanism-driven advances in synthetic organic chemistry

***Connor P. Delaney**, delaney.connor@gmail.com. The University of Texas at Dallas, Richardson, Texas, United States*

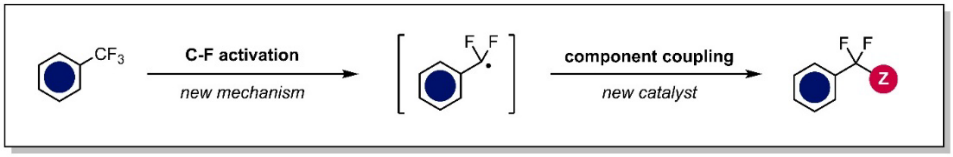
The understanding of reaction mechanisms is fundamental to the development and pedagogy of organic chemistry. I will share studies that re-evaluate the mechanisms of classic organic reactions and uncover hidden complexity. That understanding is used to develop new methods that address standing challenges in synthetic organic chemistry. In one example, our study of the cyclization step of the Blum–Ittah aziridine synthesis revealed that the reaction proceeds by a previously unconsidered concerted chain mechanism. The insight allowed us to develop new reaction conditions that afford complex aziridines in significantly higher yields than were obtained under the original conditions. The product aziridines can be used as building blocks for the construction of complex molecules, as demonstrated by our aziridine–epoxide heterocoupling approach to morpholine synthesis. In a second example, studies on Pd-catalyzed C–H activation reactions show that commonly employed ligands and silver salt additives interact to form new complexes that had not previously been considered. We show that these complexes give higher rates and yields than silver acetate in the oxidation of a model Pd(0) complex, suggesting a key role of silver-ligand interactions in the critical catalyst turnover step.

SWRM 2026 SW422

Photocatalytic C–F functionalization: Mechanism and methodology

Amit K. Jaiswal[2], Priya Saha[2], Bastian B. Skjelstad[2], Mingoo Jin[2], Ryunosuke Tomita[2], Takao Tsuneda[2], Pingyu Jiang[2], Satoshi Maeda[2], Tetsuya Taketsugu[2], ***Dennis Chung-Yang Huang****[1,2], dcyhuang@okstate.edu. (1) Department of Chemistry, Oklahoma State University, Stillwater, Oklahoma, United States(2) WPI-ICReDD, Hokkaido Daigaku, Sapporo, Hokkaido Prefecture, Japan*

Fluorinated motifs are among the most ubiquitous structural elements in modern organic and medicinal chemistry. Consequently, the selective functionalization of inert C–F bonds represents a powerful strategy for building molecular complexity. However, due to their exceptionally high bond dissociation energies, defluorinative transformations often require harsh reaction conditions that compromise chemoselectivity. Developing mild, catalytic activation modes is therefore essential to unlocking their full synthetic potential. In this presentation, two distinct photocatalytic strategies for selective C–F functionalization will be discussed. First, we describe a photoredox hydrodefluorination platform utilizing *N*-heterocyclic carbene (NHC)–boranes as hydrogen atom transfer (HAT) reagents. Detailed mechanistic investigations distinguish between two plausible pathways, complemented by a classification model that rationalizes reactivity trends across diverse borane scopes. Second, we present a defluorinative C–O coupling manifold enabled by copper photoredox catalysis, facilitating efficient access to unique difluorobenzyl ether motifs, including a compound exhibiting liquid crystalline behavior. Photochemical, photophysical, and mechanistic studies support a rare homoleptic Cu(I)–bisphosphine complex as the active photocatalyst. Together, these studies deliver practical synthetic methodologies and provide fundamental mechanistic insights into C–F activation.



SWRM 2026 SW423

Biocatalytic oxa-Pictet-Spengler reactions

David C. Miller*, dcmiller1126@gmail.com. Chemistry, Oklahoma State University, Stillwater, Oklahoma, United States*

The asymmetric oxa-Pictet-Spengler (OPS) reaction is a direct and modern approach to the synthesis of chiral dihydropyrans. Over the past ten years, the first reports for enantioselective OPS reactions for the preparation of chiral fused heterocycles such as isochromans and tetrahydropyranoindoles have emerged. While powerful, organocatalysts for these transformations (usually chiral BINOL-derived phosphoric acids and thiourea-based organocatalysts) are only available via multistep synthesis, are not readily recycled, and generally require 10 mol% loadings for efficient activity. Building upon these foundational studies, our lab's research aims to address these challenges using biocatalysis. We have discovered that squalene-hopene cyclases (SHCs) demonstrate promiscuous activity for OPS reactions using vinyl ethers as substrates. *Zmo*SHC1 demonstrates activity for the OPS reaction of tryptophol vinyl ethers for the synthesis of chiral tetrahydropyranoindoles. Directed evolution can be used to engineer variants with high activities (up to 3370 TTN) and enantioselectivities (up to 99:1 er) for this transformation. MD simulations are used to understand the role of beneficial mutations introduced during protein engineering studies, as well as the operative cyclization mode of these reactions. These initial findings are extended to substrate classes which remain unmet challenges for asymmetric organocatalysts, including substrates which lack traditional hydrogen-bonding handles required for stereoinduction and Brønsted basic heterocycles. Together,

these examples demonstrate the promise of biocatalysis to expedite access to chiral heterocyclic cores for the synthesis of bioactive small molecules.

SWRM 2026 SW424

Bifunctional boron/phosphorus organocatalysts for amide bond formation

***Christopher Sandford**, christopher.sandford@utsa.edu. Chemistry, The University of Texas at San Antonio, San Antonio, Texas, United States*

The construction of amide bonds, ubiquitous in biological molecules and pharmaceutical targets, is typically conducted with peptide coupling reagents or other stoichiometric activators that generate significant waste on process scale and are often associated with safety concerns. Boronic acid catalysts have shown promise as alternatives but are usually limited to elevated temperatures and/or have restricted substrate scopes on account of the energetic cost to eliminating water in the rate-limiting step. We have designed a new bifunctional organocatalyst that incorporates a boronic acid functionality in combination with a P(V) center as the second binding site to facilitate catalysis at room temperature with a scope of substrates that includes acyclic secondary amines and heterocycles of interest in the pharmaceutical industry. In addition to its synthetic utility, we identified novel mechanistic features that showcase how the combination of the boronic acid and phosphine oxide enable catalysis through a different monomeric mechanism to previously reported arylboronic acid catalysts, which form an activated bicyclic intermediate. In this presentation, the optimization and scope of the catalytic conditions will be discussed, applications in peptide synthesis and heterocycle formation presented, and mechanistic studies that show differences from previously published arylboronic acid catalysts will be discussed.

SWRM 2026 SW425

Cross-coupling of abundant C(sp3) electrophiles by first-row transition metal catalysts

***Reginald Mills**, lrmills2@uh.edu. Chemistry, University of Houston, Houston, Texas, United States*

Transition metal–catalyzed cross-coupling reactions are the most common strategy for carbon–carbon bond-formation in the synthesis of pharmaceuticals. While palladium-based catalysts are most often employed, other transition metals, particularly first-row and Earth-abundant metals, offer not only more economical alternatives but also unique reactivity profiles inaccessible to palladium. In first-row metal-catalyzed reactions involving C(sp3) substrates, a commonly emerging theme is the generation and capture of alkyl radicals, often implicating stepwise bond-breaking events in place of otherwise high-energy oxidative addition reactions. While open-shell catalytic pathways yield desirable opportunities for bond-breaking, paramagnetic catalytic intermediates entail unique characterization challenges, for instance due to paramagnetic line-broadening of NMR spectra, most notably 31P NMR spectra, which are otherwise invaluable for characterization of diamagnetic metal-phosphine complexes. To understand single-electron bond-breaking events by paramagnetic metals, the Mills Laboratory at the University of Houston has developed new first-row catalysts of manganese, iron, cobalt, and nickel for a variety of carbon–carbon, carbon–nitrogen, and carbon–oxygen bond-forming cross-coupling reactions under thermal conditions. This presentation will share development of such catalysts capable of functionalizing thiol-, alcohol-, and carboxylic acid–derived substrates such as thioethers, sulfones, ethers, and redox-active esters, which are used as

electrophiles in Negishi and Kumada cross-coupling reactions. Catalyst characterization techniques include paramagnetic 1H and 19F NMR spectroscopies, X-band EPR spectroscopy, and X-ray crystallography, combined with catalytic and stoichiometric studies to elucidate catalytic mechanisms and substrate design principles for future reaction development.

SWRM 2026 SW426

Decoding molecular mechanisms underpinning helium separation using halogenated polymer blends

***Michele Galizia**, mgalizia@ou.edu. The University of Oklahoma, Norman, Oklahoma, United States*

It is demonstrated that immiscible blends of halogenated polymers exhibit peculiar helium transport features, with a relevant role played by the polymer-polymer interface.
Experiments and MD simulations were combined to decode the molecular mechanisms underpinning the observed behavior.
The results indicate that the proposed blending approach provides membranes capable of operating with a wide dynamic range, with potential impact on helium harvesting from natural gas.
Fundamentals and practical implications are presented and bridged.

SWRM 2026 SW427

Lanthanide-based optical unclonable anticounterfeit features embedded in additively manufactured polymer parts

*William T. Higgins[1], Mahtab Heydari[3], Robert J. Lastowski[2], Aaron M. Tondreau[2], Bruce L. Tai[3], David D. Mascareñas[4], **Kyungtae Kim**[1], kyungtae@lanl.gov. (1) Center for Integrated Nanotechnologies, Los Alamos National Laboratory, Los Alamos, New Mexico, United States(2) Chemistry Division, Los Alamos National Laboratory, Los Alamos, New Mexico, United States(3) Department of Mechanical Engineering, Texas A&M University, College Station, Texas, United States(4) Engineering Division, Los Alamos National Laboratory, Los Alamos, New Mexico, United States*

Additive manufacturing (i.e., 3D printing) of polymeric materials contributes to mitigating carbon footprint by reducing material waste and transportation costs via on-demand, localized production. However, ensuring the authenticity of 3D-printed parts remains a critical challenge. This work aims to develop 3D-printable polymer nanocomposite materials that embed optical unclonable anticounterfeit features.
Counterfeit products threaten national security, particularly when installed in weapons, military communication systems, or nuclear power plants. These counterfeit parts often exhibit below-standard performance and can fail unexpectedly, risking the safety and reliability of mission-critical equipment and personnel. Current anticounterfeit tags and labels are intrinsically vulnerable to forgery due to their deterministic fabrication procedures. Optically verifiable unclonable features, created through unpredictable manufacturing outcomes, have been studied to prevent counterfeiting. However, these approaches have two major limitations: (i) most are made as labels that can be detached from the product surface, and (ii) the optical signals degrade over time due to photobleaching.
In this work, we developed a strategy to embed photobleaching-resistant, unclonable optical authentication features based on lanthanide complexes directly into polymer resins using pellet

extrusion 3D printing. This approach allows direct incorporation of lanthanide additives into the polymer matrix without requiring separate filament fabrication. As proof of concept, colorant masterbatches were used to visualize the random distribution of additives in printed parts. We demonstrate the ability to register and authenticate parts through optical imaging under different lighting conditions, effectively discriminating authentic parts from counterfeits.

SWRM 2026 SW428

Oxidation-mediated pathways for upcycling legacy plastics into value-added chemicals

***Hyunjin Moon**, hyunjinm@uark.edu. Chemical Engineering, University of Arkansas, Fayetteville, Arkansas, United States*

Polyethylene, polypropylene, and polystyrene account for ca. 50% of total plastic production and, correspondingly, of plastic waste generation. Plastic waste can be chemically recycled or upcycled through various processes, and this presentation focuses on how oxidation chemistry can convert these legacy plastics into upcycled products. We developed a non-catalytic oxidation process that uses peroxide to convert PP, as well as PP/PE mixtures, into polar waxes. This radical oxidation chemistry performed well on PP and PE waste containing a range of impurities. Replacing the solvent decane with the polar wax itself further demonstrated a reduction in the waste stream of the process. Next, the presentation shows how polystyrene waste can be converted into adipic acid through successive oxidative depolymerization, bioprocessing, and hydrogenation reactions. Benzoic acid was used as the solvent for the polystyrene oxidation to enhance depolymerization activity, and the reaction was carried out with an Mn/Br co-catalyst without the Co catalyst conventionally used in autoxidation, thereby reducing the environmental impact associated with Co mining. The bioprocess using *P. putida* achieved a 96% yield of *cis,cis*-muconic acid, and hydrogenation gave a quantitative yield of adipic acid, a precursor for nylon 6,6. A life-cycle assessment of the developed process showed a 66% reduction in greenhouse gas emissions, while the technoeconomic analysis indicated a higher price for adipic acid compared to its market price, requiring further improvement of the plastic upcycling system. The presentation concludes with possible directions for reducing legacy plastic waste.

SWRM 2026 SW429

Probing the influence of fixed charge chemistry on selective ion transport in cation exchange membranes

***Everett Zofchak**, ez33@rice.edu, Teja Patrice, Annie Villa, Stephen D. Sarkar, Rafael Verduzco. Chemical and Biomolecular Engineering, Rice University, Houston, Texas, United States*

Polymeric ion exchange membranes (IEMs) capable of differentiating between similarly charged ionic species are highly desirable for resource recovery applications such as lithium recovery from geothermal brines or rare earth element recovery from mine tailings. These separations are critical to a more sustainable supply chain for clean energy technologies, yet conventional IEMs lack the selectivity and throughput to be viable for these applications. Designing next-generation IEMs for these applications requires a detailed understanding of how the physicochemical properties of the membrane govern water uptake, ion partitioning, and ion diffusion. In this work, we explore the role that fixed charge chemistry plays in governing the transport properties of monovalent cations in cation

exchange membranes (CEMs). We synthesized an array of CEMs with similar backbone chemistry, network structure, and fixed charge concentration, but different fixed charge chemistries. We observe that CEMs with more delocalized, polarizable fixed charges exhibit reduced water uptake relative to their less polarizable counterparts. Despite their lower water content, these membranes show lower energetic barriers to ion transport. To rationalize these trends, we use vibrational spectroscopy to probe interactions between water, fixed charges, and counterions within the confined IEM environment. These results provide fundamental insight into how the physicochemical properties of fixed charges influence transport in IEMs, informing the design of next-generation membranes that enable more selective, energy-efficient separations for resource recovery applications.

SWRM 2026 SW430

Cellulose biomass sustainability through cellulose fiber reproduction

***Jonathan Chen**, jychen2@austin.utexas.edu. The University of Texas at Austin, Austin, Texas, United States*

Cellulose biomass is a complex of cellulose polymer abundant in natural resources and end-of-life consumer products. Conversion of cellulose biomass into new consumer products enhances sustainability of the bio-based polymer. This presentation will explicate a closed-loop roadmap to produce cellulose fiber from cellulose biomass including recycled cellulose textiles. Technical approaches for processing raw cellulose and recycled cellulose will be discussed. Wet, dry, and hybrid methods of spinning cellulose fiber will be exhibited. Finally, the presentation will give a summative comparison of these engineering methods regarding their features, feasibility, and challenges.

SWRM 2026 SW431

Sugar, polyphenolic, and catechol motifs for polymeric materials

***Samantha L. Kristufek**, samantha.kristufek@ttu.edu. Chemistry & Biochemistry, Texas Tech University, Lubbock, Texas, United States*

Bio-based small molecules are a natural resource with great potential to be incorporated into polymers due to their structural diversity and functional handles for derivatization and degradation. Particularly, polymers derived from sugars or polyphenolic compounds that contain degradable moieties in the backbone are of great promise. Incorporation into the the backbone of polymeric materials drastically changes the physical properties. Through the synthetic manipulations of these natural products, we aim to produce sustainable materials that are used for elastomers, thermosets, 3D printing, adhesives, and other applications.

SWRM 2026 SW432

Growing the future of sustainable materials with multifunctional bacterial cellulose

***Muhammad Rahman**, mmr96@cornell.edu. Mechanical and Aerospace Engineering, University of Houston, Houston, Texas, United States*

Bacterial cellulose (BC) is a bio-based renewable polymer that offers an attractive alternative to conventional non-biodegradable polymers because of its exceptional mechanical properties and hierarchical nanofibrillar structure. However, translating the intrinsic properties of BC nanofibrils into high-performance macroscopic materials remains challenging, largely because of the difficulty in achieving nanofibrillar alignment over macroscopic length scales. Additionally, poor diffusion and homogeneous integration of functional nanofillers within the three-dimensional BC network impede the development of multifunctional BC-based hybrid materials. Here, we address both critical challenges simultaneously by designing a simple, single-step biosynthesis strategy that leverages shear-induced alignment generated by controlled fluid flow in a rotational culture device during BC biosynthesis. This approach produces BC-based hybrid sheets with highly ordered nanofibrillar architectures and uniformly distributed functional nanomaterials, and the resulting materials exhibit enhanced mechanical and thermal performance. This strategy provides a versatile and potentially scalable route toward sustainable, high-performance multifunctional materials.

SWRM 2026 SW433

Elasticity dominated surface segregation in formulated products

***Buddhapriya Chakrabarti**, b.chakrabarti@sheffield.ac.uk. Physics, Kansas State University, Manhattan, Kansas, United States*

When mixtures containing both high and low molecular weight components are exposed to air, the smaller molecules tend to migrate to the surface. This phenomenon is common in industrial formulations, where the active ingredient is often a small molecule, and surface migration can lead to a significant loss of performance. I will describe a modelling framework that allows us to quantify and ultimately control this process.

SWRM 2026 SW434

Polymerized lyotropic liquid crystal membranes for monoclonal antibody concentration

***Shirin Tahazadeh**, shirin.tahazadeh@ou.edu, Reza Foudazi, Farid Talebnia Rowshan. SCBME, The University of Oklahoma, Norman, Oklahoma, United States*

This research focuses on developing nanostructured membranes using lyotropic liquid crystal (LLC) templates formed by the self-assembly of amphiphilic block copolymers. First, Pluronic P105 was functionalized to add acrylate groups at two ends (P105DA). Then, LLCs were made from solutions of P105DA with ethylammonium nitrate (EAN) ionic liquid before being cast onto a support layer and crosslinked to make ultrafiltration membranes. Polymerization conditions were optimized to preserve the ordered LLC nanostructure in polymerized LLC (polyLLC). The fabricated membrane is designed to retain monoclonal antibody (mAb) while allowing buffer components and smaller molecules to pass through the membrane. The nanostructure of the synthesized LLC and polyLLC materials was confirmed using small-angle X-ray scattering (SAXS). Molecular weight cut-off (MWCO) studies were conducted using poly(ethylene glycol) standards with different molecular weights, indicating an effective membrane pore size of approximately 5 nm. Permeability and selectivity tests demonstrated

effective mAb retention from buffered solutions. During the concentration test, the mAb concentration increased from 0.5 g/L in the initial feed to 4.4 g/L in the final retentate, corresponding to an approximately 8.8-fold increase in concentration. Electrophoretic analysis of the feed, retentate, and permeate samples further qualitatively supported the retention and concentration of mAbs by the membrane. These results demonstrate the potential of polyLLC ultrafiltration membranes for mAb concentration in biopharmaceutical processing.

SWRM 2026 SW435

Development of an interpretable machine learning framework for food additive toxicity prediction

***Sara Castillo**, scastillo20@twu.edu, Shiru Lin. Texas Woman's University, Denton, Texas, United States*

Food additives represent a chemically diverse class of compounds widely used to improve the quality, stability, flavor, and appearance of food products. Although regulatory agencies evaluate many additives prior to approval, comprehensive toxicity testing remains experimentally costly and time-consuming. As the number and complexity of food additives increase, efficient computational methods are needed to support Ames toxicity assessment. The Ames test, also known as the Salmonella/microsome mutagenicity assay, is widely used to evaluate the mutagenic potential of chemicals and is an important component of chemical safety assessment. Previous studies have demonstrated that Density Functional Theory (DFT)-derived molecular descriptors can correlate with Ames toxicity. However, models based on limited chemical datasets may have restricted predictive power and generalizability.
To address these limitations, this project proposes a structure-aware machine learning framework to predict Ames toxicity across diverse food additives. A curated dataset is constructed using publicly available food safety and chemical databases, including FDA food additive resources and PubChem. Molecular structures represented as SMILES strings are processed using RDKit and Discovery Studio to generate molecular fingerprints (Morgan/ECFP4), topological, physicochemical, and three-dimensional descriptors, while DFT calculations using DMol3 generate electronic descriptors such as HOMO/LUMO energies, chemical hardness, and dipole moments. These complementary molecular features are then integrated to train and evaluate machine learning models for Ames toxicity prediction. By combining molecular fingerprints, physicochemical descriptors, and DFT-derived electronic properties within an interpretable machine learning framework, this work aims to improve Ames toxicity prediction across structurally diverse food additives and advance computational approaches for food safety assessment.

SWRM 2026 SW436

Surrogate reference standards for RP-HPLC quantification of paracetamol: Influence of structural variability on assay values

***Japhat O. Ofosu**[1], japhat.ofosu@stu.edu.gh, Samuel Asare-Nkansah[2]. (1) Pharmaceutical Sciences, Sunyani Technical University, Sunyani, Brong Ahafo Region, Ghana(2) Pharmaceutical Chemistry, Kwame Nkrumah University of Science and Technology College of Health Sciences, Kumasi, Ashanti Region, Ghana*

The choice and application of suitable reference standards is a crucial step in High Performance Liquid Chromatography quantification as it facilitates creation of controls, calibration curves and system suitability tests. In some cases, the respective reference standard of the analyte may not be readily available or too expensive to use especially in developing countries like Ghana. In such scenarios, the use of chemically related compounds, also referred to as surrogate reference standards, can be a good substitute.The study explores the use of surrogate reference standards for RP-HPLC external calibration of paracetamol in tablets and the effect of the relative structural variations of the surrogate candidates on assay values. A cost-effective isocratic HPLC method was developed, utilizing a mobile phase of methanol and water (65:35 v/v) at pH 3.10,with a C-18 Copsil Column and UV detection at 235nm. A mixture comprising the target analyte (paracetamol) and surrogate reference standards (p-aminophenol, caffeine, acetanilide and aspirin) was analysed at a flow rate of 1.5 mL/min.The study established surrogate constant for all the surrogate reference standards and employed in a derived equation to evaluate paracetamol content.The results showed that these compounds could successfully quantify paracetamol in the absence of a paracetamol reference standard, with all measurements falling within compendial monograph limits, although structural analogs of the surrogate reference standards to the target analyte provided least mean difference of assay values and greater accuracy.These findings highlight theflexibility of reference standard selection in HPLC external calibration, offer a practical approach for researchers, small-scale pharmaceutical industries and laboratories in resource-constrained settings.

SWRM 2026 SW437

First-principles computational investigation of structural characteristics, electronic properties, and interactive coupling behavior of 12-5-12 cationic gemini surfactant

Saima Tabassum Bristi[1]*, sbristi@twu.edu, Nasrin Mirsaleh-Kohan*[1]*, Richard D. Sheardy*[1]*, Steve Bachofer*[2]*, Shiru Lin*[1]*. (1) Chemistry and Biochemistry, Texas Woman's University, Denton, Texas, United States(2) Chemistry, Saint Mary's College of California, Moraga, California, United States*

Cationic surfactants have significant importance in exhibiting unique structural, electronic, and coupling behaviors in different environments due to their dimeric structure. These surfactants are widely used in various industries, including pharmaceuticals, environmental, and materials science. This study investigates the structural characteristics, electronic properties, and coupling integrations of Cationic Gemini Surfactant:12-5-12(($CH_3(CH_2)_{11}(CH_3)_2$-N^+-$(CH_2)_5$-N^+- (CH_3 $(CH_2)_{11}(CH_3)_2$) [1]. Density Functional Theory (DFT) calculations are employed to optimize molecular structures and analyze fundamental properties across three distinct conformers: parallel, wing, and bent. Comparative stability assessments offer insight into critical surfactant characteristics, including critical micelle concentration (CMC), micelle size, and overall stability[1]. The study employs Density Functional Theory (DFT) to evaluate adsorption energies of Gemini surfactants in the presence of organic anions, Grand Canonical Monte Carlo (GCMC) simulations in Materials Studio to investigate adsorption energetics and interactive coupling behavior, and molecular dynamics simulations using GROMACS software and the CHARMM force field to investigate surfactant aggregation and micelle formation. DFT calculations show that the parallel conformer is the most thermodynamically stable (0.00 kcal/mol), followed by wing (1.24 kcal/mol) and bent (3.96 kcal/mol). GCMC simulations identify 5-phenyl-2,4-pentanedionate as the strongest single-molecule adsorber across all conformers (mean 11.197 kcal/mol), while DFT identifies ortho-bromobenzoate as the strongest binding anion (−227.47 kcal/mol with the bent conformer). MD simulations show that 5-phenyl-2,4-pentanedionate produces the strongest collective electrostatic stabilization. These results demonstrate that conformational geometry plays scale-dependent roles in governing surfactant–anion interactions, with thermodynamic stability, single-molecule adsorption, and collective aggregation

each favoring a different conformer, providing a molecular basis for the rational design of next-generation Gemini surfactants.

SWRM 2026 SW438

Chirality-induced spectral changes in multi-walled carbon nanotubes: Computational and experimental analysis

***Maya Schwickert**, mschwickert@twu.edu, Daisy Woodring, Sydney Burrows, John D. Beatty, Shiru Lin, Nasrin Mirsaleh-Kohan. Chemistry and Biochemistry, Texas Woman's University, Denton, Texas, United States*

Carbon nanotubes (CNTs), composed of rolled graphene sheets, possess unique structural and electronic properties with broad applications in materials science, electronics, and environmental technologies. This study employs Raman scattering to investigate how varying the chirality index (n,m) influences the spectral features of non-functionalized single-walled carbon nanotubes (SWCNTs) . Understanding these chirality-dependent spectra characteristics can aid in distinguishing different SWCNT structures and evaluating their selective interactions with solvents. In this study, we use Density Functional Theory (DFT) to complement the experimental analysis and provide further insight into the observed behavior. Understanding the spectral shifts is key to optimizing CNT performance and solvent adsorption applications. We analyze peak shifts, structural changes, and dispersion behavior under different laser powers and solvent exposures. Our findings offer insights into tuning CNT properties for advanced functional applications.

SWRM 2026 SW439 - Withdrawn

SWRM 2026 SW440

Octa- and tetra- Heck reaction, a novel porphyrin synthesis

***Nicholas Starrett**, colestarrett2000@gmail.com, Joaquin Bueno. Chemistry, Texas Woman's University, Denton, Texas, United States*

Porphyrins are an interesting molecule with unique photochemical uses. Ranging an abortion spectrum from around 350-450nm. These versatile properties are due to the relationship between structure and function. There is a well categorized knowledge pool of reactions in the synthesis of porphyrins. Post-synthesis tailoring of beta- and meso-pyrrole positions of core porphyrin is yet another source of attunement. Utilizing the coordination of a metal-based porphyrin bromination of all 8 available positions can be utilized using NBS reaction schemes. These brominated positions can then undergo a heck reaction giving rise to new larger multi-differential ligand porphyrins with unique properties and a larger amount of reaction sites. Key ligands containing hydrogen-bond doners and acceptors can be added increasing hydrogen bonding capabilities, framework stability, and crystalline Hydrogen organic bonding (HOF) formations.

SWRM 2026 SW441

Novel metalated porphyrin synthesis: Tuning photochemical properties for functionality

***Ireland LaBass**, ilabass@twu.edu, Nicolas Starrett, Ting Han, Katelyn Martin, Joaquin Bueno. Chemistry & Biochemistry, Texas Woman's University College of Arts & Sciences, Denton, Texas, United States*

Porphyrins have unique photochemical properties, a large absorption spectrum from 350-450nm, fluorescent and phosphorescent properties, gas storage, etc. These properties are due to the relationship between the compound's structure and function. In recent developments, the desire for metalated porphyrins has grown within the pharmaceutical and biosensor communities. Recent advances in hydrogen peroxide monitoring have large implications for improving patient monitoring. In this project, we will explore the synthetic control over the hydrolysis of platinum metalated porphyrins by tuning the reaction parameters, yield, functional groups, solubility, and other properties. Creating and characterizing a novel porphyrin with functionality, crystalline hydrogen-organic bonding formations, and stability.

SWRM 2026 SW442

Development and characterization of BSA-functionalized PNVCL particles with tunable thermoresponsive behavior for biomedical applications

***Gabriel ReCalderon**, gabrielrecalderon@my.unt.edu, Robert Smith, Tae-Youl Choi, Mohammad A. Omary. University of North Texas, Denton, Texas, United States*

Stimuli-responsive polymers have attracted significant interest for biomedical applications due to their ability to respond to environmental changes in a controlled manner. Poly(N-vinylcaprolactam) (PNVCL) is a promising thermoresponsive polymer with significant potential in biomedical applications due to extreme biocompatibility and tunable lower critical solution temperature (LCST). However, PNVCL has a native LCST of 32°C, which limits its effectiveness due to the need for a responsiveness closer to physiological temperature to execute biological applications. In this work, PNVCL will be copolymerized with acrylic acid and other hydrophilic copolymers to increase the LCST. PNVCL will also be decorated with BSA to introduce biologically relevant surface functionality and improve uptake by the pancreas and serve as an essential cog to the drug delivery system being designed. PNVCL material will be characterized through measurements of mean particle size and zeta potential to evaluate particle stability and surface properties. Thermoresponsive behavior will be investigated by monitoring optical density (OD) as a function of temperature using UV–visible spectrophotometry, allowing determination of phase transition behavior and LCST. In addition to temperature-dependent studies, the influence of environmental factors including pH and solvent composition on particle swelling, stability, and phase transition behavior will be examined. Poly(lactic-co-glycolic acid) (PLGA) systems containing BSA are prepared and characterized as a comparative control in terms of thermal response, stability, and potential suitability for biomedical delivery applications. This work seeks to establish a versatile thermoresponsive biomaterial system with tunable transition temperatures near physiological conditions, and development of protein-functionalized polymers for drug delivery.

SWRM 2026 SW443

Investigation of newly synthesized Cu(I) complex interactions with deoxyguanosine monophosphate as a model for copper and DNA interactions

***Jose E. Paniagua**, jpaniagua2@twu.edu, Haven Kennedy, Asher Johnson, Manal Rawashdeh-Omary, Nasrin Mirsaleh-Kohan. Texas Woman's University, Denton, Texas, United States*

Interactions of DNA with copper and copper complexes have attracted significant interest because of copper's ability to coordinate with nucleobases and potentially influence DNA structure and function. In particular, guanine is of interest due to its multiple coordination sites and strong affinity for copper. This study investigates the interaction between deoxyguanosine monophosphate (dGMP), a guanine-containing nucleotide, and newly synthesized Cu(I) complexes incorporating a biologically relevant ligand, as a model system for understanding copper (I)–DNA interactions. The reaction was initially monitored through visual luminescence assays, which revealed a distinct change in luminescence, suggesting an alteration in the local chemical environment. To further characterize these interactions, Fourier-transform infrared (FT-IR) and Raman spectroscopy are being used to examine changes in vibrational modes associated with functional groups in dGMP and potential copper coordination sites. Comparison of the spectra before and after reaction will provide insight into changes in the chemical environment and coordination behavior of the guanine-containing nucleotide, contributing to a better understanding of the interactions between Cu(I) complexes and DNA-related biomolecules.

SWRM 2026 SW444

Learning biochemistry: Student challenges and strategies for success

***Natalie Caracena**, ncaracena@twu.edu, **Rafaela Dominguez**, rdominguez2@twu.edu, Yunxiang Li. Texas Woman's University, Denton, Texas, United States*

Biochemistry is often perceived by students as one of the most challenging subjects in the life sciences because it requires the integration of chemical principles, molecular structures, metabolic pathways and physiological processes. From a student perspective, common difficulties include the large volume of interconnected information, difficulty visualizing molecular mechanisms, distinguishing between similar metabolic pathways and moving beyond memorization toward meaningful conceptual understanding. These challenges can be particularly significant when students encounter biochemistry for the first time. This presentation explores the major challenges students experience when learning biochemistry and the strategies they use to overcome them. Effective coping strategies include connecting new concepts to prior knowledge, using pathway maps and visual representations, practicing problem-solving rather than relying solely on memorization, studying collaboratively and seeking timely feedback from instructors and peers. The presentation will also consider how active-learning approaches and the use of real-world biological and clinical examples can help students recognize relationships among biochemical concepts. Understanding biochemistry from the student perspective can provide valuable insight for instructors seeking to improve teaching and learning. Identifying the barriers students encounter can contribute to the development of more student-centered approaches that promote conceptual understanding, confidence and long-term retention of biochemical knowledge.

SWRM 2026 SW445

Integrating competency based assessment and sustainable practices into hands-on separation methods instruction

***John D. Beatty**, jbeatty@twu.edu. Chemistry and Biochemistry, Texas Woman's University, Denton, Texas, United States*

A special topics Separation Methods course was designed to provide authentic, hands-on experience with GC-MS and HPLC while integrating competency based assessment, workforce preparation, and more sustainable laboratory practices. Rather than using traditional exams, students completed competency demonstrations and a final simulated interview for a laboratory technician position. Students participated as job candidates, brought a current résumé, and responded to interview-style questions incorporating technical competencies in sample preparation, instrument operation, calibration, data interpretation, troubleshooting, and method selection. This format connected assessment of laboratory knowledge with professional communication and preparation for technical employment. Course activities progressed from instrument fundamentals and quantitative analysis to real-sample method development using GC-MS and HPLC. Sustainability was incorporated through modifications intended to reduce solvent consumption and chemical hazards while retaining meaningful analytical experience. Liquid-liquid extractions used reduced solvent volumes, and ethyl acetate was substituted for chloroform where practical. Direct-injection mass spectrometry was also used for selected activities, reducing or eliminating mobile-phase consumption associated with chromatographic separations. These approaches emphasized waste prevention, safer solvent selection, and efficient use of existing laboratory instrumentation. This work describes the course structure, competency-based assessment model, and lower-waste GC-MS, HPLC, and MS activities that can be adapted for instrumental analysis instruction using instrumentation commonly encountered in analytical laboratories.

SWRM 2026 SW446

Discovery of selective factor XIa inhibitors as potential anticoagulant agents

***Catherine Ortiz**, CatherineOrtiz@my.unt.edu, **Savannah Bryant**, SavannahBryant@my.unt.edu, **Simran Pereira**, SimranPereira@my.unt.edu, Shakila M. Silva. Chemistry, University of North Texas, Denton, Texas, United States*

Anticoagulants are essential for treating and preventing thrombotic disorders. Most current anticoagulants target thrombin and factor Xa, central enzymes in the common coagulation pathway, and therefore carry an increased risk of bleeding. Factor XIa (FXIa), an intrinsic coagulation pathway enzyme, amplifies thrombin generation and supports clot propagation. Unlike thrombin and FXa, FXIa appears to play a greater role in pathological thrombosis than in hemostasis. This makes it an attractive target for anticoagulant development with potentially reduced bleeding risk. Despite substantial clinical interest and advancement of several FXIa inhibitors into late-stage clinical trials, no direct FXIa inhibitor has yet been approved by the FDA, underscoring the need for new inhibitor chemotypes. To identify FXIa inhibitors, we screened a focused library of glycan-based molecules, and compounds that reduced activity by at least 50% were further evaluated for potency. Michaelis–Menten kinetics, heparin competition, and salt-dependence studies probed the mechanism of inhibition and likely binding mode. Selectivity was assessed against coagulation-related serine proteases including thrombin, FXa, FXIIa, and plasmin. Coagulation assays, including prothrombin time (PT), activated partial thromboplastin time (aPTT), and kinetic PT and PTT, evaluated effects on the extrinsic and intrinsic coagulation pathways. Three compounds were found to be potent FXIa inhibitors with IC_{50} values of X, Y, and Z μg/mL. Kinetic analysis identified all three compounds as

mixed inhibitors, with increased K_m and decreased V_{max}. with increasing compound concentration. Salt-dependence studies pointed to the involvement of ionic interactions, and heparin competition studies indicated that the compounds bind at or near the allosteric heparin-binding site of the enzyme, consistent with the kinetic studies. The compounds were selective for FXIa, with no inhibitory activity against other serine proteases tested. The most potent compound did not affect PT and kPT but prolonged aPTT and kPTT in a dose-dependent manner, which is indicative of an effect on the intrinsic coagulation pathway. Together, these results identify selective mixed inhibitors of FXIa with anticoagulant properties and support further development of direct FXIa inhibitors as safer therapies for preventing life-threatening thrombotic events.

SWRM 2026 SW447

Switching luminescence through solvent effects and mechanochemistry in copper(I) chloride–niacinamide complexes

***Manal Rawashdeh-Omary**, momary@twu.edu, Mekdelawit Muleta, Habiba Kouadio, Poorna Babu. Chemistry and Biochemistry, Texas Woman's University, Denton, Texas, United States*

Copper(I) halide complexes have attracted considerable interest because of their diverse structures, tunable photophysical properties, and the abundance and low cost of copper compared with precious metals. Their luminescent properties are particularly sensitive to changes in molecular structure and chemical environment, making them attractive for applications in sensing, catalysis, and energy-related technologies. This work investigates the synthesis and photophysical properties of new Cu(I) chloride complexes containing niacinamide (vitamin B3), focusing on how synthetic methods and solvent environments influence their luminescence. Complexes are prepared using both conventional solution-based Schlenk techniques and solvent-assisted mechanochemical methods involving minimal solvent. The effects of solvent polarity, coordinating ability, and reaction conditions on emission wavelength and intensity are examined and compared with products obtained through mechanochemical synthesis. The complexes are characterized using photoluminescence spectroscopy, FT-IR, NMR, and TGA to explore relationships between synthetic conditions, structural properties, and luminescent behavior.

SWRM 2026 SW448

Mixed-ligand design of sustainable luminescent Cu(I) halide complexes: Synthetic control of structure and photophysical properties

***Manal Rawashdeh-Omary**, momary@twu.edu, Asher Johnson, Katherine Branch, Ahmad Tantish. Chemistry and Biochemistry, Texas Woman's University College of Arts & Sciences, Denton, Texas, United States*

Coinage metal complexes have attracted significant interest for applications in catalysis, sensing, energy-related technologies, and optoelectronics. Among these systems, Cu(I) halide complexes are particularly attractive because of copper’s abundance, relatively low cost, and diverse structural and photophysical properties. These characteristics make copper-based materials promising and more sustainable alternatives to precious-metal-based systems for applications such as organic light-emitting diodes (OLEDs) and volatile organic compound (VOC) sensing.
This work focuses on the synthesis and characterization of new Cu(I) iodide mixed-ligand complexes

incorporating niacinamide (vitamin B3) and another diimine ligands. We investigate how ligand identity, ligand combinations, and synthetic conditions influence the resulting structures and photophysical properties. Particular emphasis is placed on understanding how mixed-ligand environments can be used to tune the luminescence of Cu(I) complexes.
The complexes are prepared using complementary approaches, including solution-based synthesis under an inert nitrogen atmosphere, solvent-assisted mechanochemical methods, and thermally induced synthesis. These approaches provide a means of examining how reaction conditions and synthetic pathways influence structural formation and luminescent behavior.
The resulting complexes are characterized using photoluminescence, FT-IR, NMR, and UV-Vis spectroscopy to establish relationships among ligand composition, synthetic conditions, molecular structure, and optical properties.

SWRM 2026 SW449

Automating and standardizing green microplastic extraction from terrestrial soil matrices

***Jay Payne**, jpayne7@twu.edu. Chemistry & Biochemistry, Texas Woman's University, Denton, Texas, United States*

Terrestrial soils are a vital environmental sink for microplastics, yet compared with methods available for aquatic matrices, standardized extraction techniques with high recovery rates remain poorly established. Current soil methods often rely on hazardous heavy-metal salts (such as $ZnCl_2$) or involve labor-intensive manual procedures that lead to operator variability and contamination from ambient fibers. In keeping with green chemistry principles, we developed a standardized extraction procedure that uses environmentally friendly, multi-stage saline solutions (NaCl and $CaCl_2$) alongside selective oxidation of soil organic matter. Method validation uses fluorescent polyethylene microsphere standards to quantitatively assess recovery rates across spiked composite soil samples. To overcome the operational constraints of manual benchwork and prevent throughput bottlenecks, we propose incorporating benchtop robotic arms into the extraction process. Articulated robotic handling addresses several key weaknesses in the analysis by providing programmable Z-axis precision to skim floating microplastic layers without disturbing settled soil mineral deposits, enabling automated reagent delivery, and reducing background fiber contamination within a closed workstation. Pairing green density separation with robotic handling establishes a safer, high-throughput pipeline for routine soil monitoring.

SWRM 2026 SW450

Target-responsive nanointerfaces for amplified optical and electrochemical biosensing

***Sicheng Wang**, sichengwang@txwes.edu. Chemistry and Biochemistry, Texas Wesleyan University, Fort Worth, Texas, United States*

Sensitive bioanalysis depends on efficiently converting molecular recognition into measurable signals. This presentation describes a unified biosensor strategy based on target-responsive nanointerfaces that regulate fluorescence, electron transfer, and plasmon-enhanced emission. Functional nanomaterials were used as active signal-control elements: glutathione removed a MnO_2 quenching shell to restore emission from Ru(bpy)3^{2+} confined in UiO-66; target DNA closed horseradish-peroxidase-functionalized DNA tweezers to enable mediator-free electron transfer

to a porous carbon nanotube electrode; and miRNA-21 triggered catalytic hairpin assembly coupling silver-nanocluster electrochemiluminescence with gold-nanoparticle plasmonic enhancement. These dynamic structural changes reduced background and signal loss while producing amplified responses. The platforms achieved detection limits of 0.28 μM for glutathione, 2.62 ± 0.02 μM for H_2O_2 with a response time below 3 s, and 0.96 aM for miRNA-21. They also supported intracellular glutathione monitoring and miRNA analysis in real samples. Together, these studies demonstrate that engineering nanoscale organization provides a versatile strategy for sensitive optical and electrochemical biosensing.

SWRM 2026 SW451

Enhancing ionic conductivity and electrochemical stability of zinc-ion batteries via optimized PAM hydrogel matrix

***Chaekyung Kim**, chaekyungkim@my.unt.edu. Material science and Engineering, University of North Texas, Denton, Texas, United States*

Flexible aqueous zinc-ion batteries (ZIBs) have attracted growing interest for wearable electronics, owing to their high theoretical capacity, low toxicity, and low cost. However, flexible ZIBs in practice remains challenging because conventional hydrogel electrolytes tend to be mechanically weak, making them susceptible to internal short circuits and performance loss under repeated bending or stretching. Here, we introduce a polyacrylamide (PAM) hydrogel electrolyte chemically crosslinked with poly(ethylene glycol) dimethacrylate (PEGDMA) to address this limitation. According to prior literature, when comparing the properties of polymer electrolytes with different polymer chains, PAM has been reported to show the highest ionic conductivity among them. However, that high conductivity comes with a challenge that mechanical strength tends to be pretty weak, which ends up being a critical weakness for long-term stability. So, with that in mind, we carried out work aimed at improving the mechanical strength. Incorporating PEGDMA into the PAM network yields a dual-crosslinked architecture with markedly improved tensile strength and toughness relative to pristine PAM hydrogels. The denser polymer network physically impedes zinc dendrite propagation and better accommodates electrode volume changes during charge–discharge cycling. Electrochemical testing confirms that ZIBs using the PAM/PEGDMA electrolyte deliver 99% of stable capacity retention and consistent voltage profiles long-term cycles of 1000. Cycling data by pouch cell further reveals that the cells maintain their electrochemical performance even under sustained mechanical deformation. Overall, PEGDMA-reinforced PAM hydrogels offer a straightforward route toward flexible zinc-ion batteries capable of withstanding the mechanical demands of real wearable applications.

Get involved with the ACS Division of Chemical Education

***Alena Moon**[2], Alena.Moon@unt.edu, Joshua D. Edwards[1]. (1) Chemistry, Texas A&M University, College Station, Texas, United States(2) Chemistry, University of North Texas, Denton, Texas, United States*

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SWRM 2026 SW453

Design, synthesis, and characterization of functional Zr(IV) and Eu(III) macrocycle-based metal–organic frameworks for sensing applications

Habiba A. Kouadio[1,2]*, habibakouadio00@gmail.com, Charu Charu*[2]*, Manal Rawashdeh-Omary*[1]*, Shengqian Ma*[2]*. (1) Chemistry and Biochemistry, Texas Woman's University, Denton, Texas, United States(2) Department of Chemistry, University of North Texas, Denton, Texas, United States*

Metal–organic frameworks (MOFs) are highly tunable porous materials with promising applications in sensing, molecular separations, and environmental monitoring. Incorporating macrocyclic ligands into MOF structures provides additional control over pore environments and host–guest interactions, creating opportunities to develop selective and functional materials.
As part of an undergraduate Research Experiences for Undergraduates (REU) project, this work focuses on the synthesis and characterization of two new MOF systems incorporating Zr(IV) and Eu(III) metal centers with the aza-macrocyclic ligands Cyclen and TACN. The target ligands were prepared through multistep organic synthesis and characterized using H NMR spectroscopy and mass spectrometry. The resulting MOFs were synthesized using solvothermal methods and characterized to evaluate their structural, morphological, and photophysical properties.
Powder X-ray diffraction (PXRD) was used to assess crystallinity and structural integrity, while scanning electron microscopy (SEM) coupled with energy-dispersive X-ray spectroscopy (EDS) provided information on morphology, elemental composition, and distribution. Preliminary photoluminescence studies demonstrated that the Eu(III)-based MOFs exhibit strong emission, with luminescence that can be modulated or quenched by external analytes, highlighting their potential for sensing applications.
This research provides valuable hands-on training in organic synthesis, MOF fabrication, materials characterization, and photophysical analysis, while advancing the development of functional MOF materials for sensing and environmental applications.

SWRM 2026 SW454

Biocompatible polymer–gold nanoparticle composites for photothermal therapy and controlled drug delivery

Anna Ilundu[1,2]*, Annallundu@my.unt.edu, Nur Rabah*[2]*, Bisola Adeyemi*[2]*, Yonas Amare*[2]*, Mohammad A. Omary*[2]*. (1) Texas Woman's University, Denton, Texas, United States(2) University of North Texas, Denton, Texas, United States*

Conventional cancer treatments, including surgery, chemotherapy, and radiation therapy, are associated with significant toxicity and adverse side effects, motivating the development of more targeted therapeutic approaches like photothermal therapy. This project investigates gold nanoparticles (AuNPs) within biocompatible polymers as a platform for plasmonic photothermal therapy (PPTT) and controlled drug delivery. Poly(N-isopropylacrylamide) (PNIPAm); a

thermoresponsive hydrogel, and polymethyl methacrylate (PMMA); a biocompatible polymer with low cytotoxicity, were investigated as polymer components. Dynamic light scattering (DLS), ultraviolet-visible (UV-Vis) spectroscopy, and Fourier-transform infrared spectroscopy (FTIR) were used to characterize particle size, optical properties, and chemical structure, respectively. AuNPs were characterized by scanning electron microscopy (SEM) and UV-Vis-NIR spectroscopy.
DLS measurements demonstrated that PNIPAm exhibited a particle size change from approximately 50 nm in the collapsed/non-swollen state to 340.8 nm in the swollen state, confirming its thermoresponsive behavior. The PNIPAm exhibited a lower critical solution temperature (LCST) above 37.5 °C, supporting its potential for physiological applications. UV-Vis-NIR spectroscopy revealed localized surface plasmon resonance peaks at 548 nm and 947 nm, with broad near-infrared absorption indicating the ability of the AuNPs to absorb NIR light and generate localized heat. Incorporation of AuNPs into PNIPAm is expected to allow photothermal heating to raise the hydrogel above its LCST, causing polymer collapse and triggering controlled drug release. FTIR characterization confirmed successful PMMA synthesis, including the disappearance of the double-bonded carbon signal. Jurkat cells from acute T-cell lymphoblastic leukemia (T-ALL) were cultured successfully for PPTT application. The cells were recovered averagely at ~1,300,000 cells/mL and 90% viability. Overall, characterization confirmed successful synthesis of the polymer systems, incorporation of AuNPs, thermoresponsive PNIPAm behavior, and strong NIR photothermal properties. These findings support continued investigation of the polymer–AuNP platform for stimulus-responsive drug delivery and photothermal cancer therapy.

SWRM 2026 SW455

Isomorphous series of lanthanide adipate 2-bromoterephthalate coordination polymers, $Ln_2(Adip)(TPBr)_2(H_2O)_2$

Vinson Ratcliffgardy[1]*, vratcliffgardy@angelo.edu,* ***Megan Walsh***[2]*, mwalsh3@angelo.edu,* ***Sophia Nguyen***[2]*, snguyen8@angelo.edu, Thomas Hodge*[1]*, Ralph A. Zehnder*[1]*. (1) Chemistry & Biochemistry, Angelo State University, San Angelo, Texas, United States(2) Biology, Angelo State University, San Angelo, Texas, United States*

Work with actinides is very restricted due to their scarcity and them exhibiting serious radiation hazards, which is why researchers commonly use the lanthanide elements as surrogates for the actinide analogs. The feasibility of this approach in *f*-element science has been demonstrated for decades as the actinides share numerous chemical similarities with the lanthanide elements. In this work we demonstrate how variation of ligands in series of lanthanide coordination polymers changes the resulting network topologies, and coordination numbers. Reaction of various lanthanide(III) oxides, Ln_2O_3, with adipic acid and 2-bromoterephthalic acid under hydrothermal conditions resulted in the formation of $Ln_2(Adip)(TPBr)_2(H_2O)_2$. The resulting three-dimensional network consists of LnO_8 coordination polyhedra assembling as Ln_2O_{14}-clusters via edge sharing of two oxygen atoms stemming from adipate carboxylates. The adipate 2-bromoterephthalates with coordination number 8 exhibit the smallest and most shielded lanthanide coordination centers as compared to what we found in lanthanide pimelate 2-bromoterephthalates, $Ln_2(pim)_2(TPBr)(H_2O)_2$ (CN = 9), and lanthanide glutarate 2-bromoterephthalates, $Ln(glut)_2(TPBr)(H_2O)_4{*}4H_2O$ (CN = 10). We are anticipating that these networks may serve as matrices to gain access to related air stable uranium(III) networks, which would be unprecedented for U(III) mixed ligand networks that incorporate organic linking entities.

SWRM 2026 SW456

Switching emission pathways via molecular engineering in hybrid metal halides for scintillation and neutron detection

***Muhammad Sani Muhammad**, muhammad.sani@ou.edu, Bayram Saparov. Chemistry and Biochemistry, The University of Oklahoma, Norman, Oklahoma, United States*

Hybrid organic–inorganic metal halides have emerged as versatile platforms for rational materials design. Traditionally, their functional properties are primarily governed by the inorganic framework, while organic components contribute to structural stability, tunability, and processability. Here, we present a design strategy in which the organic sublattice plays a central role in determining photophysical behavior. By incorporating a stilbene-based organic emitter within two-dimensional (2D) and pseudo-2D cadmium- and zinc-based halide frameworks, we develop layered hybrid architectures in which the organic component serves as the primary luminescent center, while the inorganic framework provides structural confinement and, in cadmium-containing systems, neutron-interaction functionality. The materials were synthesized and grown as high-quality single crystals via solution-based methods, enabling precise control over composition and structure. Through optical spectroscopy and theoretical calculations, we establish structure–property relationships linking molecular design, crystal packing, and emission efficiency. Notably, incorporation of the stilbene-based emitter within the hybrid lattice results in enhanced luminescence compared with the corresponding precursor organic salt, highlighting the role of the inorganic framework in modifying excited-state dynamics and suppressing non-radiative pathways. Confinement of the organic emitter within the inorganic layers provides an additional means of controlling the emission response through its molecular and structural environment. Cadmium provides a strong neutron-interaction pathway as well, while the organic component can convert deposited energy into a measurable optical response. Integrating neutron interaction and scintillation within a single crystalline architecture provides a promising strategy for developing compact neutron-sensitive scintillating materials. Overall, this work demonstrates a generalizable approach to engineering hybrid materials in which the organic and inorganic components can be deliberately differentiated and optimized: the organic sublattice controls the emission pathway, while the inorganic framework provides structural confinement and, in Cd-containing systems, neutron-interaction functionality. This strategy opens opportunities for efficient light-emitting, scintillating, and neutron-sensitive hybrid materials for radiation detection.

SWRM 2026 SW457

Unveiling the factors governing structural evolution in entropy-stabilized cation-disordered Li_2TiO_3

***Wolalorm M. Zudor**, zudorwolalorm@gmail.com, Tianyu Li. Department of Chemistry, Louisiana Tech University, Ruston, Louisiana, United States*

Cation-disordered rocksalt (DRX) oxides represent one of entropy-stabilized materials, which exhibit high compositional tunability. However, traditional synthesis of these complex multi-component oxides relies heavily on empirical trial and error, owing to a poor understanding of the mechanisms underlying formation mechanisms. In particular, the role of pre-existing rock-salt precursors, such as lithium fluoride (LiF), in stabilizing the disordered structure remains unclear. In this work, we employ the Li_2TiO_3-$(LiF)_x$ (x = 0 to 1.0 in 0.25 increments) system as a model framework to systematically investigate how the pre-existing rock-salt precursor (LiF) drives phase formation and structural evolution from an ordered layered system to a disordered framework. Samples across the

compositional series were synthesized by solid-state reaction at 800°C. Combined X-ray diffraction (XRD) and Raman spectroscopy reveal that incorporating controlled stoichiometries of $(LiF)_x$ induces a continuous, systematic phase transition from an ordered monoclinic structure to a disordered cubic rocksalt framework (Fm-3m). Rietveld refinement confirms an increment in disordering between Li and Ti layers, characterized by a decrease in intensity of (002) reflections in the diffraction pattern and shows a concurrent reduction in cell volume across the series with the increase of LiF addition. Scanning electron microscopy indicates that the continuous incorporation of LiF leads to larger particles with more defined morphology. Furthermore, in situ synchrotron XRD data collected at the Advanced Photon Source track the reaction pathways in real time, demonstrating that LiF directly alters the solid-state reaction pathway, thereby lowering the activation barrier for DRX formation. This study aims to elucidate the role of pre-existing rocksalt precursors in driving DRX phase formation, establish structure–property–phase relationships in the entropy-stabilized oxide, and lay a framework for model-guided solid-state synthesis.

SWRM 2026 SW458

Elucidating mechanisms of chirality transfer in circularly polarized luminescent phosphors

***Victor Caycedo**, victorcay18@gmail.com, Shruti Hariyani. The University of Texas at Dallas, Richardson, Texas, United States*

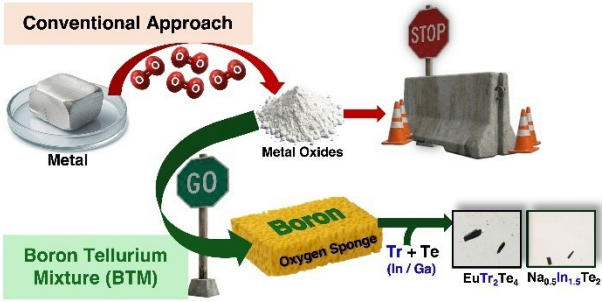
Optical encryption technologies are currently at the forefront of cyber and data security applications, given the increasingly sophisticated nature of modern cyberattacks. Luminescent materials such as rare-earth substituted inorganic phosphors offer a unique combination of robust chemical stability and precise control over optical properties, making these materials exceptional candidates to advance the field. In this work, we seek to enhance the capability of these phosphors through the introduction of circularly polarized luminescence (CPL). While inorganic phosphors lack the inherent chirality required to produce CPL, we are imparting chirality to our luminescent materials through surface functionalization with chiral ligands. The success of chirality transfer was first probed through structural characterization including powder X-ray diffraction and Fouirer transform infrared spectroscopy, as well as photoluminescence spectroscopy and circular dichroism measurements. By further exploring the mechanisms controlling chirality transfer in periodic solids and their resulting CPL properties, we aim to develop advanced tunable phosphors which can emit light into left- and right-handed polarized states to more effectively encrypt data. By performing surface treatments using chiral organic molecules such as cysteine, we have been able to observe unique circular dichroism (CD) signals, with g_{CD} values around 10^{-4}. These preliminary experiments demonstrate that we were able to impart chirality from the ligands to the surface of our materials. We have successfully performed this surface functionalization on several phosphor hosts with varied photoluminescence profiles, including $BaMgAl_{10}O_{17}:Eu^{2+}$, $Y_3Al_5O_{12}:Ce^{3+}$, and $Sr_2Si_5N_8:Eu^{2+}$

SWRM 2026 SW459

Synthesis of low-dimensional metal tellurides from boron-mediated flux mixtures

***Chirantha P. Edirisinghe**, chirantha_edirising1@baylor.edu, Subhendu Jana, Paul A. Maggard. Chemistry and Biochemistry, Baylor University, Waco, Texas, United States*

Low-dimensional telurides represent a structurally diverse class of materials. However, new synthetic discoveries remain challenging due to the limitations in conventional solid-state reactions, which often limit access to metastable and structurally complex phases. We demonstrate boron-tellurium mixtures (BTMs) as reactive fluxes that enable the synthesis of low-dimensional tellurides from binary metal oxides, avoiding the handling challenges associated with elemental or binary metal precursors. Using this approach, we synthesized single crystals and pure polycrystalline phases of ternary tellurides MTr_2Te_4 (M = Eu, Sr; Tr = In, Ga), which feature one-dimensional $[Tr_2Te_4]^{2-}$ chains separated and charge-balanced by divalent metal cations. All compounds exhibit semiconducting properties with direct band gaps of 0.93 to 1.10 eV. Extending this synthetic strategy to alkali metal-telluride systems, we accessed a TlSe-type solid-solution series $[Na_xIn_{1-x}]InTe_2$ (x = 0.5, 0.75, 1.0), stabilizing the relatively rare In(I) oxidation state with Na(I) cations sharing the same crystallographic site. This low-dimensional telluride framework consists of infinite $[In_2Te_4]^{2-}$ chains along the *c*-axis with mixed monovalent Na/In sites between the chains. Progressive substitution of In(I) for Na(I) expands the unit cell and increases interatomic distances, demonstrating the tolerance of this structure type toward mixed low-valent cations without disrupting the telluride framework. This structural evolution is further reflected by a systematic decrease in the bandgap from 0.95 to 0.79 eV with increasing In(I) content. Electronic structure calculations reveal that changes in the Na/In molar ratio selectively perturb the cation-derived conduction band while leaving the Te-5p-derived valence band associated with the one-dimensional chains largely unchanged. These findings establish boron-mediated flux mixtures as a broadly applicable synthetic strategy to expand the landscape of low-dimensional tellurides, enabling access to new structural motifs and unusual oxidation states.



SWRM 2026 SW460

How incorporating Zn into $Sn_2Nb_2O_7$ affects structure and properties for pigment applications

***Mariah Carrillo**, mariah.n.carrillo@gmail.com, Melvin Balderas, Bita Amiri, Robin T. Macaluso.*
Chemistry, The University of Texas at Arlington, Arlington, Texas, United States

The search for inorganic pigments that reduce or eliminate the use of toxic metals is an outstanding challenge of the pigment industry. The objective of this study was to investigate the substitution limits and examine structural trends in a new family of compounds, $Sn_{2-x}Zn_xNb_2O_7$. To accomplish this, we conducted solid-state synthesis for $0 \leq x \leq 1$ and structural analysis by powder X-ray diffraction (XRD). XRD results show that Zn is successfully incorporated into $Sn_2Nb_2O_7$, which possesses a cubic pyrochlore structure ($A_2B_2O_7$). Theory suggests that the Zn^{2+} substitution occurs at the A-site, replacing the Sn^{2+}. However, XRD analysis also shows that Zn substitution reaches a solubility limit of $x = 0.4$ and that the reaction produces $ZnNb_2O_6$ as a side product. Visible observations show a color shift in the pigment from yellow to orange. Furthermore, diffuse reflectance spectroscopy (DRS) demonstrates a tunable band gap from 2.39 eV to 2.27 eV, highlighting the role of Zn substitution for optimizing the optical properties for inorganic pigments that possess lower environmental and biological risk.

SWRM 2026 SW461

Rare earth metal (Ce and Pr) doped lanthanum cuprate (La_2CuO_4) aerogel based composite for hybrid supercapacitor application

***S M ANYET ULLAH SHOHAG**, anyetullah@gmail.com, Kenneth J. Balkus Jr.. Chemistry and Biochemistry, The University of Texas at Dallas School of Natural Sciences and Mathematics, Richardson, Texas, United States*

Hybrid supercapacitors have become attractive options for effective and sustainable energy storage solutions. It heats up in tandem with the switch to renewable energy sources and the development of electrified transportation networks. Supercapacitors meet the needs of increased energy density storage and high-power density. This research explains Perovskite composites for hybrid supercapacitor electrodes include Ce and Pr doped La_2CuO_4, Templated Carbon (TC) and Carbon Nanotube (CNT). Ce and Pr doped La_2CuO_4 was synthesized using a modified sol-gel method as shown in the figure 1. The structural morphology and size of the perovskites were characterized using XRD, SEM, TGA and DLS as shown in the figure 2. The particle size was found around 300nm with a BET Surface Area of 1.98 m^2/g. Cyclic voltammetry was used to get the initial electrochemical performance of the working electrode. The outcomes demonstrate encouraging redox peaks in between 0.5 to 1.5V for both Ce and Pr doped La_2CuO_4. Galvanostatic charge-discharge (GCD), electrochemical impedance spectroscopy, and cycling stability tests are underway and will be ready before November (ACS SWRM 2026).

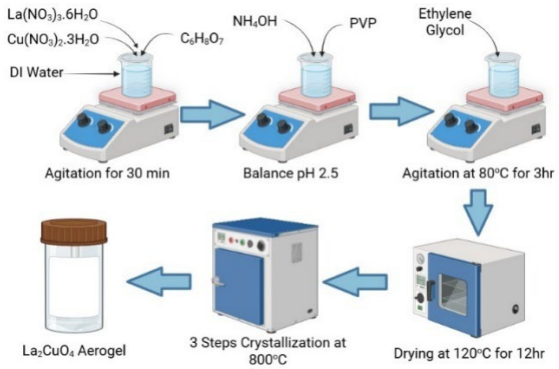


Figure 1: Synthesis of Ce and Pr doped La_2CuO_4 using a modified sol-gel method.

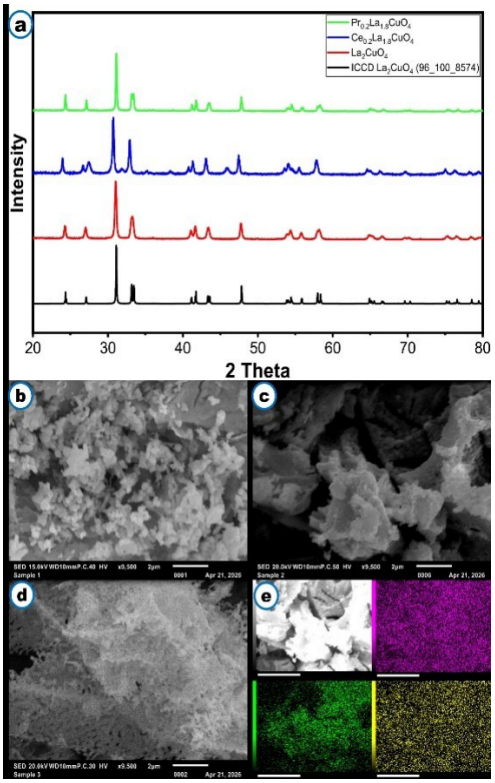


Figure 2: (a) X-ray diffraction patterns of La_2CuO_4, $La_{1.8}Ce_{0.2}CuO_4$ and $La_{1.8}Pr_{0.2}CuO_4$ perovskite samples, (b) SEM image of La_2CuO_4, (c) SEM image of $La_{1.8}Ce_{0.2}CuO_4$, (d) SEM image of $La_{1.8}Pr_{0.2}CuO_4$, (e) EDS image of La_2CuO_4.

SWRM 2026 SW462

Exploring multimetal coordination in salophene-based complexes

Tanzim Ahsan, *dal127363@utdallas.edu, Connor Naseiro, Kenneth J. Balkus. The University of Texas at Dallas School of Natural Sciences and Mathematics, Richardson, Texas, United States*

Supercapacitors are devices that have longer operation life and a faster rate of discharge when compared to a normal battery. They have applications in various fields such as transportation. In this study, the goal is to produce a supercapacitor with multiple redox active metals in an electrode using a multi-metallic covalent organic framework (COF). To synthesize the COF, Nickel Acetate and Copper Acetate were dissolved in Dimethylformaldehyde under N2 atmosphere. After 30 minutes, the organic linker 1,3,5-tris-(4-aminophenyl) triazine was added and the solution was mixed overnight at 100 C. The resulting product was isolated using vacuum filtration to obtain Ni-Cu COF. The COF was characterized through Infrared Spectroscopy, Thermogravimetric Analysis, X-Ray Diffraction, and Raman Spectroscopy to confirm the structure and assess stability. The CV will show multiple redox peaks within the operational voltage window, confirming the redox activity of the multi metal COF. The enlarged closed area proves the increased energy storage capabilities. In conclusion, the multiple redox active metals have led to increased energy storage capabilities of supercapacitors and highlight the application of mixed metal COF in supercapacitor storage, especially in renewable energy.

SWRM 2026 SW463

Frustrated Lewis pair-functionalized PCN-333(Cr) for enhanced hydrogen binding and storage at ambient temperature

***Roknuzzaman Roknuzzaman**, fnuroknuzzaman@my.unt.edu, Shengqian Ma. Chemistry, University of North Texas College of Science, Denton, Texas, United States*

Enhancing the interaction of molecular hydrogen with porous materials is crucial for improving hydrogen storage at ambient temperature because the low polarizability of hydrogen results in weak van der Waals interactions with conventional adsorbents. Metal–organic frameworks (MOFs) have been widely investigated for high-pressure hydrogen storage because of their high surface areas, tunable pore structures, and chemical versatility. However, the relatively weak interactions between hydrogen and most MOFs limit their hydrogen binding energies and consequently their storage capacities at ambient temperature. Herein, we incorporated frustrated Lewis pairs (FLPs) into PCN-333(Cr) (FLP@PCN-333(Cr)) through a solvent-assisted ligand incorporation strategy to introduce additional binding/interaction sites for hydrogen. Successful incorporation of the FLP components was investigated using FTIR, NMR spectroscopy, SEM, and XPS, while PXRD measurements confirmed retention of the framework structure following functionalization. In situ FTIR spectroscopy was employed to probe the interactions between molecular hydrogen and FLP@PCN-333(Cr), while in situ DRIFTS measurements provided further insight into the hydrogen binding environment. Analysis of temperature-dependent spectroscopic data using the van't Hoff relationship yielded an apparent hydrogen binding energy of approximately 17.9 kJ/mol. Finally, high-pressure (100 bar) hydrogen adsorption measurements revealed a significant enhancement in hydrogen uptake for FLP-functionalized MOFs compared with the corresponding pristine frameworks at 298K. These findings demonstrate that inclusion of molecular FLP sites in porous frameworks offers a viable method for increasing hydrogen–framework interactions in near-ambient conditions. In a broader sense, our work offers a molecular-level understanding of the rational design of FLP-functionalized porous materials for hydrogen storage and other small-molecule activation processes.

SWRM 2026 SW464

Discovery of 2D perovskite $Cs_2CdI_2Cl_2$ & role of ns^2 lone pair-driven anharmonicity in $Cs_2MI_2Cl_2$ (M = Cd, Sn) local structure

*Kulatheepan Thanabalasingam[1], Mihir S. Singh[1], Douglas H. Fabini[3], Milinda Abeykoon[2], **Kyle McCall**[1], kylemccall2014@u.northwestern.edu. (1) The University of Texas at Dallas Erik Jonsson School of Engineering and Computer Science, Richardson, Texas, United States(2) Brookhaven National Laboratory Energy & Photon Sciences Directorate, Upton, New York, United States(3) Paul Scherrer Institut PSI, Villigen, AG, Switzerland*

Halide perovskites are next-generation photovoltaic candidates due to their remarkable properties, such as defect tolerance, low thermal conductivity, and efficient light emission, which arise in part from the structural dynamics and disorder of the crystal lattice. However, the limits of this disorder are unclear – that is, how far can the perovskite structure be stretched while maintaining similar properties? The 2D Ruddlesden-Popper perovskites (RPs), $A_{n+1}B_nX_{3n+1}$, are quasi-2D <100> structure variants of 3D perovskites. However, only a few inorganic 2D perovskites are known, with the most promising semiconductors uniformly based on ns^2 cations. Here we report the synthesis and characterization of the new 2D RP perovskite $Cs_2CdI_2Cl_2$, along with pair distribution function results indicating dynamic symmetry breaking in $Cs_2SnI_2Cl_2$ that is absent in the non-ns^2 $Cs_2CdI_2Cl_2$

counterpart. The new semi-transparent heteroleptic 2D RP perovskite, $Cs_2CdI_2Cl_2$ crystallizes in the prototypical K_2NiF_4 structure type (*I*4/*mmm* space group) with lattice parameters ***a*** = ***b*** = 5.4450(11) Å and ***c*** = 18.135(6) Å. This is the highest allowable symmetry for Ruddlesden-Popper perovskites, and is isostructural with $Rb_2CdI_2Cl_2$, $Cs_2SnI_2Cl_2$, and $Cs_2PbI_2Cl_2$ analogues. Photoluminescence measurements show warm yellow broadband emission peaking at 570 nm, with dual excitation at 270 nm and 340 nm and a large Stokes shift of 1.47 eV. Density functional theory calculations show a surprisingly dispersive band structure for electrons in all 3 dimensions despite the anisotropy of this 2D crystal structure, with electron effective masses of $0.44m_e$ in-plane and $0.33m_e$ out-of-plane. Comparison of $Cs_2CdI_2Cl_2$ with the $5s^2$-bearing compound $Cs_2SnI_2Cl_2$ enables us to connect structural features to the presence or absence of a lone pair. Here, we present preliminary local structural data derived from X-ray scattering data from 5 to 400 K. Pair distribution function (PDF) analysis highlights a strong local structure deviation in $Cs_2SnI_2Cl_2$ that is not found in $Cs_2CdI_2Cl_2$, indicating the lone pair drives dynamic structural deviations. Importantly, powder X-ray diffraction confirms that the long-range crystal structure does not change over this temperature range, showcasing that the local and long-range order differ. This work provides insight into the behavior of lone pair electrons in an anisotropic, mixed-anion environment, building towards achieving high-quality semiconductors with complex compositions.

SWRM 2026 SW465

Isomorphous series of lanthanide pimelate 2-bromoterephthalate coordination polymers, $Ln_2(pim)_2(TPBr)(H_2O)_2$

Chanvisal Tith[2]*, ctith@angelo.edu,* ***Evan Hernandez***[1]*, ehernandez147@angelo.edu,* ***Stephen Hale***[2]*, shale9@angelo.edu, Jackson Turner*[1]*, Ralph A. Zehnder*[1]*. (1) Chemistry & Biochemistry, Angelo State University, San Angelo, Texas, United States(2) Biology, Angelo State University, San Angelo, Texas, United States*

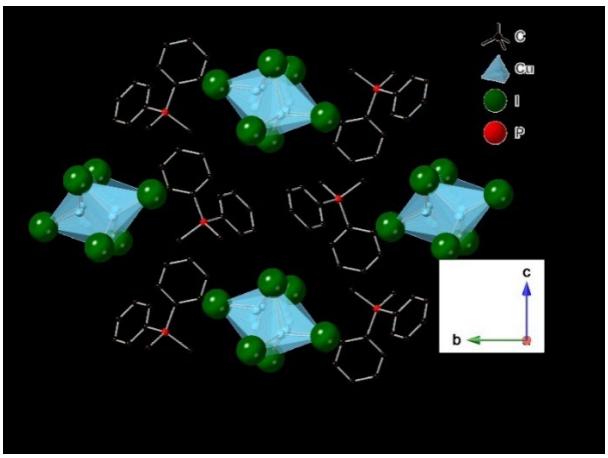
Studying extended series of lanthanide coordination compounds has been utilized to draw conclusions for their potential actinide analogs. Due to the sparse availability and the radioactivity of the actinides, particularly the trans uranium elements, scientific studies have been very challenging and restricted. Due to the chemical similarities between the actinide and non-radioactive lanthanide elements nuclear science has advanced by frequently utilizing the lanthanide elements as surrogates for their actinide counterparts. In this work we are showcasing an extended series of lanthanide pimalate 2-bromoterephthalates. At first we synthesized neodymium pimalate bromoterephthalate, $Nd_2(pim)_2(TPBr)(H_2O)_2$, utilizing hydrothermal methods. This compound forms a three-dimensional network of NdO_9-coordination polyhedra interlinked via the pimelate and 2-bromoterephthalate entities. Previously, we created a small series of lanthanide glutarate 2-bromoterephthalates, $Ln(glut)_2(TPBr)(H_2O)_4{*}4H_2O$, with Ln = La, Ce, Pr, and Nd. In contrast to the pimelate analogs, the glutarates form a coordination network of interlinked LnO_{10}-polyhedra. We have been unsuccessful in extending that series beyond neodymium, which we attribute to the rather large coordination number of ten and the decreasing ionic radius of the lanthanide cation along the series. This work is about accessing the pimaletes beyond the Nd-counterpart as a potential result of the reduced coordination number of nine.

SWRM 2026 SW466

Synthesis, crystal structure and optical properties of $(CH_3)_2(C_6H_5)_2PCu_2I_3$

***SHAK ABIR HOSSAIN**, shak.abir.hossain-1@ou.edu, Bayram Saparov. Chemistry and Biochemistry, The University of Oklahoma, Norman, Oklahoma, United States*

Recently, copper(I)-based hybrid metal halides have attracted significant attention as promising alternatives to lead-based halide perovskites because of their earth-abundant, non-toxic, cheap elemental compositions, solution processability and excellent photophysical properties. Copper(I) metal halides belonging to “123” family often show low photoluminescence quantum yields due to short Cu-X interchain distances that promote rapid energy transfer. In this work, we present a new hybrid organic-inorganic metal halide $(CH_3)_2(C_6H_5)_2PCu_2I_3$, synthesized as single crystals with lengths up to 0.7 cm using anti-solvent diffusion method. The compound crystallizes in the monoclinic $P2_1/n$ space group, featuring one-dimensional edge sharing $[Cu_2I_3]^-$ chains separated by $[(CH_3)_2(C_6H_5)_2P]^+$ organic cations. Their structural and optical properties are investigated using single crystal X-ray diffraction, photoluminescence (PL) and photoluminescence excitation (PLE) spectroscopy measurements. The single crystals exhibit a broad emission band centered at 533 nm when excited at 370 nm, corresponding to a large Stokes shift of 163 nm. These studies provide important insights into the composition-structure-optical property relationships in this important class of new Cu(I)-based optical materials.



One dimensional crystal strucrure of $(CH_3)_2(C_6H_5)_2PCu_2I_3$

SWRM 2026 SW467

Synthesis, structural diversity, and optical properties of a series of hybrid organic-inorganic copper(I) bromides

***Tamanna Akhter Pinky**, tamanna.pinky@ou.edu, Kanika Parashar, Bayram Saparov. Chemistry and Biochemistry, The University of Oklahoma, Norman, Oklahoma, United States*

Recently, hybrid organic-inorganic copper(I) metal halides have attracted significant attention due to their intriguing optical properties and low-cost solution processability. Here, we report a series of trimethylphenylammonium ($TMPA^+$)-based copper(I) bromides synthesized through a slow-evaporation method. By controlling the stoichiometry of CuBr and TMPABr precursors, distinct copper(I) bromide structural units $[Cu_2Br_4]^{2-}$, $[Cu_6Br_{10}]^{4-}$, and $[Cu_4Br_6]^{2-}$ can be obtained. Each compound demonstrates distinct emission colors of blue, orange, and greenish-yellow, corresponding to $[TMPA]_2[Cu_2Br_4]$, $[TMPA]_4[Cu_6Br_{10}]$, and $[TMPA]_2[Cu_4Br_6]$, respectively. The first two compounds have zero-dimensional (0D) crystal structures, whereas $[TMPA]_2[Cu_4Br_6]$ features a unique one-dimensional (1D) structure. Interestingly, the observed greenish-yellow emission of $[TMPA]_2[Cu_4Br_6]$

is also unique, in contrast to the typical orange-red emission of 0D $[Cu_4Br_6]$-based compounds. This study emphasizes the influence of structural dimensionality on photoluminescence. The tunable optical properties highlight the potential of these materials for applications such as multicolor photopatterning, information encryption, and anti-counterfeiting.

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SWRM 2026 SW469

Exploring the structural and functional properties of a novel category of hybrid double metal halide perovskites

***Kanika Parashar**, kanika.parashar-1@ou.edu, Tamanna Akhter Pinky, Bayram Saparov. Department of Chemistry and Biochemistry, The University of Oklahoma, Norman, Oklahoma, United States*

Layered hybrid double metal halides have recently gained attention as promising lead-free alternatives to address the instability and toxicity issues associated with lead in metal halide perovskites. So far, only Ag(I)-based double metal halides have been explored, with very few reports on Cu(I)-based alternatives. In this work, we investigate the synthesis and properties of a new category of layered hybrid double metal halides: two pure bromide compounds, $(C_2H_{10}N_2)_4CuBiBr_{12}$ and $(C_2H_{10}N_2)_4AgBiBr_{12}$, and two mixed bromide/iodide compounds, $(C_2H_{10}N_2)_4CuBiBr_5I_7$ and $(C_2H_{10}N_2)_4AgBiBr_5I_7$. These compounds display a two-dimensional layered structure with a unique arrangement of organic layers, featuring an extra halide interlayer between them, achieved using the smallest diammonium cation, ethylene diammonium. With their semiconductor band gaps, they exhibit anisotropic charge transport properties with low semiconductor resistivities. Moreover, unlike typical layered metal halides, all these compounds demonstrate an unexpected conductive ab-plane, highlighting the potential influence of the interhalide layer on their electronic structure. These exciting findings are discussed alongside thermal properties, density functional theory calculations, and optical characterization experiments.

SWRM 2026 SW470

Degradation and fouling of anion-exchange membranes in a semi-pilot MEC treating fermented food waste

***Minsu Noh**[1,2], shalstn23@kier.re.kr, Hwi Jong Jung[1,2], Yuri Kim[1,2], Jiye Lee[1], jaewoo jeong[1], EunJeong Shin[1], KoChang Hyun[2], LeeJi Eun[2], Soo Youn Lee[1], Sahng Hyuck Woo[3]. (1) Korea Institute of Energy Research, Daejeon, Daejeon, Korea (the Republic of)(2) Chonnam National University, Buk-gu, Gwangju, Korea (the Republic of)(3) Anyang University, Anyang-si, Gyeonggi-do, Korea (the Republic of)*

Microbial electrolysis cells (MECs) are promising for sustainable hydrogen production, yet their practical application remains constrained by the limited durability of ion-exchange membranes (IEMs), which act as critical solid-state electrolytes. In this study, we investigated the physicochemical degradation of the AMI-7001 anion exchange membrane (AEM) in a 50 L semi-pilot MEC system fed with fermented food waste.

SEM, EDS, and FTIR-ATR analyses were performed to evaluate the structural and chemical changes of the membrane surface. The results indicated the accumulation of inorganic foulants (e.g. calcium-based scales and organic acids derived from fermented food waste), along with the irreversible degradation of quaternary ammonium functional groups within the polymer matrix during prolonged alkaline operation. These alterations increased membrane resistance and impeded hydroxide (OH^-) ion migration. Electrochemical impedance spectroscopy (EIS) confirmed that rising internal resistance corresponded with surface fouling accumulation, leading to a proportional decline in electrochemical performance (peak current density: 2.3 A/m^2, applied voltage: 1 V, hydrogen yield: 4.17 L-H_2/g TCOD). Although chemical oxygen demand (COD) removal efficiency remained stable near 70%, system performance deteriorated due to the decoupling of organic substrate oxidation from ionic flux. Furthermore, a preliminary TEA regarding membrane management using 0.5 M NaOH cleaning demonstrated its potential as an effective strategy to mitigate such fouling. Overall, these findings provide practical insights into key factors that must be addressed to enhance membrane durability in MEC systems.

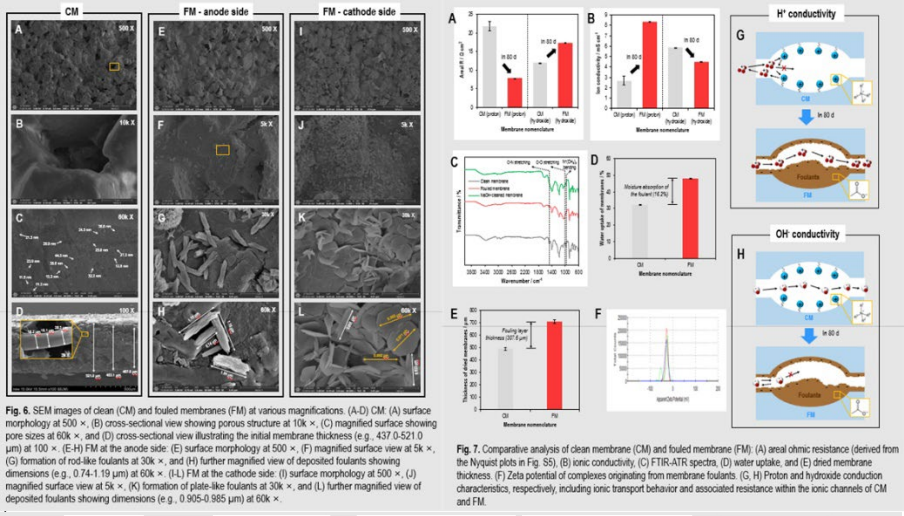


Fig. 6. SEM images of clean (CM) and fouled membranes (FM) at various magnifications. (A-D) CM: (A) surface morphology at 500 ×, (B) cross-sectional view showing porous structure at 10k ×, (C) magnified surface showing pore sizes at 60k ×, and (D) cross-sectional view illustrating the initial membrane thickness (e.g., 437.0-521.0 μm) at 100 ×. (E-H) FM at the anode side: (E) surface morphology at 500 ×, (F) magnified surface view at 5k ×, (G) formation of rod-like foulants at 30k ×, and (H) further magnified view of deposited foulants showing dimensions (e.g., 0.74-1.19 μm) at 60k ×. (I-L) FM at the cathode side: (I) surface morphology at 500 ×, (J) magnified surface view at 5k ×, (K) formation of plate-like foulants at 30k ×, and (L) further magnified view of deposited foulants showing dimensions (e.g., 0.905-0.985 μm) at 60k ×.

Fig. 7. Comparative analysis of clean membrane (CM) and fouled membrane (FM): (A) areal ohmic resistance (derived from the Nyquist plots in Fig. S5), (B) ionic conductivity, (C) FTIR-ATR spectra, (D) water uptake, and (E) dried membrane thickness. (F) Zeta potential of complexes originating from membrane foulants. (G, H) Proton and hydroxide conduction characteristics, respectively, including ionic transport behavior and associated resistance within the ionic channels of CM and FM.

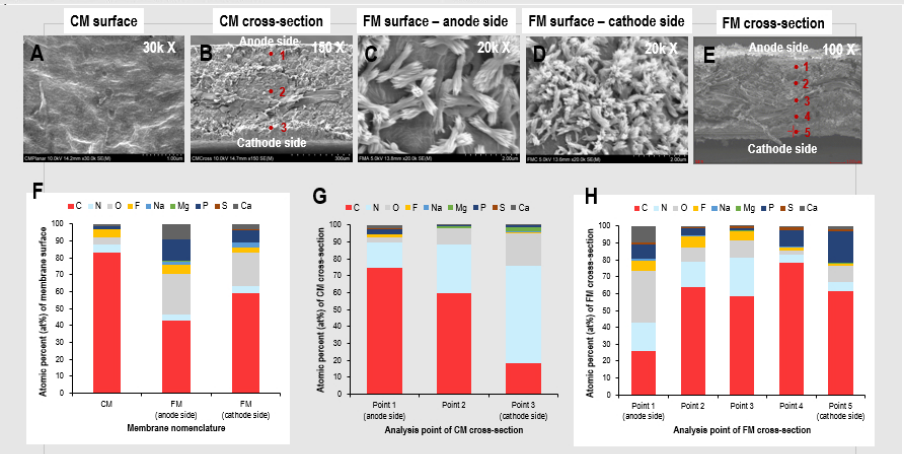


Fig. 8. Chemical composition analysis of the clean membrane (CM) and fouled membrane (FM): (A) surface image of CM, (B) cross-sectional image of CM with the analysis point, (C) surface image of the anode side of FM, (D) surface image of the cathode side of FM, (E) cross-sectional image of FM with the analysis point, (F) atomic percentages of CM and FM surfaces, (G) atomic percentages of the CM cross-section, and (H) atomic percentages of the FM cross-section. EDS mapping results for the CM surface, FM surface, and FM cross-section are provided in the Supporting Information (Fig. SX).

SWRM 2026 SW471

Effects of a NiO coating on FTO|WO_3-$BiVO_4$ photoanodes for TEMPO mediated conversion of HMF to DFF

***Md Lutfor Rahman**, lutfor.rahman@tcu.edu, Benjamin D. Sherman. Department of Chemistry and Biochemistry, Texas Christian University, Fort Worth, Texas, United States*

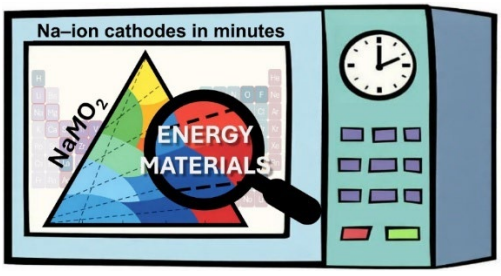
2,5-Diformylfuran (DFF) is a significant intermediate material in pharmaceuticals, fine chemicals, and biodegradable polyester and is produced from carbohydrate converted biomass followed by selective oxidation of 5-hydroxymethylfurfural (HMF). Critical to the oxidative formation of DFF is avoiding the formation of byproducts (viz., 2,5-furandicarboxylic acid (FDCA) or 5-hydroxymethyl-2-furan carboxylic acid (HMFC)), low faradic efficiency, and low percent yield. To overcome this constraint, a NiO layer has been incorporated on FTO|WO_3-$BiVO_4$ where NiO acts as an effective hole transport layer due to its favorable valence band alignment and hole mobility relative to traditional materials. In the current research, FTO|WO_3-$BiVO_4$-NiO electrodes are being used for driving TEMPO-mediated HMF to DFF conversion in acetonitrile solution. Photoelectrochemical investigations including cyclic voltammetry, chronoamperometry, and electrochemical impedance spectroscopy are being used to evaluate the influence of NiO on interfacial charge transfer and the photoelectrosynthetic performance of the system. Comparative study with FTO|WO_3-$BiVO_4$ and FTO|WO_3-$BiVO_4$-NiO photoanodes shows promising improvements in the photocurrent performance and faradaic efficiency for the formation of DFF attributed to the presence of the NiO layer coating.

SWRM 2026 SW472

Layered Na-ion cathodes in minutes: Microwave synthesis as a platform for phase and composition control

***Matthew Wright**, matthew-alex-wright@hotmail.com, Ram Seshadri. Materials, University of California Santa Barbara, Santa Barbara, California, United States*

Layered Na*M*O_2 oxides are leading Na-ion cathode candidates, but conventional solid-state routes are slow, require sacrificial excess Na, and give limited access to specific stacking polymorphs. We present a susceptor-assisted microwave heating procedure that prepares these materials in minutes, and show that the speed of the reaction is itself a synthetic handle. Because the reaction is short, Na is not lost to volatilization, so target stoichiometries are reached directly from stoichiometric precursors, and phases that sit outside the equilibrium phase field become accessible. Which stacking sequence forms is set by the Na content of the precursor alone, with all other conditions held fixed, so a single route delivers several polymorphs of the same composition and allows their electrochemistry to be compared directly. *Operando* diffraction and impedance analysis across these polymorphs show that the dominant kinetic limitations arise from stacking rearrangements and Na–vacancy ordering in the bulk rather than from interfacial charge transfer. The method extends across a broad transition-metal composition space, where compositions are prepared at near-target stoichiometry on minute timescales, making it a practical platform for fast exploration of compisitional space — one particularly well suited to layered Na cathodes.



SWRM 2026 SW473

Engineering thermal transport in multifunctional liquid crystal elastomers via sequential infiltration synthesis

***Akhila Joy**, akhilajoy@my.unt.edu. Materials Science and Engineering, University of North Texas College of Engineering, Denton, Texas, United States*

Artificial intelligence, soft robotics, and human-machine interfaces require compliant functional materials that combine adaptive mechanical behavior with efficient thermal management. Liquid crystal elastomers (LCEs) have emerged as highly promising candidate materials due to their reversible stimulus-responsive capabilities; however, intrinsically low thermal conductivity caused thermal gradients normally hinder thermally driven actuation and heat dissipation. Conventional conductive fillers can improve heat transport but often aggregate within the matrix or compromise compliance. Here, sequential infiltration synthesis is applied for the first time to a thiol-based polydomain LCE film of 85μm thickness. The mechanisms governing metal precursor transport and inorganic incorporation are investigated by varying trimethylaluminum exposure, purge duration, and temperature. Density functional theory calculations further identify ether sites as the strongest interaction sites for precursor binding and subsequent Al-OH formation. The combination of accessible polar reaction sites and free volume in LCEs enables precursor diffusion and reaction throughout the LCE bulk. The hybrid films performed 28% faster thermal response with increased Young's modulus up to 2.5 MPa and enabled tunable tensile strength and optical absorbance. The *in-situ* nucleation and growth of inorganic species in LCEs open up broad prospects for the development of LCE-based multifunctional materials for 3D packaging, soft robotics, and sensors.

SWRM 2026 SW474

Effects of Fe-doping on surface polarity, morphology, and antibacterial action in microscale ZnO

***John H. Brannon**[1], j.h.brannon@tcu.edu, Joshua Humphrey[1], Rachel Hull[2], Henry Henken[3], Landon Davies[1], Gursaroop Kahlon[1], Arihant Gauttam[1], Pavan Ahluwalia[4], Parmeet Jodhka[4], Alexander Baumann[4], Shauna McGillivray[5], Yuri Strzhemechny[1]. (1) Physics and Astronomy, Texas Christian University, Fort Worth, Texas, United States(2) Physics, Hollins University, Roanoke, Virginia, United States(3) Physics, The University of Texas at Austin, Austin, Texas, United States(4) Biology, Tarrant County College - Northwest Campus, Fort Worth, Texas, United States(5) Biology, Texas Christian University, Fort Worth, Texas, United States*

ZnO exhibits notable antibacterial activity against both Gram-positive and Gram-negative microorganisms. As the demand for alternative antimicrobial materials continues to grow, a more comprehensive understanding of the mechanisms governing ZnO antibacterial behavior is needed, particularly regarding the relative contributions of its various mechanisms. In our previous work, we proposed that the antibacterial activity of ZnO is primarily associated with surface-defect-mediated dissolution. To further examine this model, we modify hydrothermally synthesized ZnO microparticles to systematically control their antibacterial properties. We propose that the observed instability of ZnO under antibacterial conditions results from defect-driven reconstruction of its polar surfaces, which is influenced by the substantial internal dipole moment of the ZnO lattice and interactions between the material, surrounding medium, and bacterial surfaces. Incorporating Fe ions into the ZnO lattice may theoretically compensate for this dipole moment and improve surface stability without producing secondary crystalline phases. To investigate this possibility, the hydrothermal synthesis procedure is

modified to produce ZnO microparticles with controlled Fe incorporation and distinct morphologies containing different proportions of polar surfaces. The resulting materials are then systematically characterized using scanning electron microscopy, energy-dispersive X-ray spectroscopy, X-ray photoelectron spectroscopy, X-ray diffraction, and photoluminescence spectroscopy, both before and following exposure to *Staphylococcus aureus* in different nutrient media. These analyses allow us to evaluate changes in ZnO surface stability and determine how surface reconstruction is related to Fe concentration, particle morphology, and antibacterial performance.

SWRM 2026 SW475

Polyphosphazene based solid state electrolyte for Li-ion batteries

***Mayank Tiwari**, mxt230015@utdallas.edu. The Department of Chemistry & Biochemistry, The University of Texas at Dallas, Richardson, Texas, United States*

The development of safe and efficient solid-state lithium-ion batteries requires polymer electrolytes that combine high ionic conductivity, electrochemical stability, and suitable mechanical properties. In this work, poly[bis(2-(2-(2-methoxyethoxy)ethoxy)ethoxy)phosphazene] (MEEEP) was investigated as a polyphosphazene-based solid polymer electrolyte for lithium-ion battery applications. The polymer was synthesized and characterized using spectroscopic and chromatographic techniques to confirm its chemical structure and molecular weight characteristics. Lithium bis(trifluoromethanesulfonyl)imide (LiTFSI) was incorporated into the polymer at different ethylene oxide-to-lithium (EO:Li) ratios to investigate the effect of salt concentration on electrolyte properties. Electrochemical impedance spectroscopy was used to evaluate ionic conductivity over a range of temperatures. The electrolyte exhibited temperature-dependent ionic conductivity, with the highest conductivity observed for the 20:1 EO:Li ratio, reaching 4.46E-5 S/cm at 30 degrees C under the investigated conditions. The activation energy increased from 0.230 eV for the 20:1 ratio to 0.319 eV for the 50:1 ratio. Electrochemical characterization was further performed to evaluate the stability of the polymer electrolyte for battery applications. These results demonstrate the potential of MEEEP-based polyphosphazene electrolytes as tunable solid polymer electrolyte materials and provide a foundation for further structural modification to improve lithium-ion transport and electrochemical performance.

SWRM 2026 SW476

Electrochemistry in air: Coupled electron and phase transfer at three-phase interfaces enabled by electric-field spillover

***Kenta Kawashima**[1], u6071200@utah.edu, Mark C. Cisewski[1], Parinaz Nasehi[1], Jong Ho Choi[2], Joshua Bilsky[1], Andrew D. Pendergast[3], Vee C. Sutton[1], Salvador Gutierrez-Portocarrero[4], Gregory A. Voth[2], Aurora E. Clark[1], Rodrigo Noriega[1], Henry S. White[1]. (1) Chemistry, The University of Utah, Salt Lake City, Utah, United States(2) Chemistry, The University of Chicago, Chicago, Illinois, United States(3) Chemistry, University of Florida, Gainesville, Florida, United States(4) Chemistry, Idaho State University, Pocatello, Idaho, United States*

Coupled electron- and phase-transfer (CEPhT) reactions are ubiquitous in many energy conversion and electrochemical technologies but remain poorly understood at multiphase boundaries. In this study, scanning electrochemical cell microscopy together with finite element simulations is used to probe CEPhT at air/water/electrode interfaces. By comparison with toluene/water/electrode systems,

we also assess how solvation in the dielectric phase affects reaction kinetics and energetics. The results identify electric-field spillover at the three-phase boundary as a key driving force for CEPhT processes (i.e., concerted CEPhT), providing mechanistic insight into three-phase electrochemistry at complex interfaces.

SWRM 2026 SW477

Occurrence and quantitation of perfluoroalkyl substances (PFAS) in wastewater samples from an activated wastewater treatment plant in Deep East Texas (USA)

***Kefa K. Onchoke**, kefaon@yahoo.com, Michael Janusa, Jamie Humphries, Ken Fiffick, Anthony M. Broom, Thanh Dao, Imani Harris. Chemistry & Biochemistry, Stephen F Austin State University, Nacogdoches, Texas, United States*

Per- and polyfluoroalkyl substances (PFAS) pose environmental and human health concerns and contribute to disease burden and disability across the lifespan. A new developed method using ultra performance liquid chromatography-tandem mass spectrometry (UHPLC/MS/MS) was used to quantitate concentrations of eleven PFAS in wastewater treatment stages from Nacogdoches Wastewater Treatment Plant and Deep East Texas (USA). PFAS were detected in all treatment stages with concentration ranges (in ng/g): PFPeA (0 - 0.58), PFHxA (3.26 – 26.45), PFHpA (0.675 - 13.985), PFOA (14.17 - 123.00), PFNA (0.81 - 8.86), PFDA (7.91 - 1303.15), PFOS (8.81 - 1013.84), PFTrDA (0.116 - 10.39), PFDS (0.931 - 6.02), PFUdA (0.097 - 5.91), PFDoA (2.19 - 11.17). PFDA, PFOA and PFOS were the predominant species. Principal component analysis showed very strong correlations (> 0.99) between most PFAS substances. Further studies are essential for examination of PFAS concentration amounts from WWTPs over long periods of time. Data from this study is useful for risk asssessment potential on exposure to PFAS of ≤ 12 carbons and implications for regulatory agencies. This information is useful for public health concerns, and possible interventions for enactment of necessary policies to reduce exposure to PFAS.

SWRM 2026 SW478 - Withdrawn

SWRM 2026 SW479

Abraham solvation parameter model: Experiment based solute descriptor values for potential medicinal candidates, dietary healthcare supplements and pharmaceutical formulation ingredients

***Chelsi Wilson**, ChelsiWilson@my.unt.edu. Chemistry, University of North Texas, Denton, Texas, United States*

Experiment-based Abraham model solute descriptors have been determined for oxibendazole which prevents parasitic infection, 3,3’-diindolylmethane which regulates hormones, meglumine which improves solubility and bioavailability of lipophilic medicines, N-acetyl-L-phenylalanine an anti-inflammatory drug and tranilast anti-allergic medicine for asthma. These solute descriptors are based on recently published mole fraction solubility data. The calculated descriptor values, when inserted into the respective Abraham model correlation, provided a reasonably accurate mathematical

description of the observed solubility behavior, with deviations between the measured and back-calculated values being on the order of ±0.17 log units (or less). The calculated solute descriptors will allow academicians and design engineers to predict the solubility of the five potential medicinal candidates, dietary healthcare supplements and pharmaceutical formulation ingredients compounds in more than 130 different organic solvents of varying polarity and hydrogen-bonding character using previously published Abraham model predictive expressions. The Abraham model solute descriptors have been determined for more than 8,000 compounds. Such predictions enable researchers to possibly identify more environmentally compatible, renewable solvent alternatives to replace the more harmful, petroleum-based and volatile organic compounds that are currently being utilized in many of today's chemical manufacturing processes. Solvent selection is extremely important in the pharmaceutical industry as government regulations often limit the quantity of residual solvents that can remain in medicinal compound or drug formulation. In this presentation, I will describe 1) The Abraham model correlations and solvent parameters that enable academicians and design medicinal engineers to predict the solubility of potential medicinal candidates, dietary healthcare supplements and pharmaceutical formulation ingredients compounds in more than 130 different organic solvents and 2) explain how advanced analytical instrumentation is critical for providing parameters needed to make successful prediction.

SWRM 2026 SW480

Hydrophilic interaction chromatography coupled with evaporative light scattering detection for inorganic cations and anions

***Reza Salehi**, rxs5765@mavs.uta.edu. The University of Texas at Arlington, Arlington, Texas, United States*

The chromatographic analysis of inorganic ions typically relies on ion chromatography with conductivity detection because many ionic species lack chromophores suitable for conventional UV detection. In this study, hydrophilic interaction liquid chromatography coupled with evaporative light scattering detection (HILIC-ELSD) was investigated as an alternative platform for the separation and detection of inorganic cations and anions. Cyclofructan-based stationary phases were evaluated with highly organic, volatile mobile phases containing acetonitrile and aqueous ammonium formate. A structurally diverse set of monovalent and divalent cations and inorganic anions was examined to evaluate chromatographic retention, selectivity, and ELSD response. Significant differences in retention were observed among the investigated ions, reflecting differences in charge, ionic size, hydration, polarizability, and interactions with the stationary phase. ELSD parameters were also optimized to maximize analyte response while maintaining effective evaporation of the volatile mobile phase. Detector response was found to be strongly dependent on both analyte identity and operating conditions. These results demonstrate that HILIC-ELSD provides a versatile approach for the separation and direct detection of UV-transparent ionic species and offers a complementary strategy to conventional conductivity-based ion analysis.

SWRM 2026 SW481

Simple salt assisted liquid-liquid extraction method for analysis of poly- and perfluoroalkyl substances in meconium

***Chimauchem V. Odinaka**, cvo7937@mavs.uta.edu, Pranta Acharjee, Charles P. Shelor. Department of Chemistry and Biochemistry, The University of Texas at Arlington, Arlington, Texas, United States*

Per- and polyfluoroalkyl substances (PFAS) are persistent contaminants linked to adverse developmental and immune outcomes. Exposure risk of PFAS to the developing fetus is not yet fully understood. Further, assessing prenatal exposure remains challenging because placental transfer is not well characterized and noninvasive biomarkers are limited. Cord blood is most widely used but only reflects exposure at delivery. Additionally, PFAS in paired mother blood samples decrease substantially throughout gestation but don't show a similar increase in infant cord blood samples suggesting that the majority of PFAS remain unaccounted for. Measurement at birth of either mother or infant blood then likely underestimates true prenatal exposure. In order to close the PFAS mass balance and provide a non-invasive cumulative measure of PFAS exposure, we are investigating meconium. Meconium is the infant's first stool which is produced throughout the last 2 trimesters of gestation and consists mainly of epithelial cells, mucus, amniotic fluid, bile, and lanugo (fine hair). As the fetus constant imbibes amniotic fluid, compounds may be concentrated within the meconium. Analysis of PFAS is difficult as sample sizes are small (especially for pre-term births), concentrations of interest are typically in pg/g, and are prone to contaminantion due to PFAS ubiquity in the environmental and laboratory. We have developed a simple salt assisted liquid-liquid extraction protocol that minimizes sample handling followed by ultrahigh performance liquid chromatography high resolution mass spectrometry (UHPLC-HRMS). Meconium samples (<0.2g) were dried, weighed, and slurred with water to which was added acetonitrile, graphitized carbon black, and salt. Quantitative recovery of 24 PFAS compounds was achieved (58-148%) using 10:1 sample:acetonitrile allowing efficient concentration of PFAS into the supernatant avoiding the need for solid phase extraction or solvent evaporation. Limits of detection ranged from 6.6 – 53.3 pg/g. Overall, this study demonstrates an efficient, simple, inexpensive approach for PFAS biomonitoring, providing valuable insight into maternal-fetal transfer and prenatal exposure burden.

SWRM 2026 SW482

Flow-through fluorescence detection of fluoride using the zirconium–calcein blue system

***Pranta Acharjee**[1], pxa2738@mavs.uta.edu, Memona Zulafiqar[1], Ranvit Pakala[2], John Guzman[3], Arya Mojahed Naghi[1], Charles P. Shelor[1]. (1) Analytical Chemistry, The University of Texas at Arlington, Arlington, Texas, United States(2) Newman Smith High School, Carrollton, Texas, United States(3) The University of Texas at Arlington, Arlington, Texas, United States*

Poly- and Perfluoroalkyl substances (PFAS) are a broad range of anthropogenic persistent organic pollutants. PFAS have been shown to be ubiquitous in the environment and concentrations of concern are often in low part per trillion. Targeted methods are based on liquid chromatography tandem mass spectrometry (LC-MS/MS), but this can only measure a few of the 15,000 identified compounds and is expensive. An alternative is to measure all organic fluorine species present by combustion ion chromatography (CIC). In CIC, PFAS are first absorbed on a granular activated carbon sorbent. The sorbent is combusted in a high temperature furnace under a stream of oxygen, argon, and water vapor to liberate fluorine as HF which is bubbled through a trapping solution. The solution is then measured by ion chromatography (IC) for fluoride content. Unfortunately, IC is typically only able to measure low part per billion making it insufficient for ultra trace screening. Further, fluoride is poorly retained and presence of significant concentrations of other species may compromise to separation. Alternative sensitive and selective fluoride detections methods are required. The Zirconium (IV)–Calcein Blue (Zr–CB) system offers exceptionally sensitive fluorescence-based fluoride detection; however, despite a half century of analytical use, its underlying

solution chemistry remains incompletely resolved. Published studies report strongly condition-dependent spectral behavior, complex formation, stability, and fluoride response, leaving important questions regarding the fluorescent species and reaction pathway under dynamic analytical conditions. This study addresses these questions while translating Zr–CB chemistry into a mechanistically optimized flow-through fluorescence detector. Fluoride produced stable, concentration-dependent fluorescence responses over 0.1–5.0 µM. Detector performance was strongly influenced by acid conditions, with the highest HCl response near 12.5 mM and markedly lower signals at higher acidity and in sulphuric acid. The current detection limit is ~80 ng/L fluoride, supporting application to PFAS-related fluorine analysis. These findings establish the Zr–Calcein Blue system as a rapid, reproducible, and chemically tunable flow-through detector, offering a compact alternative to ion chromatography for combustion-derived fluoride in total organic fluorine and PFAS workflows.

SWRM 2026 SW483

Simultaneous deep-UV fluorescence and high-dynamic-range absorbance detection in a liquid-core waveguide flow cell

***Charles P. Shelor**, shelor@uta.edu. Chemistry and Biochemistry, The University of Texas at Arlington, Arlington, Texas, United States*

Liquid-core waveguide (LCW) flow cells guide light through total internal reflection at the lower-refractive-index capillary wall, providing high optical throughput and low relative transmission noise for sensitive absorbance measurements. However, conventional axial LCW detection does not extend the detector's dynamic range, complicating simultaneous quantification of trace and major constituents. Here, a thin-walled fused-silica LCW (0.53 mm i.d., 6 cm length) was configured for simultaneous axial absorbance, radial absorbance, and deep-UV-excited fluorescence detection. Radial measurements used fiber-coupled 280 nm LEDs and paired photodiodes positioned 1 cm apart, creating a shorter optical path that extended the absorbance range by more than two orders of magnitude. Performance was demonstrated with a homologous series of aliphatic ketones. The photodiodes also detected broadband fluorescence, while the low-loss LCW suppressed excitation stray light. A deuterium lamp, with strong output near 200 nm, efficiently excited compounds having negligible absorbance above 225 nm. Several unconventional fluorophores emitted near 300 nm, corresponding to Stokes shifts approaching 18,000 cm^{-1}. Modulation of the radial LEDs enabled separation of transmittance and background/fluorescence signals, yielding absorbance noise as low as 10 µAU. Radial detection further revealed that axial measurements underestimated the true chromatographic dispersion at the cell outlet and showed asymmetric flow caused by small inlet/outlet geometric differences. This multimode LCW platform therefore expands quantitative range, enables deep-UV fluorescence measurements, and provides diagnostic information on flow-cell dispersion within a compact optical configuration.

SWRM 2026 SW484

Exploring the spectrochemical behavior of derivatized amino acids for HPLC-fluorescence detection

***Sakil Islam**, sxi9741@mavs.uta.edu, M. Farooq Wahab, Ryan J. Burk, Daniel W. Armstrong. Chemistry and Biochemistry, University of Texas at Arlington Research Institute, Arlington, Texas, United States*

Precolumn derivatization remains widely used for liquid chromatography-fluorescence detection (HPLC-FLD) of amino acids, but reagent performance is often evaluated without considering how eluent environment and detector optics alter fluorescence response. Here, seven representative amino acids were derivatized with 6-aminoquinolyl-N-hydroxysuccinimidyl carbamate (AQC), 9-fluorenylmethyl chloroformate (FMOC), or dansyl chloride (DNS) and compared under a common reversed-phase gradient at pH 2.9 and 6.5 using first-order fluorescence (FL), zero-order fluorescence (ZoFL), and ultraviolet (UV) detection. Most AQC derivatives shifted from approximately 260/473 nm at pH 2.9 to 247/407 nm at pH 6.5, whereas FMOC and DNS derivatives were largely pH insensitive. FMOC gave the highest FL calibration sensitivity for all analytes except tryptophan, while AQC gave the strongest UV response for most analytes. ZoFL response depended strongly on emission region: DNS derivatives increased 3.1-3.9 fold relative to FL, whereas non-tryptophan FMOC derivatives decreased 7.1-7.7-fold relative to their original FL response. AQC- and FMOC-derivatized tryptophan showed pronounced fluorescence suppression relative to other derivatives within their reagent classes, whereas DNS-tryptophan did not. In solvent-composition experiments with Glu, Phe, and Val, DNS fluorescence increased approximately 17-fold across 20-80% acetonitrile at pH 2.9, FMOC remained invariant, and AQC showed pronounced pH-dependent spectral changes. Derivatized amino acids' fluorescence cannot be solely attributed to derivatizing reagents; analyte structure, fluorescent solvatochromism, and detector optics jointly influence analytical performance. Emission-order settings should be evaluated under the actual chromatographic and detector conditions used for method development and transfer from one FLD to another due to the undisclosed grating blaze angle.

SWRM 2026 SW485

Identifying and eliminating systematic errors in laboratory gas permeability and non-Darcy flow measurements

***Deborah O. Rufus**, deborahrufus@ou.edu, **Mashhad Fahes**, mashhad.fahes@ou.edu. Mewbourne School of Petroleum and Geological Engineering, The University of Oklahoma, Norman, Oklahoma, United States*

The non-Darcy flow coefficient β is a critical parameter in subsurface energy applications including hydrocarbon recovery, carbon storage, and geothermal energy extraction, where accurate characterization of high-velocity gas flow through porous media is essential.
Despite its importance, laboratory measurements of β show significant variability across studies, and several investigators have reported that β increases dramatically as core sample length decreases. Whether this apparent length dependence reflects a genuine rock property or a measurement artifact has remained unresolved for nearly four decades.
This study presents a systematic experimental investigation designed to isolate and eliminate the sources of this apparent length effect. Steady-state nitrogen flow measurements were conducted on Berea sandstone core plugs of two diameters and lengths ranging from 0.446 to 11.561 inches, using a dual pressure transducer configuration that recorded inline and separate line measurements simultaneously on every sample. A progressive series of core holder modifications, including spacer placement tests, washer distribution experiments, and large-bore rod substitution, identified two experimental factors responsible for the apparent length dependence: the restrictive geometry of the narrow-bore spacer face and the inline pressure measurement configuration.

When both factors were corrected, β values were consistent across all tested lengths, with remaining differences within 3% attributable to natural rock heterogeneity. The Forchheimer model is confirmed as an accurate description of high-velocity gas flow in Berea sandstone, and β is confirmed as a true intrinsic rock property when measurements are made with appropriately designed apparatus.

SWRM 2026 SW486 - Withdrawn

SWRM 2026 SW487

Micro solid phase extraction-liquid chromatography tandem mass spectrometry strategy for evaluating subcutaneous enzyme replacement therapy in Fabry disease

Sabrina Islam[1]*, sxi0536@mavs.uta.edu, MJ Cao*[2]*, Kevin Schug*[1]*. (1) The University of Texas at Arlington, Arlington, Texas, United States(2) Kinetiq Therapeutics LLC, Fort Worth, Texas, United States*

Fabry disease is an inherited lysosomal storage disorder associated with inadequate activity of the enzyme α-galactosidase A, leading to the accumulation of globotriaosylceramide (Gb3), a glycosphingolipid consisting of a ceramide backbone linked to a trihexose sugar moiety. This buildup occurs across multiple tissues, particularly the kidney, liver, and heart, contributing to disease progression. Enzyme replacement therapy (ERT) is the current established treatment approach, however challenges with administration and tissue distribution create necessity for improvement. This study focuses on a new subcutaneous self-administrable ERT, BrySQ, using a Fabry disease mouse model. The effectiveness of the treatment is being assessed by monitoring Gb3 concentrations. Gb3 is extracted from biological matrices using micro-solid phase extraction (MSPE), followed by quantitative analysis using a liquid chromatography – tandem mass spectrometry workflow. Chromatographic separation is performed using reversed-phase liquid chromatography on a Evosphere C12 column, coupled with triple quadrupole mass spectrometry operated in multiple reaction monitoring mode. Samples from treated and control groups are being analyzed, and matrix effects associated with different tissue types are being evaluated to ensure accurate quantification of glycolipids. The findings from this study are expected to contribute to the evaluation of BrySQ as a subcutaneous therapeutic approach and provide insight into its ability to reduce glycolipid accumulation in tissues affected by Fabry disease.

SWRM 2026 SW488

Evaluating column selectivity for forensic applications: A comparison of diphenyl, C18/AR, and C12 phases using liquid chromatography-mass spectrometry

Kei Osawa[1,2]*, kaosawa@tarrantcountytx.gov, Robert Johnson*[2]*, Kevin Schug*[1]*. (1) The University of Texas Arlington College of Science, Arlington, Texas, United States(2) Tarrant County Medical Examiner, Fort Worth, Texas, United States*

There are numerous reversed-phase stationary phases, which provide significant differences in retention and selectivity. Three such phases—diphenyl, C18/AR, and C12—were investigated along with mobile phase selection using liquid chromatography coupled with triple quadrupole mass

spectrometry. A sample mixture of 107 commonly encountered over-the-counter drugs, prescription drugs, and drugs of abuse was analyzed using scouting gradient without further optimization, since the goal was simply to observe the phases' variable retention and selectivity under generic conditions. The chromatographic results showed wide variations in peak shape and selectivity across the parameters tested. For example, among the polar, early-eluting compounds, morphine and hydromorphone demonstrated poor chromatography on the C12 column and performed better on the diphenyl column. The addition of ammonium formate and formic acid to the mobile phase, rather than formic acid alone, also improved peak shape. The kratom alkaloids further illustrate the observed selectivity differences. The stereoisomers mitragynine, speciogynine, speciociliatine, and mitraciliatine demonstrated different degrees of separation, exhibiting poorer separation with methanol than with acetonitrile, while use of C12 or C18/AR columns showed better results than the diphenyl column. Overall, column selection will ultimately depend on the analytes being examined, and there is no one-size-fits-all solution. However, the C18/AR column may offer the best of both worlds—combining a longer carbon chain with aromatic character, which could make it a versatile first choice across a broad panel of compounds.

SWRM 2026 SW489

PFAS screening by real-time tandem mass spectrometry

***Raghvendra Sengar**, Raghvendra.Sengar@bruker.com, Artem Filipenko. Bruker Scientific, Billerica, Massachusetts, United States*

Per- and polyfluoroalkyl substances (PFAS) are synthetic chemicals known as "forever chemicals" because they persist in the environment and accumulate in living organisms. The Environmental Protection Agency (EPA) currently employs liquid chromatography-tandem mass spectrometry (LC-MS/MS) for PFAS analysis in various matrices. However, high concentrations of PFAS in samples frequently cause carryover in LC-MS/MS, resulting in false-positive peaks in subsequent analyses. Eliminating these contaminants necessitates an extensive cleaning process. This study proposes the use of direct analysis in real time tandem mass spectrometry (DART-MS) to pre-screen samples, thereby avoiding the analysis of high-concentration samples by LC-MS/MS and reducing carryover. Preliminary findings indicate that samples prepared according to EPA Method 1633 can be rapidly analyzed by DART-MS within seconds. These results suggest that DART-MS may serve as an effective screening tool for identifying high-concentration samples prior to LC-MS/MS analysis, thereby minimizing carryover.

SWRM 2026 SW490

Novel triple quad approaches for sensitive quantification of 1000 compounds in single runs

***Raghvendra Sengar**, Raghvendra.Sengar@bruker.com, **Artem Filipenko**, Artem.Filipenko@bruker.com. Bruker Corporation, Billerica, Massachusetts, United States*

Pesticides represent the most frequently analyzed hazardous compounds in food and feed. The analysis of an ever-increasing number of diverse pesticides in a single LC/MS run and the demand for higher sample throughput are key challenges. A rapid LC-TQ quantitative analysis method addressing both throughput and the high number of target pesticides is presented. For the evaluation of the analytical performance, the new method was optimized in a real scenario in common matrices

for > 700 pesticides in positive/negative mode with the focus on how the speed, number of compounds and other parameters influence the sensitivity and robustness. UHPLC gradients with water (A) and methanol (B) (0.01% FA, 2 mM ammonium formate) at a 15-100% B gradient in 0.5-8min were used at a runtime of 9.2 min with subsequent 2.5 min equilibration. 2 uL sample were injected on an Intensity Solo 2.0 100x2.0 mm column at 45 C. A novel triple quadrupole was used in MRM Compound Based Scanning. With a scan time for each compound of 4-11 ms, the method accommodates >1000 pesticides in fast polarity switching with ≥ 2 transitions in a single run. A probe temperature program reduced the impact for thermolabile compounds. A calibration curve containing 520 pesticides was prepared in pepper matrix (QuEChERS) with five calibration levels at 0.2-50 ppb. The analysis speed fits to generate a high number of data points for each peak to ensure accurate analysis. Statistics demonstrate even with different acquisition speeds and polarity switching a reproducibility of 2.6% within 10 consecutive injections. Calibration curves show R^2 >0.99 for 95% of the compounds with < 10% ion ratio deviation and RSD < 10% for most pesticides is achieved in real matrix spiked with 2 ppb in total. Different methods have been completed for >765 pesticides in a single run with positive/negative switching. Due to the high instrument sensitivity, samples and standards can be diluted to reduce matrix effects, leading to less interference and use of one matrix to calibrate similar samples. Novel electronics and rapid polarity switching ensure consistent intensity and ion ratio regardless of the scan speed. All these parameters indicate robust and reliable screening and quantitation up to 1000 pesticides in a single run. Higher throughput, less maintenance and downtime can be achieved. Finally, 30 real samples prepared with the same extraction method were analyzed afterward to quantify the potential pesticides.

SWRM 2026 SW491

Selective oxidation of ethylene–vinyl alcohol facilitates multilayer plastic film recycling

Mohammad Reza Razzaghi*, razzaghi.mreza@ou.edu, Samira Abdolbaghi, Dai-Phat Bui, Steven Crossley, Lance Lobban. Sustainable Chemical, Biological and Materials Engineering, The University of Oklahoma, Norman, Oklahoma, United States*

Multilayer plastic films (MLFs) are widely used in packaging applications but remain difficult to recycle due to the presence of minor polar components including ethylene–vinyl alcohol (EVOH), adhesives, dyes, and resin additives, which are incompatible with polyolefin recycling streams. Selective catalytic conversion of these minor components into smaller oxygenated molecules offers a potential strategy to improve recyclability while preserving the polyethylene-rich matrix. In this work, both molten-phase and solvent-assisted catalytic oxidation approaches for EVOH removal are investigated. Heterogeneous oxide catalysts, particularly CeO_2-based catalysts previously investigated for EVOH transformation, provide an effective way for selective oxidation of the polar layer while exhibiting negligible conversion of polyethylene. Tailoring the properties of these oxide catalysts can further enhance catalytic activity and improve selectivity toward oxygenated products, including aldehydes, ketones, and carboxylic acids, while minimizing complete oxidation to CO and CO_2. To date, CeO_2 nanorods have been shown to increase the reaction rate by nearly an order of magnitude compared with CeO_2 nanoparticles. Several solvents were evaluated based on polymer solubility, thermal stability, and practical considerations. Among the candidates examined, γ-valerolactone (GVL) was identified as a promising solvent due to its ability to dissolve EVOH, its relatively high boiling point (207°C), and its renewable origin. Experiments were conducted near 195–205°C using molecular oxygen (5% O_2) as the oxidant. NMR analysis indicates that GVL remains largely stable under the reaction conditions. Compared with non-solvent systems, the presence of a solvent significantly increased conversion to gas-phase products, indicating improved catalyst-polymer interaction and enhanced mass transfer. These results suggest that solvent-assisted catalytic oxidation may provide

a viable strategy for selective removal and chemical conversion of polar minor components in multilayer plastic films, offering a potential route toward improved recycling of complex packaging materials.

SWRM 2026 SW492

Lyotropic liquid crystal templated ultrafiltration membranes for virus removal in mAb purification

***Mostafa Tabatabaei**, smtabatabaei.76@ou.edu, Shirin Tahazadeh, Farid Talebnia Rowshan, Reza Foudazi. School of Chemical, Biological & Materials Engineering, The University of Oklahoma, Norman, Oklahoma, United States*

Lyotropic liquid crystals (LLCs) form through the self-assembly of amphiphilic block copolymers in selective solvents, creating nanostructured mesophases, such as hexagonal, lamellar, and cubic phases. These LLCs can serve as templates for polymerization, producing membranes with potential applications in separation processes. This study explores the self-assembly of Poloxamer 407-diacrylate in ethylammonium nitrate, demonstrating the formation of face-centered cubic. UV crosslinking of these templates results in membranes with a pore size of approximately 20 nm, a hydrophilic surface resistant to fouling, and a narrow pore size distribution. These characteristics make LLC-templated membranes highly suitable for biopharmaceutical applications, particularly in virus separation for monoclonal antibody production, improving the sustainability of the downstream of bioprocessing.

SWRM 2026 SW493

Polymerization of Frank-Kasper A15 phase formed by Pluronic P105-diacrylate and ethylammonium nitrate mixtures

***Shirin Tahazadeh**, shirin.tahazadeh@ou.edu, Reza Foudazi, Farid Talebnia Rowshan. School of Sustainable Chemical, Biological and Materials Engineering, The University of Oklahoma, Norman, Oklahoma, United States*

Lyotropic liquid crystals (LLCs) formed by the self-assembly of amphiphilic block copolymers provide an attractive template for creating ordered nanostructured materials with tunable domain dimensions. In this study, the self-assembly behavior of Pluronic P105 in ethylammonium nitrate (EAN), a protic ionic liquid, was investigated, with emphasis on the formation and polymerization of an ordered LLC structure. Pluronic P105 was first functionalized with acrylate end groups to enable subsequent polymerization of the assembled structure, and NMR spectroscopy was used to confirm successful diacrylation. The thermal behavior of the P105/EAN system was characterized by differential scanning calorimetry (DSC) to identify thermal transitions associated with micellization and mesophase formation. Small-angle X-ray scattering (SAXS) was used to characterize the nanoscale organization of the LLC, revealing the formation of spherical micelles and their organization into an ordered Frank-Kasper A15 phase with symmetry. Following polymerization and solvent exchange, the resulting hydrogels were characterized by measuring their swelling ratio and equilibrium water content to evaluate water uptake and swelling behavior. Overall, these results demonstrate the formation and subsequent polymerization of an ordered Frank-Kasper A15 structure in the P105/EAN system and provide a basis for developing nanostructured hydrogels derived from polymerized LLCs.

SWRM 2026 SW494

Study of the segmental dynamics in PEO-based polymer electrolytes using quasi-elastic neutron scattering

Pattuwe A. Pattuwearachchi[1]*, anuradhapattuwearachchi@ou.edu, Fatemeh Naderi Samani*[1]*, Naresh Osti*[2]*, Reza Foudazi*[1]*. (1) School of Sustainable Chemical, Biological and Materials Engineering, The University of Oklahoma, Norman, Oklahoma, United States(2) Oak Ridge National Laboratory, Oak Ridge, Tennessee, United States*

This study investigates model polymer electrolytes based on a short-chain poly(ethylene oxide)-block-polyethylene (PEO-b-PE) block copolymer doped with ionic liquids (ILs) and/or Li and Mg salts. Movement of ions as charge carrying components in the system is tied with the polymer segmental dynamics. Using quasi-elastic neutron scattering (QENS), the governing diffusion mechanism of hydrogen atoms of polymer chains be used to investigate segmental dynamics. Jump diffusion better explains the dynamics in a pure block copolymers, while mixed electrolyte segmental relaxation is more tied to Fickian diffusion. All samples show a reduction of the segmental diffusion coefficient upon addition of salts due to the strong coordination bonds between PEO and metal cation. Most fitted diffusion coefficients fall in the 10^{-10} m^2s^{-1} range, which is consistent across systems, that is inline with findings in the literature.

SWRM 2026 SW495

Minimalist peptide assemblies as metal-free catalysts for esterase activity

Shams Aaghaz*, aaghazshams100@gmail.com, Liam R. Marshall, Ivan V. Korendovych. Chemistry and Biochemistry, Baylor University, Waco, Texas, United States*

Short peptide assemblies can serve as minimalist catalysts that mimic enzymatic activity. In this work, we describe the ability of *de novo*-designed 7-amino-acid peptides to catalyze *p*NPA hydrolysis in the absence of metal and how the amino acid sequence influences catalytic efficiency. These peptides self-assemble into amyloids containing a catalytically active Cys-His dyad. We observe sequence-activity relationships that switch between enzyme-like burst-phase behavior and steady-state kinetics. The most active peptide, Ac-FHFHFCF-NH_2, shows a k_{cat}/K_M of 6.9 ± 1.6 M^{-1} s^{-1} in the absence of metal. These findings suggest that we can incorporate entire active sites within a single amyloid strand, simplifying synthesis while expanding the reaction space.

SWRM 2026 SW496

Polydiacetylene-based colorimetric detection of PFAS

Nicholas Payne*, nicholas.payne@ttu.edu, Kaleb Jewell, Joshua Tropp. Chemistry and Biochemistry, Texas Tech University, Lubbock, Texas, United States*

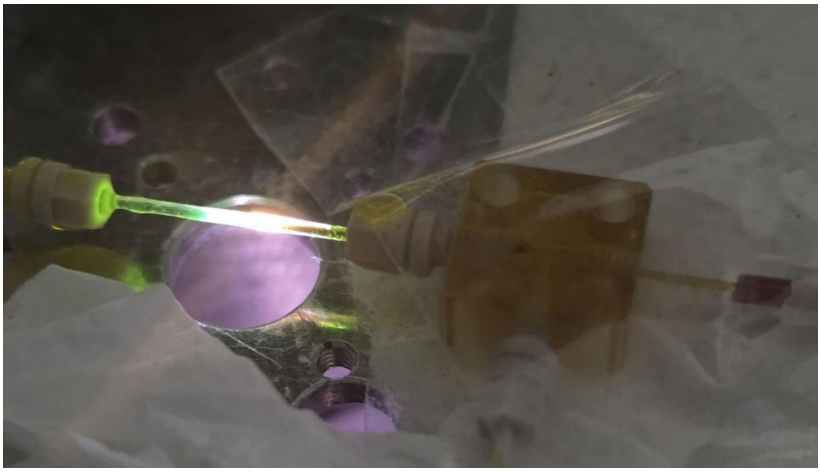
Per- and polyfluoroalkyl substances (PFAS) are environmentally persistent synthetic chemicals that can accumulate in humans and ecosystems through contaminated food and water. Exposure to certain PFAS has been associated with adverse health effects, creating a need for accessible methods to monitor these contaminants. Current analytical methods for PFAS detection, including liquid chromatography-tandem mass spectrometry, provide high sensitivity and selectivity but require costly instrumentation, extensive sample preparation, and trained personnel. As a result, these methods are not well suited for rapid, on-site screening. Polydiacetylenes (PDAs) are a class of conjugated polymers that act as signal-transducer platforms through a characteristic blue-to-red color transition in response to external stimuli. In this study, functionalized diacetylene monomers with varied headgroup structures were synthesized and self-assembled into aqueous nanoparticles. Monomer synthesis was evaluated using ^{1}H NMR spectroscopy, while the corresponding nanoparticles were then characterized using dynamic light scattering, zeta-potential measurements, nanoparticle tracking analysis, and UV-Vis spectroscopy. Following photopolymerization, the nanoparticle systems exhibited the characteristic blue phase of PDA and produced measurable colorimetric responses following exposure to selected PFAS. These responses were monitored spectroscopically and quantified using changes in the blue- and red- phase absorbance bands; limits of detection ranged from nanomolar to picomolar concentrations in aqueous environments. The selectivity of certain cationic surface chemistries to specific PFAS may give insight into what electrostatic interactions promote PFAS selectivity in polymer interfacing technologies.

SWRM 2026 SW497

Deep ultraviolet fluorescence detection using liquid core waveguide flow cells

ANIKA HAIDER*, axh1587@mavs.uta.edu. Chemistry & Biochemistry, The University of Texas at Arlington, Arlington, Texas, United States*

Fluorescence detection is one of the most sensitive techniques available for trace analyte quantitation. However, it is less widely used than absorbance detection as it is widely accepted that only a fraction of species (usually aromatics) have appreciable fluorescence while almost all species absorb. We show that this is not true and nontraditional fluorophores may be excited when deep UV excitation (<220 nm) is used. Conventional spectrofluorimeters rely on high brightness Xe arc lamps to achieve sensitivity in the near UV and and visible, but their output decreases exponentially in UV (<400 nm). Deuterium (D_2) lamps by contrast increase in intensity in the UV peaking at ~200 nm using fused silica; at this wavelength all organic species absorb. To maximize illumination intensity, we have constructed a liquid core waveguide (LCW) flow cell utilizing broadband excitation and emission. Light from a focused D_2 lamp radially illuminates a thin wall fused silica capillary. Fluorescent light emits in all directions but a portion of the light undergoes total internal reflection at the silica/air interface and propagates along the length of the capillary. The light enters into a fiber optic inserted into the lumen of the capillary and detected. The LCW prevents most of the excitation light from reaching the detector preventing the need for additional monochromators or filters. Fluorescent impurities were detected in various solvents following reverse phase separation but the compounds showed no appreciable absorbance >220 nm suggesting the species were not aromatics. We investigated various simple heteratom containing species and found that all ethers (including carbohydrates!) showed measurable fluorescence when excited at low wavelengths and emitted around ~300 nm while no appreciable fluorescence was observed for similar peroxides or alcohols. We found that hydrophobic and polyethers were the most sensitive.



SWRM 2026 SW498

Symmetric azobenzene photoswitches in multiple solvents

***Nicole Litvak**, nicole.123.l.321@gmail.com, Caleb Griffin, Alex R. Lippert. Department of Chemistry, Southern Methodist University, Dallas, Texas, United States*

Photoswitches change their molecular geometry, such as a rotation around a double bond, in response to energy from the electromagnetic spectrum. This research is focused on synthesizing azobenzene photoswitches, which respond to light of different wavelengths, causing them to change between E and Z isomers. The solvent affects photoswitching, which is studied herein. Azobenzene photoswitches have many versatile applications in materials and biological tools.

SWRM 2026 SW499

1,2-dioxetane probe for imaging of select reactive oxygen species

***Caleb Griffin**, calebgriffin@smu.edu, Alex R. Lippert. Chemistry, Southern Methodist University Dedman College of Humanities and Sciences, Dallas, Texas, United States*

Neutrophils are a type of white blood cell that play a vital role in the body's innate immune system. These neutrophils use reactive oxygen species (ROS) like hypochlorous acid (HOCl) to attack and neutralize unwanted pathogens found in the body. This research utilizes a Schaap's 1,2-dioxetane chemiluminophore to study the concentration of HOCl and select ROS in vitro, which will be expanded to living cells. The findings of this research will gain insight into the innate immune system and how ROS are used as a tool to fight pathogens.

SWRM 2026 SW500

Cucurbit[6]uril-β-cyclodextrin PEG-based polyrotaxanes and interlocked slide-ring materials

Aunindya Jyoti[1,2]*, aunindya.jyoti@gmail.com, SOUMEN PRADHAN*[1,2]*, Brennan Curole*[2]*, Amman Nadeem*[2]*, Mahi Ahmad*[2]*, Husain Kagalwala*[1]*, Scott M. Grayson*[2]*, Janarthanan Jayawickramarajah*[1,2]*. (1) Chemistry, Southern Methodist University, Dallas, Texas, United States(2) Chemistry, Tulane University, New Orleans, Louisiana, United States*

Mechanically interlocked materials (MIMs), specifically polyrotaxanes, have become an important area of study for materials scientists due to their exceptional mobility, stimuli responsiveness, and their application as molecular machines; however, more innovative approaches are needed to produce functionalizeable polyrotaxanes that exhibit stoichiometric threading on a large-scale. Here we report an example of a hetero-macrocyclic poly(ethylene glycol) (PEG)-based polyrotaxane (Mn= 203 kDa, determined via 1H-NMR spectroscopy) which was synthesized in water under mildly acidic conditions. The self-assembly of positively charged biphenyl bis-azidoethylamine guest (BABP2+) and bis-alkynyl ammonium PEG is promoted by β-cyclodextrin (β-CD) and cucurbit[6]uril (CB[6]) host-guest interactions, as well as by CB[6]-catalyzed azide-alkyne cycloaddition (CBAAC), with N-(tert-butyl)prop-2-yn-1-amine (TPBA) stoppers terminating the growth of the polymer chains. This synthetic strategy has many advantages, including, the effective threading of β-CD onto PEG (historically non-optimal in solution), controlled coverage, pH-driven slide-ring propensity, and scalability on a tens of grams scale. Moreover, the benefit of having functionalizable macrocycles on polyrotaxanes is demonstrated, yielding slide ring hydrogels via effective cross-linking of the β-CDs. These novel heteromacrocylic polyrotaxanes provide a platform for future functional slide-ring materials and hydrogels.

SWRM 2026 SW501

Programming multidomain peptides with molecular frustration into biomolecular condensates

Debdatta Das*, dxd4526@mavs.uta.edu. Department of Chemistry and Biochemistry, The University of Texas at Arlington, Arlington, Texas, United States*

Biomolecular condensates formed through liquid-liquid phase separation (LLPS) provide dynamic, membraneless compartments with emerging potential for engineering functional biomaterials. Here, we demonstrate a molecular frustration-based strategy for programming LLPS in rationally designed multidomain peptides (MDPs). These peptides balance a central domain that promotes assembly with charged terminal domains that oppose excessive molecular ordering, enabling control over peptide phase behavior. Systemic variation of peptide chemistry and domain architecture revealed that primary structure directly regulates secondary structure and, consequently, macroscopic phase behavior. Spectroscopic characterization showed that peptides that formed condensates adopt partially ordered β-sheet structures, whereas increased intermolecular ordering favours formation of hydrogel. Confocal Raman microscopy further revealed contributions from hydrogen bonding, van der Waals interactions, and hydrophobic interactions toward condensate formation. The resulting simple coacervates exhibit liquid-like behaviour as observed in fluorescence recovery after photobleaching (FRAP) experiment. Incorporation of polyanions enables formation of coacervates at lower critical peptide concentrations and substantially enhance condensate stability. Isothermal titration calorimetry of peptide-polyanion complexation indicates contribution from both enthalpy and entropy to the overall free energy of coacervation. Finally, phosphorylation of specific residues in the peptide sequence supresses coacervate formation, while alkaline phosphatase (ALP)-mediated dephosphorylation restores LLPS in bacterial culture, enabling ALP to act as a molecular switch. Together, these results indicate that partial molecular ordering is essential for LLPS and establishes the foundation for development of antibacterial peptides condensates with targeted therapeutic applications.

SWRM 2026 SW502

pH-sensitive peptide nanofibers and: Innovations in self-assembling peptides with ionizable non-coacervatesn-natural amino acids

***Jenny Nguyen**, hoang.nguyen8@mavs.uta.edu. Chemistry and Biochemistry, University of Texas at Arlington Research Institute, Fort Worth, Texas, United States*

The development of "smart" biomaterials those capable of sensing and responding to environmental triggers is a cornerstone of modern nanomedicine and tissue engineering. Among these, pH-responsive multidomain peptides (MDPs) and peptide-polymer conjugates have emerged as highly versatile building blocks due to their predictable self-assembly and biological compatibility. We will study the antimicrobial activity of peptides and cytocompatibility of peptide self-assembly. Recent research has focused on two critical advancements in this field: pH-sensitive peptide assembly incorporating histidine residues and pH-sensitive peptide self-assembly derived from protein architectures. This study discusses recent endeavors in developing peptide-polymer conjugate hydrogels, leveraging a double network comprising both covalent and non-covalent interactions. The resulting double network significantly enhances the storage modulus of peptide-based hydrogels. To address antimicrobial properties, antimicrobial peptides were encapsulated. The alternating hydrophobic and hydrophilic residue pattern of antimicrobial peptide facilitates favorable interactions with the peptide component of the hydrogel sharing the same pattern. This enables immobilization within or on the hydrogel network surface, imparting desired antimicrobial activity with low cytotoxicity. This innovative approach based on a covalent-noncovalent double network holds promise in constructing peptide-based hydrogels with tailored rheological properties and diverse biological functionalities, opening new avenues for biomedical applications.

SWRM 2026 SW503

Optimizing DNA-barcoded peptides for the detection of disease-relevant proteases

***Gabriel Pohlman**, gabepohlman@yahoo.com, Devleena Samanta. The University of Texas at Austin, Austin, Texas, United States*

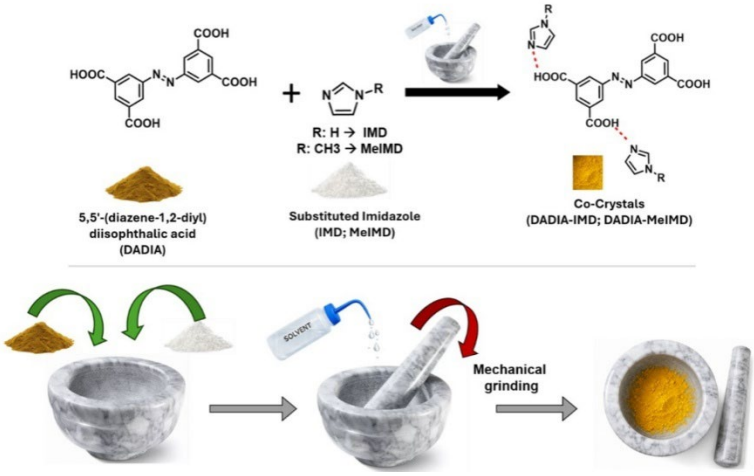
Proteases, enzymes responsible for cleaving peptide bonds within proteins, have received attention as potential disease biomarkers due to their roles in various pathophysiological processes. These enzymes, often dysregulated in disease states, exhibit distinct substrate specificity, enabling them to selectively cleave specific peptide sequences. Our lab has developed protease sensors in which a protease-cleavable peptide is conjugated to a unique DNA sequence. The DNA acts as a barcode helping to identify the protease and acts as a handle for signal amplification. Therefore, by detecting the DNA as a proxy for protease activity, highly sensitive detection of proteases down to 58 pM is possible. My work focuses on understanding how the DNA tag impacts the rate of proteolytic cleavage. Specifically, I am investigating how the length and sequence of the DNA tag along with its position relative to the peptide cleavage site affects proteolysis and subsequent detection sensitivity. Through optimizing these DNA-tagged peptides, our goal is to improve the design of probes. These enhanced probes will enable the detection of multiple proteases at once by tracking the DNA tags, which serve as markers for protease activity. We can utilize various techniques for this purpose, including PCR, CRISPR, and Next-Generation Sequencing (NGS), to facilitate efficient and accurate monitoring of protease activity.

SWRM 2026 SW504

Mechanochemical synthesis and co-former-controlled assembly of azobenzene polycarboxylate organic salts: From framework node to passive guest in HOF-like architectures

JYOTISHKA NATH[1]*, jxn230017@utdallas.edu, Ashutosh Shrivastava*[1]*, Madison Rader*[2]*, Mihaela C. Stefan*[1]*, Michael C. Biewer*[1]*. (1) Department of Chemistry and Biochemistry, The University of Texas at Dallas, Richardson, Texas, United States(2) Department of Chemistry, Radford University, Radford, Virginia, United States*

Hydrogen-bonded co-crystals are versatile supramolecular materials whose architecture can be tuned through co-former selection. Here we report two multicomponent crystals of the azobenzene polycarboxylic acid 4,4′-(diazene-1,2-diyl)bis(3,5-dicarboxybenzoic acid) (DADIA): one with imidazole (DADIA:IMD) and one with N-methylimidazole (DADIA:MeIMD). Both were prepared by mechanochemical grinding followed by recrystallization from methanol. In each case, proton transfer from the carboxylic acid groups to the imidazole nitrogen gives charge-assisted hydrogen bonds, so the materials are best described as organic salts. Single-crystal X-ray diffraction shows that DADIA:IMD crystallizes in a monoclinic and DADIA:MeIMD in a triclinic, both forming two-dimensional HOF-like architectures. In DADIA:IMD, protonated imidazole acts as an active framework node, generating channels occupied by disordered solvent. In DADIA:MeIMD, the 2D sheet is stabilized by hydrogen bonding between DADIA host molecules, with protonated N-methylimidazole housed in the pores as a passive guest. The compounds were further characterized by proton NMR, FT-IR, PXRD, and TGA. These results show how a single N-methyl substituent switches the co-former between the framework node and the guest, with implications for gas storage, separation, and drug delivery.

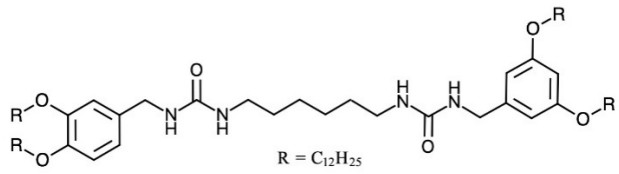


SWRM 2026 SW505

Synthesis and characterization of mixed-ratio bis-urea organogelator systems

Caroline Ceballos, ***Andrew J. Carr****, acarr@austincollege.edu. Chemistry, Austin College, Sherman, Texas, United States*

Oil spills continue to negatively affect marine life despite current remediation and operational safety practices, which has led to growing interest in low molecular weight organogelators (LMWOGs) as a potential clean-up method. In this experiment, five bisurea organogelators derived from 3,4- and 3,5-dihydroxybenzaldehyde were synthesized by a three step procedure- alkylation of the phenols with docecyl bromide followed by reductive amination via an oxime intermediate, the resulting amine was them reacted with 1,6-diisocyanatohexane to for the desired bis ureas pure 3,4-isomer (G3,4), pure 3,5-isomer (G3,5), and (3,4:3,5) 1:1, 1:3, and 3:1 mixtures. Each gelator was confirmed by ^{1}H NMR in $CDCl_3$, and gelation efficiency was tested by measuring the critical gelation concentration (CGC) of each organogelator in motor oil, toluene, and octane. Every mixed ratio gave a lower CGC than either pure isomer in all three solvents, with the 1:1 mixture performing best in motor oil (1.56 mM, 0.21 wt%) and octane (1.61 mM, 0.25 wt%) and the 1:3 (3,4:3,5) mixture performing best in toluene (1.42 mM, 0.16 wt%). This trend suggests that mixing the two isomers disrupts the tight, ordered packing seen in the pure isomers and instead favors the fibrillar network needed for gelation. Additionally, mixed ratiosmay allow for more van der Waals interactions between alkyl tails with solvent producing a stronger network overall. These results show that mixing isomers is an effective way to improve the gelation efficiency of bisurea organogelators and supports their potential use in oil spill remediation and transportation.

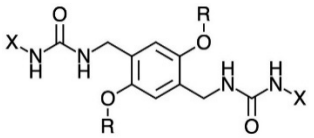


SWRM 2026 SW506

Synthesis and characterization of 2,5-dihydroxytereohthaldehyde derived organogelators

*Katherine J. Riemer, **Andrew J. Carr**, acarr@austincollege.edu. Chemistry, Austin College, Sherman, Texas, United States*

Low molecular weight organogelators (LMWOGs) are small molecules that immobilize organic solvents through the formation of supramolecular gels. LMOWGs self-assemble through a combination of intermolecular forces (hydrogen bonding, π–π stacking, and Van der Waals interactions) and further aggregate to create a complex matrix that immobilizes solvents. LMOWGs possess a variety of applications such as environmental remediation, use in cosmetics, and oil spill recovery. In this experiment, three different 2,5-dihydroxyterephthalaldehyde-derived bisurea organogelators were synthesized via a three step protocol-alkylation with an alkyl bromide(dodecyl, octadecyl, benzyl), reductive amination through an oxime intermediate, followed by reaction with an isocyanate. The performance of each gelator was evaluated by determining the critical gelation concentrations (CGCs) via the vial inversion test in toluene, octane, and motor oil. All three derivatives performed at similar CGC values in toluene, suggesting that gelation efficiency is governed by the bisurea groups and aromatic core and not the alkyl or benzyl tails. However, when examining octane and motor oil it was clear that alkyl/benzyl tail identity significantly impacts CGC values. The benzyl derivative performed the worst in octane, with it being completely insoluble, and in motor oil, with it possessing the highest CGC (0.573 wt%). Meanwhile, the dodecyl tail derivative performed the best in octane (2.25 wt%) and motor oil (0.200 wt%), possessing the lowest CGCs across the three derivatives.



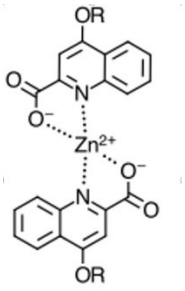
R = $C_{12}H_{25}$, X = $C_{12}H_{25}$, $C_{18}H_{37}$, benzyl

SWRM 2026 SW507

Synthesis and characterization of quinoline-based ligands for metalorganic gelators

*Denton N. Reese, Bradley W. Smucker, **Andrew J. Carr**, acarr@austincollege.edu. Chemistry, Austin College, Sherman, Texas, United States*

A series of alkoxy-substituted quinoline ligands and zinc-containing derivatives were synthesized as potential metalloorganic gelators. The project was designed to investigate how alkoxy chain length affects synthesis, product isolation, Zn(II) coordination, and possible gelation behavior. Methyl 4-hydroxyquinoline-2-carboxylate was first alkylated using iodomethane, bromobutane, or bromododecane to form the corresponding methoxy, butoxy, and dodecyloxy quinoline ester derivatives. The alkylation reactions gave isolated yields of 45.7%, 65.6%, and 67.8%, respectively. The ester products were then hydrolyzed to form the corresponding alkoxy-substituted quinalic acid ligands. Saponification gave a low yield for the methoxy derivative, a moderate yield for the butoxy derivative (56.6%), and near quantatative yeild for the dodecyloxy derivative. The butoxy and dodecyloxy ligands were then reacted with zinc acetate to form zinc quinaldinate complexes, which were isolated in 67.7% and 87.5% yield, respectively. NMR and Single-crystal X-ray diffraction confirmed the structure of methyl 4-butoxyquinoline-2-carboxylate, verifying successful O-alkylation and retention of the methyl ester group before hydrolysis. Overall, the results show that alkyl chain length strongly influenced product recovery throughout the synthetic sequence, with the longer-chain derivatives giving higher isolated yields and providing the most promising candidates for metallogelator testing.



R= CH_3, C_4H_9, $C_{12}H_{25}$

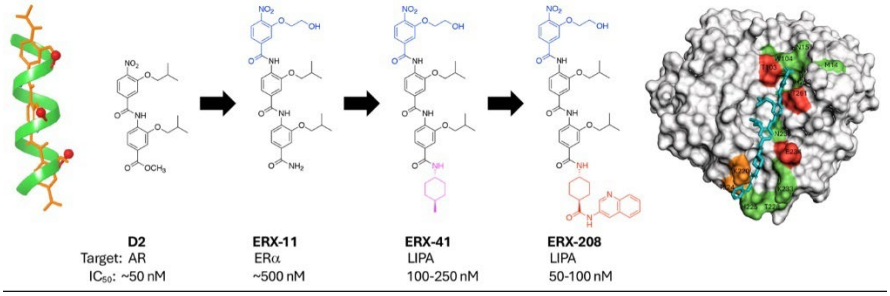
Expected complexation of quinolinic ligands with zinc

SWRM 2026 SW508

Structure-based design of alpha-helix mimetics for inhibiting protein-protein interactions and treating cancers

***Jung-Mo Ahn**, jungmo@utdallas.edu. Chemistry and Biochemistry, The University of Texas at Dallas, Richardson, Texas, United States*

We have designed an oligo-benzamide scaffold as a rigid template to replicate protein helices. It presents side chains of the amino acid residues found at the *i*, *i+4*, and *i+7* positions in a helix in addition to two substituents at its N- and C-termini for achieving higher affinity, selectivity, and improved physicochemical properties. It has demonstrated outstanding mimicry of LXXLL motifs that is critical to facilitate protein-protein interactions between nuclear receptors and their coactivators. Bis-benzamide D2 was found to disrupt androgen receptor and its coactivators effectively in prostate cancer models, whereas tris-benzamide ERX-11 showed potent inhibition of estrogen receptor in breast cancer models. Recently, our efforts to further improve these leads identified a new therapeutic target, lyososomal acid lipase A (LIPA) for treating hard-to-kill cancers like triple-negative breast and ovarian cancers. Tris-benzamide-based ERX-41 was found to induce endoplasmic reticulum (ER) stress, resulting in cell death. Mechanistically, ERX-41 binding to LIPA decreases expression of multiple ER-resident proteins involved in protein folding. This targeted vulnerability has a large therapeutic window with no adverse effects either on normal mammary epithelial cells or in mice. It is also found to be metabolically stable and orally available.



SWRM 2026 SW509

Phagophore-associated protein-inspired antibody-fusion degraders for targeted clearance of intracellular protein aggregates

***Tianqi Wang**, tianqiwang992@gmail.com, Ziwen Jiang. Chemistry and Biochemistry, The University of Texas at Dallas, Richardson, Texas, United States*

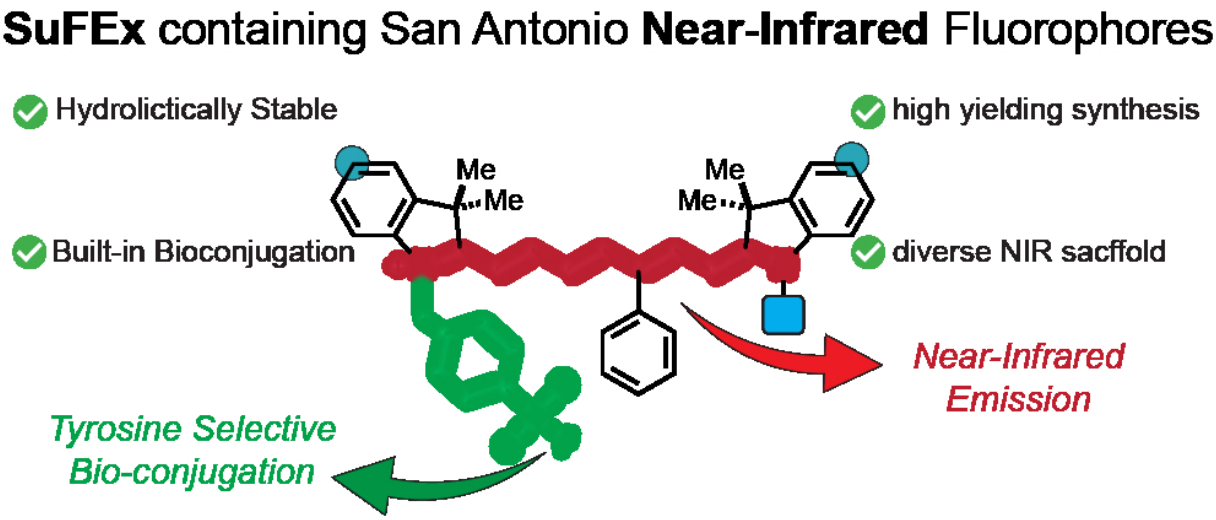
Autophagy is the primary clearance pathway for intracellular protein aggregates. Here, we developed a targeted degradation system by fusing target-specific antibodies directly with mammalian ATG8 proteins. We tested all six ATG8 family members through the antibody-fusion strategies, resulting in a series of ATG8-based antibody degraders. As a result, the degrader specifically recognizes the target protein through the antibody binding, meanwhile the fused ATG8 compoenent directs it toward the forming autophagosomal membrane (*i.e.*, phagophore). Overall, this design promotes selective degradation of intracellular protein aggregates through autophagy, providing a modular and potent strategy for autophagy-based targeted clerance of protein aggregates.

SWRM 2026 SW510

SuFEx-enabled tyrosine specific bioconjugation of near-infrared fluorophores

Syed Usama[1], *syedmuhammad.usama@utsa.edu, Paula Mckay*[1], *Stefan Nashawati*[1], *Mohan Kodisana*[1], *Jude Aden*[1], *Wendell Griffith*[1], *Kirsten Hanson*[2]. *(1) Chemistry, The University of Texas at San Antonio, San Antonio, Texas, United States(2) Molecular Microbiology and Immunology, The University of Texas at San Antonio, San Antonio, Texas, United States*

Sulfur (VI) fluoride exchange (SuFEx) chemistry has been widely applied in small-molecule medicinal chemistry, but its translation to near-infrared fluorophores and application to antibody labeling remain largely unexplored. Here, we report a general synthetic approach for the preparation of aryl sulfonyl fluoride-functionalized indolenines and their incorporation into heptamethine cyanine (Cy7) fluorophores. The strategy is compatible with several substituted indolenines that enabled development of a library of water-soluble, SuFEx-enabled Cy7 fluorophores. Using SAT-NIR-746-SF, we demonstrate that the aryl sulfonyl fluoride handle is stable under physiologically relevant conditions ($t_{1/2}$ >18h at pH 7.4) and enables efficient antibody labeling (DOL up to 6.1). The DOL can be systematically controlled by varying reaction pH, incubation time, and reagent stoichiometry. The strategy was successfully applied to therapeutic monoclonal antibodies, and the resulting conjugates were stable under acidic, physiological, and serum conditions. Amino acid selectivity assays and tandem mass spectrometry-based proteomics of labeled trastuzumab confirmed modification exclusively at tyrosine residues, establishing the tyrosine-selective nature of this conjugation platform. SAT-NIR-746-SF-conjugated secondary antibodies provided specific labeling of phospho-histone H3 (H3S10P) in confocal immunofluorescence microscopy. These results establish SuFEx-enabled Cy7 fluorophores as a practical platform for tyrosine-selective antibody bioconjugation and demonstrate their utility in fluorescence imaging applications.



SWRM 2026 SW511 - Withdrawn

SWRM 2026 SW512

Killing time: Rapid kinetic profiling for antiparasitic drug discovery

Jordon A. Ma[1], *Melanie Arlsanian*[1], *Joshua A. Solorzano*[1], *Alexandra M. Yokomizo*[1], *Claire Hartwell*[1,2], *David C. Swinney*[3], ***Brad A. Haubrich***[1], *bhaubric@touro.edu. (1) Touro University Nevada College of Osteopathic Medicine, Henderson, Nevada, United States(2) University of Nevada Las Vegas Kirk Kerkorian School of Medicine, Las Vegas, Nevada, United States(3) DC Swinney Consulting, Belmont, California, United States*

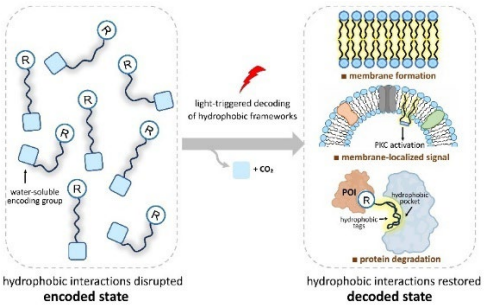
Increasing biological complexity from proteins to cells to organisms leads to many failures in drug discovery as molecules are advanced to the next stage. Extending residence time, to the point of essential irreversibility on a physiological time scale ('pseudoirreversibility'), can help molecules overcome metabolism and excretion in biological systems, if there is selectivity for the pathogen protein. However, detailed measurements of binding kinetics and residence time are costly, making them impractical for large numbers of compounds, particularly when most compounds screened will not exhibit slow-binding behavior. We have adapted a four-point rapid assay to rapidly check for slow-binding behavior early in the discovery process. The assay uses high and low substrate concentrations to assess competitiveness and 0- and 30- minute protein-inhibitor preincubation to identify slow-binding before substrate addition. Compounds displaying differential inhibition after preincubation can then be prioritized for more detailed kinetic characterization. We applied this paradigm to compounds screened against glycogen synthase kinase (GSK from *Trypanosoma cruzi*. The four-point assay distinguished a few slow binders, including human GSK inhibitor TUN-00001, as well as non-GSK-targeting molecules TUN-00004 and TUN-00066, which were more potent *in vitro* with preincubation. Other compounds tested exhibited competitive behavior and rapid equilibrium kinetics, with several possessing micromolar potency. Follow up kinetic assays confirmed slow-binding of the three hits. This slow-binding activity may have been missed in canonical inhibitor screens. Future studies will evaluate slow-binding compounds in microbiological assays and investigate their structure-activity relationships. These results support rapid kinetic profiling as a strategy for prioritizing small-molecule inhibitors in early antiinfective drug discovery.

SWRM 2026 SW513

Light-triggered decoding of hydrophobic interactions in living systems

***Peng Ji**, peji@ucsd.edu, Neal K. Devaraj. Chemistry and Biochemistry, University of California San Diego, La Jolla, California, United States*

The hydrophobic effect is central to biological organization, underlying membrane assembly, molecular recognition, and protein folding. Despite its importance, spatiotemporal control of hydrophobicity is challenging because it emerges from collective solvation free-energy effects around hydrocarbon frameworks whose C(sp3)–H bonds are chemically inert. Here we show that hydrophobic interactions can be encoded and decoded on demand under physiological conditions using water-soluble functional groups and visible light. Aliphatic carbon frameworks are encoded in charged radical precursors, significantly reducing the free-energy penalty of aqueous solvation. Light-triggered single-electron decarboxylation converts these precursors into nonpolar hydrocarbon products, restoring hydrophobic interactions. This transition drives emergent behaviors including membrane self-assembly, lipid-mediated signaling, and targeted protein degradation in living cells.



SWRM 2026 SW514

Quantitative evaluation of bacterial binding affinity of self-bacterial panning-derived silver nanoparticles using Kd analysis

***James Cho**, james.cho@selu.edu, Logan McCarthy, Mckenzie Miller, William Dodson, Samyra Gipson-Gordones. Chemistry and Physics, Southeastern Louisiana University College of Science and Technology, Hammond, Louisiana, United States*

Silver nanoparticles (AgNPs) have demonstrated broad-spectrum antibacterial activity. However, improving their interaction with specific bacterial targets may provide a strategy for enhancing their antibacterial performance. In this study, we investigated a Self-Bacterial Panning (SBP)-based approach for developing silver nanoparticles toward *Klebsiella pneumoniae*. SBP was used to enrich bacterial surface-associated components with affinity for *K. pneumoniae*, which were subsequently incorporated into the nanoparticle system. The bacterial binding characteristics of the resulting SBP-derived AgNPs were quantitatively evaluated using the dissociation constant (Kd) as a measure of binding affinity. Comparative Kd analysis was used to characterize the interaction between the nanoparticles and bacterial cells and to evaluate the effect of SBP-derived biological components on bacterial association. The resulting nanoparticles were further evaluated for their antibacterial activity against *K. pneumoniae*. Together, these analyses provide a quantitative framework for linking the bacterial binding properties of SBP-derived AgNPs with their antibacterial performance. This study demonstrates the potential of Self-Bacterial Panning as a strategy for engineering bacteria-associated nanomaterials and highlights Kd-based analysis as a useful approach for quantitatively characterizing nanoparticle–bacteria interactions.

SWRM 2026 SW515

Pulsed blue light as a potential approach for modulating *Lactobacillus* survival and bacterial-host interactions

***Violet Bumah**, violet.bumah@sfasu.edu. Chemistry and Biochemistry, Stephen F Austin State University, Nacogdoches, Texas, United States*

The increasing prevalence of antimicrobial resistance has created a need for alternative approaches to bacterial control. Pulsed blue light (PBL) is a promising non-antibiotic antimicrobial strategy, but its effects on beneficial microorganisms and bacterial-host interactions require further investigation. This study evaluated the effects of PBL on three lactic acid bacterial strains—*Lactiplantibacillus plantarum* (F201), *Pediococcus pentosaceus* (K18F), and *Pediococcus acidilactici* (K19D)—and examined preliminary interactions between F201 and human dental fibroblasts. Bacterial growth was monitored over 48 hours using optical density measurements. Single cultures, co-cultures, and tri-cultures were exposed to 405, 410, 425, and 450 nm PBL at an irradiance of 10 mW/cm^2 and radiant exposure of 36 J/cm^2. Following treatment, bacterial survival was determined by colony-forming unit enumeration. Initial dental fibroblast adhesion and invasion assays were also conducted using F201. The results demonstrated that PBL activity varied according to wavelength, bacterial strain, culture composition, and growth phase. For instance, in single-culture experiments, F201 showed survival rates of approximately 19.6%, 41.1%, 74.1%, and 83.3% following exposure to 405, 410, 425, and 450 nm, respectively. Mixed cultures demonstrated additional variation in response. For example, stationary-phase F201 + K19D cultures showed survival values ranging from approximately 6.5% to 42.5%, while K19D + K18F cultures exhibited survival between approximately 8.2% and 13.7%. Tri-culture experiments containing all three strains also demonstrated wavelength-dependent survival.

Preliminary dental fibroblast experiments showed variable recovery of F201 following PBL treatment in both adhesion and invasion assays. These findings suggest that PBL can influence Lactobacillus survival while demonstrating that bacterial responses become more complex in mixed microbial and host-associated environments. Continued optimization of irradiation conditions and fibroblast adhesion and invasion assays will help clarify the potential application of PBL as a targeted antimicrobial approach.

SWRM 2026 SW516

Probing alternative reaction pathways in complex condensed-phase systems via first-principles machine-learning force fields

***Deepa Ranabhat**, deeparanabhat@my.unt.edu, Peyton Calvert, Bharatha K. Gunawardana, Hsin-Yu Ko. University of North Texas, Denton, Texas, United States*

Reactive processes in condensed-phase environments are fundamental to chemistry, biology, and materials science. Compared with gas-phase processes, condensed-phase chemical reactions are strongly influenced by local solvation structures and interfaces, thereby increasing the number of viable reaction pathways. Understanding these pathways and their relative importance requires reaction free-energy profiles under realistic condensed-phase conditions. In this work, we develop a high-throughput first-principles framework to systematically compute the reaction free-energy profiles of alternative reaction pathways in complex condensed-phase systems. This framework seamlessly integrates: (1) constrained molecular dynamics within the reliable hybrid density functional theory (DFT) level; (2) adaptive quadrature for free-energy integration; and (3) reactive machine-learning force fields for >10^6x speedup without losing reliable DFT accuracy. As a proof of concept, we apply the framework to high-pressure radical polyethylene polymerization, focusing on chain-growth and the competing chain-transfer pathways. This development paves the way towards a full first-principles framework for probing reaction networks during the real-time evolution of complex condensed-phase reactive systems.

SWRM 2026 SW517

Computational identification of microRNAs as potential biomarkers and follistatin-targeting therapeutic candidates in ischemic heart disease

***Nethania Ajan**[2,1], ajannethania@gmail.com, Gaurav Sharma[1]. (1) Eigen Sciences, Apex, North Carolina, United States(2) Westwood High School, Austin, Texas, United States*

Ischemic heart disease (IHD) remains a leading cause of mortality, highlighting the need for new biomarkers and therapeutic strategies. MicroRNAs (miRNAs) regulate gene expression and may serve as circulating biomarkers or modulators of proteins involved in cardiovascular remodeling. This study used an in-silico workflow to identify miRNAs with potential affinity for follistatin, a protein associated with tissue repair and cardiovascular signaling. We obtained human mature miRNA sequences from miRBase, aligned them using MAFFT, and evaluated them through phylogenetic and sequence-based analyses. Ten representative miRNAs were selected and their secondary and three-dimensional structures were generated using RNAstructure, Forna, and ROSIE. We modeled the follistatin structure using AlphaFold and assessed its localization, disorder, transmembrane regions, and potential binding sites using SignalP, DeepLoc, IUPred3, TMHMM, P2Rank. Follistatin-miRNA

docking was performed using HADDOCK, followed by interaction and binding-energy analyses. Among the evaluated complexes, Docking Job 5 produced the most favorable HADDOCK score (-62.8 ± 1.9), Z-score (-2.2), van der Waals energy (-61.1 ± 3.9), and buried surface area (1648.7 ± 54.8 $Å^2$). However, IEM rescoring identified R1-22 as the most energetically favorable complex, with an estimated interaction energy of -47.66, followed by R6-26 at -39.07. These findings identify promising miRNA–follistatin complexes for further molecular-dynamics simulations and experimental validation. The study demonstrates a computational framework for investigating miRNAs as candidate biomarkers and potential therapeutic regulators in IHD.

SWRM 2026 SW518

Computational prediction of solvent-dependent NMR chemical shifts in flexible macrocycles

***Kien Tran**, taosongduoirac@gmail.com, Benjamin G. Janesko. Chemistry and Biochemistry, Texas Christian University, Fort Worth, Texas, United States*

Large molecules can adopt multiple solution-state conformations, complicating structural assignment efforts based on their nuclear magnetic resonance (NMR) spectra. Prediction of NMR chemical shifts has traditionally focused on improving the accuracy of electronic structure calculations, with recent approaches incorporating rovibrational effects and machine-learning models. However, these approaches do not necessarily account for flexible molecules whose experimental chemical shifts reflect solvent-dependent conformational ensembles. We have developed a computational workflow for systematic prediction of solvent-dependent NMR spectra that prioritises agreement with experiment rather than the accuracy of individual chemical-shift calculations at a single geometry. The workflow includes conformational sampling, structure refinement with density functional theory, chemical shift prediction, and Boltzmann-weighted ensemble averaging. This approach is being applied to macrocycles exhibiting hinging motions in different solvents, with computed chemical shifts compared directly with experiment. Initial results indicate that averaging over low-energy sampled structures improves agreement with experiment, particularly for methyl groups whose individual hydrogen shieldings differ substantially in a static geometry. The calculations also reveal that continuum solvation may be insufficient for specific local solute-solvent interactions; inclusion of a single explicit solvent molecule near a hydrogen-bonding proton substantially improves the predicted chemical shift of that proton. These results demonstrate how systematic ensemble-based NMR prediction can account for dynamic averaging and local solvent effects in experimental spectra, providing a framework for interpreting solvent-dependent NMR measurements of flexible molecules and, ultimately, their conformational dynamics.

SWRM 2026 SW519

GauOpen: An interfacing toolkit

***Edward N. Brothers**, chicoraed@gmail.com, Fernando R. Clemente, Michael J. Frisch. Gaussian Inc, Wallingford, Connecticut, United States*

GauOpen is a toolset designed to make the results of calculations accessible in a modern collaborative ecosystem. It allows intermediate and final calculated quantities from Gaussian to be accessible in a workflow without requiring the workflow to be Gaussian-centric. GauOpen is comprised of two main parts. The first portion is an unformatted file type that stores both calculation

results, such as energies and atomic gradients, as well as intermediate quantities, such as four-center two-electron integrals. This file is self-defining to allow numerous data types to be added to the file by other programs for subsequent manipulation. The second part is a set of subprograms in C, FORTRAN, Perl, and Python that make accessing and utilizing these quantities seamless in modern modular codes. In addition, but separate from GauOpen, code has been added to Gaussian to make interacting with the new file type simple, although this is distinct from the interfacing tools. GauOpen thus makes it far simpler to utilize properties, integrals, etc., calculated via a quantum chemistry code in other software without any knowledge of the original program's data structures and conventions. This talk will focus on GauOpen's efficacy in automation, prototyping, data exchange between programs, the post-processing of results, and pedagogy.

SWRM 2026 SW520

Accurate and time-efficient condensed-phase free energy simulations with reaction-specific delta-machine learning potentials in CHARMM

Saroj Kumar Panda[1]*, saroj.panda2@uta.edu, Abdul Raafik Arattu Thodika*[1]*, Xiaoliang Pan*[2]*, Yihan Shao*[3]*, Kwangho Nam*[1]*. (1) Chemistry and Biochemistry, The University of Texas at Arlington, Arlington, Texas, United States(2) Chemistry and Biochemistry, The University of Oklahoma, Norman, Oklahoma, United States(3) Chemistry, Brandeis University, Waltham, Massachusetts, United States*

The application of machine learning potentials (MLPs) to accurately simulate enzymatic reactions remains challenging. This is primarily due to the high dimensionality and structural heterogeneity of enzyme systems, as well as the need to incorporate off-equilibrium and transition state conformations into the training data. Integrating MLPs into a quantum mechanical/molecular mechanical (QM/MM) framework through either direct learning or Δ-learning, together with reaction-specific training strategies, can help overcome these limitations. In this work, we present an integrated workflow for MLP/ΔMLP-assisted QM/MM simulations that achieves *ab initio* (*ai*) or density functional theory (DFT)-level accuracy in predicting enzyme reaction thermodynamics. Developed within CHARMM and tightly integrated with the *mlp_qmmm* Python package, the workflow automates training-data generation, data sanitization, MLP/ΔMLP training and deployment of trained models in QM/MM molecular dynamics (MD) simulations. In addition, a low-overhead interface implemented in CHARMM enables efficient model inference on both CPU and GPU during simulations. The workflow further incorporates an iterative model-refinement strategy that systematically improves predictive performance through successive rounds of sampling, high-level labeling, and retraining. The capabilities of the approach are demonstrated using the hydride-transfer reaction catalyzed by four variants of dihydrofolate reductase (DHFR). Compared with conventional ai/DFT-QM/MM simulations, the ΔMLP-assisted approach achieves more than 500-fold acceleration while maintaining sub-kcal/mol accuracy in the predicted reaction free energies and free-energy barriers. Iterative refinement further improves the underlying energy and force predictions, leading to more accurate thermodynamic and structural properties obtained from QM/MM simulations with only modest additional computational cost. Overall, this work establishes a scalable and extensible workflow for the systematic development and iterative refinement of reaction-specific MLP/ΔMLP models, enabling highly accurate and computationally efficient simulations of enzyme-catalyzed reactions.

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Discovery of a novel KEAP1 inhibitor screened via a virtual screening workflow and validated biologically

***Nitish Kumar**, nitishsanotra@live.com, Kayla N. Green. Chemistry and Biochemistry, Texas Christian University, Fort Worth, Texas, United States*

Chronic oxidative stress (OS) is a primary cause of Alzheimer's disease and cardiovascular disorders. As a result, recent approaches to treating these diseases focus on reducing chronic OS. The human body naturally regulates oxidative stress through the NRF2 transcription factor, which is controlled by interactions with the KEAP1 protein. However, in the presence of reactive oxygen species, NRF2 is released from KEAP1. Both aging and genetic mutations have been shown to lead to a desensitized or malfunctioning KEAP1 protein, preventing the release of NRF2. This blockage lowers antioxidant expression and increases ROS-induced damage in the body.
Small molecules have been hypothesized to increase cellular NRF2 levels by inhibiting the KEAP1-NRF2 binding domain. KEAP1 inhibitors have been reported as both active and potent but have failed in clinical trials due to off-target effects, poor ADME, and high toxicity. In the era of Computers and Artificial intelligence, using Computer-aided drug design tools to design novel molecules increases efficacy and reduces failures. Therefore, this study presented here focused on screening a large chemical database using molecular docking, molecular dynamics simulations, and IC_{50} predictions via the QSAR-ML webserver. The potency of the most potent compounds was further validated using *in vitro* biological assays, including the KEAP1 inhibition assay, NRF2 expression assay, and endothelial stress assay. This screening identified seven molecules for experimental validation.

SWRM 2026 SW522

Exploring chameleonicity of PROTACs via atomistic simulation

***Kabita Sharma**, kabitasharma@my.unt.edu, Shikshya Bhusal, Omar Valsson. University of North Texas, Denton, Texas, United States*

PROTACs (proteolysis-targeting chimeras) are heterobifunctional molecules consisting of two protein binding moieties connected by a linker. They induce proximity between Protein of Interest (POI) and E3 ligase to form a ternary complex, leading to ubiquitination and the subsequent degradation of the targeted protein. As a result, PROTACs have the potential to address difficult drug targets and reduce drug resistance. Variation in linker length, rigidity, and chemical composition can significantly affect the conformational behavior of PROTACs. However, the large size and flexibility of PROTACs presents challenges in understanding the membrane permeability and their cellular uptake. PROTACs are chameleonic and can adapt to different conformations according to the environment which is thought to improve permeability. Here, using atomistic simulations, we investigate the chameleonicity of different PROTACs with flexible and rigid linkers including those in clinical trials or have been approved by the FDA. We use Parallel-Bias Metadynamics to study their conformational behavior in different solvents, including water, chloroform, and DMSO. Here, chloroform is considered to be a proxy for the membrane environment due to its similar dielectric constant. Our results show that PROTACs with rigid linkers exhibit similar conformational distributions across different solvents. In contrast, PROTACs with flexible linkers display solvent-dependent conformational distributions, adopting collapsed conformations in water and chloroform, and extended conformations in DMSO. Previous studies indicate that folded conformations in apolar environment correlate with greater membrane permeability. Consistently, we observe collapsed conformations for PROTACs with flexible linkers. These findings highlight the importance of the linker in determining the physicochemical properties of PROTACs, but also shows that further investigations are needed to

better understand the relationship between the linker architecture and PROTACs membrane permeability.

SWRM 2026 SW523

Design and insight into the photophysics of photochromic dyes: A DFT and ML study

Juganta K. Roy[1]*, jroy@wtamu.edu, Ruben Nunez*[1,2]*, Emma Doucette*[1,2]*. (1) Chemistry & Physics, West Texas A&M University, Canyon, Texas, United States(2) Engineering, West Texas A&M University, Canyon, Texas, United States*

Semi-transparent solar cells are emerging as promising devices for building integrated photovoltaics due to their stability and attractive color. However, limited optical transmission in daylight or under weather conditions hinders their use as photovoltaic windows. A solution to this issue could be the development of smart transparent photovoltaic windows that can adjust their absorption under intense illumination to generate energy without external intervention. To tackle this challenge, a strategy based on photochromic molecules emerged. Herein, we designed a series of napthopyran-based photochromic dyes with different donor groups (carbazole, indoline, and phenothiazine) and their substituents to examine the effect of the electron-donating group on the optoelectronic properties. We explore the frontier energy distributions and charge-transfer mechanisms of the different fragments of the designed photochromic dyes using Density Functional Theory (DFT) and Time-dependent DFT. Our results revealed that substituting diphenylamine with carbazole, indoline, and phenothiazine donor groups lowers the energy of the highest occupied molecular orbital (HOMO) and shifts the UV-Vis spectra to higher wavelengths. We also implemented a machine learning model to explore the chemical space to optimize the photophysical properties of photochromic dyes. This combined approach provides insights into rational molecular design and photophysics that can guide the development of efficient photochromic dyes.

SWRM 2026 SW524

Pyridinium-derived carbene ligands in nickel-catalyzed carbon–heteroatom coupling

William G. Whitehurst*, william.whitehurst@ttu.edu, Maedeh Bagheri. Chemistry & Biochemistry, Texas Tech University, Lubbock, Texas, United States*

Metalation of a pyridinium group at its 2-position results in the formation of a pyridylidene *N*-heterocyclic carbene that is less stabilized and more strongly electron-donating than established imidazolium-derived *N*-heterocyclic carbenes. Replacement of pyridyl donors within multidentate ligands of transition metal complexes with pyridylidenes retains the ligand framework but incorporates a strong-field donor that could be used to tune the electronic structure and reactivity of the metal center for catalytic applications. Isomeric bipyridine (*iso*-bpy) ligands derived from metalation of *N*-2-pyridyl pyridinium salt precursors were explored in nickel-catalyzed carbon–heteroatom coupling reactions with aryl halides. A series of structurally defined Ni(*iso*-bpy) complexes containing a square planar Ni(II) center were synthesized by C–H activation or oxidative addition into 2-chloropyridinium salts. An optimal Ni(*iso*-bpy) precatalyst was discovered which enabled the coupling of electron-rich aryl chlorides with aliphatic alcohols using low catalyst loadings, overcoming current limitations of thermally sustained, light-free processes using conventional nickel–bipyridine catalysts.

SWRM 2026 SW525

Highly Lewis acidic main group cations partnered with carborane anions as catalysts for hydrodefluorination of PFAS

***Oleg Ozerov**, ozerov@chem.tamu.edu, Joshua H. Daum, Jack P. Raker, Yu-Hsin Chen. Chemistry, Texas A&M University, College Station, Texas, United States*

Catalytic hydrodefluorination (HDF) under highly Lewis acidic conditions is a potentially promising process for the destruction of undesirable per- and polylfluoroalkyl substances (PFAS). Previous work in our group showed that halogenated carboranes as weakly-coordinating anions enable high-turnover silylium-catalyzed HDF of sp^3 C-F bonds in perfluoroalkyl-containing organic molecules. More recently, we were able to access more electron-deficient silylium cations for dramatically improved catalytic HDF reactivity. By analogy, we have begun investigating the potential of borinium and other boron cations as either the reactive species in HDF instead of silylium, or as an activator for the silylium-catalyzed process. The presentation will delve into the fundamental reactivity of these species and their potential relevance in catalysis.

SWRM 2026 SW526

Exploring ligand noninnocence towards s-block-mediated hydrofunctionalization

***Samantha Yruegas**, sy71@rice.edu. Chemistry, Rice University Wiess School of Natural Sciences, Houston, Texas, United States*

C-H functionalization reactions are dominated by precious metal catalysts (i.e. Pd, Pt, Ir) functioning through two-electron redox processes such as oxidative addition and reductive elimination. Comparatively, C-H activation methods with alkaline earth metals (i.e. Mg and Ca) are fundamentally unexplored as redox cycling is inaccessible, thereby restricting directed activation of organic substrates. Noninnocent ligands have enabled first row 3d metals to cooperatively engage in redox cycling by tuning electronic properties or acting as electron reservoirs, emulating oxidative and reductive processes for C-H activation. Strategies to employ redox noninnocent scaffolds onto alkaline earth metals have proven unsuccessful due to their heightened Lewis acidity, Bronsted basicity, and proclivity to undergo facile and fast kinetic ligand redistribution unlike the 3d metals. Our research group has advanced this area through the development of synthetic strategies to access Mg and Ca complexes with noninnocent ligand frameworks, utilizing pincer ligands with pyridine donors in highly delocalized systems to effectively “tame” the electronics at the metal center as our main approach.

SWRM 2026 SW527

Fascinating chemistry of coinage metal ions supported by fluorinated *N*-heterocycles

***Rasika Dias**, dias@uta.edu. Chemistry and Biochemistry, The University of Texas at Arlington, Arlington, Texas, United States*

This presentation explores how fluorinated substituents on ligands impart unique properties to metal complexes, focusing on our recent work with fluorinated pyrazolyl and pyridyl ligands coordinated to copper and silver. Significant advances in photoluminescent materials and gas separation technologies using these metal-fluorinated ligand combinations will be highlighted, along with comparative analyses of non-fluorinated analogs.

SWRM 2026 SW528

Design and synthesis of multifunctional tetra-aza macrocycles for antioxidant and redox applications

Kayla N. Green*, kayla.green@tcu.edu, Hannah K. Pyle, David Mingle, Sarah Dunn. Chemistry & Biochemistry, Texas Christian University, Fort Worth, Texas, United States*

The development of multifunctional small molecules capable of addressing complex chemical and biological challenges requires precise control over molecular architecture. Our laboratory focuses on the synthesis of tetra-aza macrocyclic ligands and their transition metal complexes as versatile platforms for redox-active and antioxidant applications. These systems provide opportunities to systematically modify donor atom identity, ring rigidity, electronic properties, and pendant functional groups to tune reactivity and biological activity. We have developed synthetic strategies that enable the preparation of structurally diverse pyclen-derived macrocycles containing electronically tunable substituents and biologically relevant functionalities. Modification of macrocyclic frameworks has generated compounds capable of supporting transition metal ions while also exhibiting complementary antioxidant properties. Structure-property investigations reveal that ligand architecture strongly influences metal coordination behavior, redox activity, catalytic hydrogen peroxide disproportionation, superoxide scavenging activity, and cellular protection from oxidative stress. These studies demonstrate that strategic synthetic modification can be used to incorporate multiple functional attributes within a single molecular scaffold. Ongoing efforts are focused on expanding the chemical space of these macrocyclic systems and establishing design principles that connect molecular structure with antioxidant function. Collectively, this work highlights the power of synthetic inorganic and bioinorganic chemistry to generate multifunctional molecules with applications ranging from catalysis to therapeutic antioxidant development.

SWRM 2026 SW529

Carborane substituted boron compounds

Caleb Martin*, caleb_d_martin@baylor.edu. Baylor University, Waco, Texas, United States*

Dodecacarborane clusters ($C_2B_{10}H_{12}$) have been known for 60 years yet their application as an electron withdrawing group is not well established. Our group has been preparing boron complexes that feature two or three *ortho*-carboranes as bulky electron withdrawing groups on boron to enhance the Lewis acidity. The reactivity of the new boranes is compared to the state-of-the-art boranes with fluoroaryl groups revealing significantly greater Lewis acidity. In addition to stabilizing electrophilic centers, the electron withdrawing effects can be leveraged to stabilize boryl anions. The properties of the feature compounds, mechanisms of the reactions, and isolation of reactive intermediates will be discussed.

SWRM 2026 SW530 - Withdrawn

SWRM 2026 SW531

Alkyl/aryl phosphido ligands as tunable bridging ligands for controlling dipolar coupling interactions in Ln-cluster single-molecule magnets

Trevor Latendresse[1]*, trechem@gmail.com, Jeffrey D. Rinehart*[2]*, James Vanjak*[1]*, Maximilian G. Bernbeck*[2]*. (1) Chemistry, University of Houston System, Houston, Texas, United States(2) University of California San Diego, La Jolla, California, United States*

Single-molecule magnets (SMMs) are discrete molecules having magnetic anisotropy of purely molecular origin. The realization of SMMs has garnered significant interest in their utilization as synthetically modifiable spin units in quantum-based processing and data-storage technologies. Lanthanide cluster SMMs, which utilize Ln-Ln interactions to improve SMM performance, have emerged as some of the top performing SMMs to date with selected examples featuring magnetic hysteresis near liquid N_2 temperatures and coercive field strengths rivaling bulk magnetic materials. The performance of Ln-cluster SMMs is strongly dependent on the strength and nature of the magnetic coupling interactions between lanthanide ions in a molecule. As such, developing systems in which the Ln-Ln interactions can be manipulated in a predictable manner will be key to further advancement of SMMs toward their practical application. Herein, we show that the highly modifiable steric and electronic profiles of alkyl/aryl phosphido ligands can be used to predicably control Ln-Ln interactions in cluster SMMs. The synthesis, structural, and magnetic characterization of a new family of phosphido-bridged lanthanides cluster SMMs will be discussed and the observed magneto-structrual correlations will be corroborated with computational methods. In all, this study highlights the utility of unconventional phosphido ligands in controlling Ln-Ln interactions, and hence the performance, of lanthanide cluster SMMs.

SWRM 2026 SW532

Photochemical reactivity trends of early transition metal oxos for sustainable oxidation catalysis

Matthew B. Chambers*, chambers@lsu.edu. Chemistry, Louisiana State University System, Baton Rouge, Louisiana, United States*

Toward the development of sustainable methodologies for hydrocarbon functionalization, we have recently reported a Mo dioxo platform that mediates C–H activation upon irradiation at 365 nm. The organic products resulting from the reaction are found to disproportionately disfavor oxygenation relative to high-valent Fe and Co counterparts due to the thermodynamically stronger interaction between the intermediate hydroxyl moiety and the early transition metal. This makes a more diverse array of products available, including new C–C bonds via homocoupling, and halogenations, among others. The original platform employed a weakly coordinating bpy ligand supporting an inorganic MoO_2Cl_2 core that was activated via a bpy to Mo ligand-to metal charge transfer. Photocatalysis can be achieved through the inclusion of a sacrifical oxygen atom donor, but is stifled by bpy ligand lability. This work will present new efforts to develop robust ancillary ligand environments while

maintaining the critical photochemical properties needed to support photochemical reactivity towards enhancing and broadening the photocatalytic performance of the Mo dioxo complexes. Strategies for supporting similar reactivity using blue light via ancillary ligand modifications will also be discussed. Additionally, preliminary successes in developing monometallic Ti(IV) mono-oxo complexes with suitable lifetimes and excited-state electronic structure for photochemical reactivity will be presented. Initial observations of light-initiated oxygen atom transfer reactivity from these platforms suggest that they transiently generate reduced Ti(II) complexes, which can be thermally reoxidized by H_2O to regenerate the high-valent Ti(IV) oxo. This enables photocatalysis that leverages H_2O as a benign source of terminal oxygen atoms. Underlying synthetic, mechanistic, and selectivity challenges will be addressed.

SWRM 2026 SW533

Molecular design for uranyl coordination and reactivity

***Anne E. Gorden**, anne.gorden@ttu.edu. Chemistry and Biochemistry, Texas Tech University, Lubbock, Texas, United States*

The coordination chemistry of the uranyl ion is strongly influenced by the electronic and structural environment surrounding the uranium center, yet establishing clear relationships between ligand structure and uranyl properties remains challenging. Our research uses molecularly tunable Schiff-base ligands to investigate how changes in the equatorial coordination environment influence uranyl structure, noncovalent interactions, and redox behavior. Recent studies of naphthylsalophen and pyrasal complexes demonstrate that relatively subtle changes in the equatorial ligand framework can significantly alter the uranyl oxo environment. In one pyrasal complex, hydrogen bonding between a coordinated water molecule and a uranyl oxo ligand results in asymmetric elongation of the U–O bonds. Building on these structural studies, a series of monohalogenated naphthylsalophen complexes containing F, Cl, or Br substituents was used to examine the effect of the fifth coordination site on uranyl redox chemistry. Coordination of acetate shifts the apparent U(VI)/U(V) reduction potential to more negative values, demonstrating increased stabilization of U(VI). At the same time, removal of the anionic ligand enables access to uranium-centered reduction. The magnitude and reversibility of these responses also vary with ligand substitution. Together, these results demonstrate that both the Schiff-base ligand framework and the fifth coordination site provide molecular handles for controlling the electronic structure and reactivity of uranyl.

SWRM 2026 SW534

Diarylselenides potentiated by carbenium functionalities: Synthesis, reactivity and catalytic studies

***Arkamitra Roy**, arkamitraroy2001@tamu.edu, Francois P. Gabbai. Chemistry, Texas A&M University System, College Station, Texas, United States*

Our ongoing studies of cationic main group compounds have motivated us to explore how electron-rich heavy p-block elements interact with, and are influenced by, a proximal carbenium (C^+). In this work, we focus on systems where a diaryl selenium moiety is positioned in the immediate vicinity of carbenium center. Due to the proximity of these functionalities, Se->C^+ intramolecular donor-acceptor interaction becomes possible. The goal of this study is to test whether such interactions can modulate

the redox properties of the selenium center, with possible applications in catalysis. These concepts will be demonstrated through a presentation of the catalytic properties that these systems display in various reactions, including halogenation and oxidation reactions.

SWRM 2026 SW535 - Withdrawn

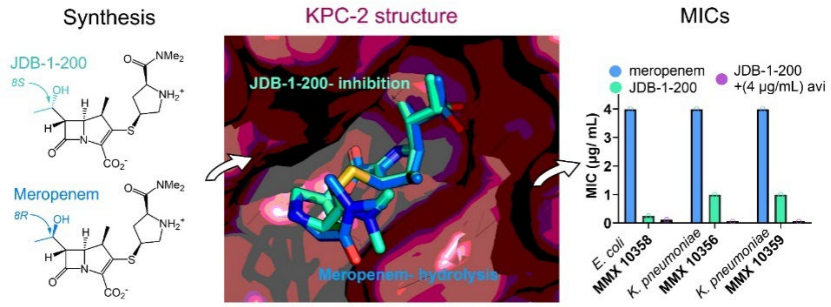
SWRM 2026 SW536 - Withdrawn

SWRM 2026 SW537

Synthesis and evaluation of a carbapenem C8 diastereomer with standalone activity against KPC-producing Enterobacterales

Md Mahbub K. Khan[1]*, mdmahbubkabirk@smu.edu, Pojun Quan*[1]*, Jonathan Cox*[1]*, Maidileyvis Castro Cabello*[1]*, Lucas Webster*[1]*, Matthew McLelland*[1]*, Sarah Tadesse*[1]*, Miriam Hagen*[1]*, Srilaasya Thadiboyina*[1]*, Sara Vijay*[1]*, Anisha Puri*[1]*, Amey Jayaprakash*[1]*, Ava Brown*[1]*, Diego Villareal*[1]*, Rob Lane*[1]*, Ben Radko*[1]*, Lakshitha BhatlaPenumarthi*[1]*, Connie Zhao*[1]*, Bryan Li*[1]*, Aditya Zanzaria*[1]*, Megha Pillai*[1]*, Param Shah*[1]*, James Spencer*[2]*, Catherine Tooke*[3]*, John D. Buynak*[1]*. (1) Chemistry, Southern Methodist University, Dallas, Texas, United States(2) School of Cellular and Molecular Medicine, University of Bristol, Bristol, United Kingdom(3) Department of Life Sciences and Centre of Evolution, University of Bath, Bath, England, United Kingdom*

The carbapenem class of antibiotics represents a crucial last line of defense against resistant bacteria. Unfortunately, the 21st century has seen the development of carbapenem resistance especially in clinically important Gram-negative pathogens. Carbapenem Resistant Enterobacterales (CRE), including *Escherichia coli* and *Klebsiella pneumoniae* are increasingly common pathogens. Resistance in CRE is often associated with production of *K. pneumoniae* (KPC) carbapenemases. The Buynak research group at SMU has been systematically exploring structural alterations of carbapenems with the objective of improving efficacy against resistant microbial strains. Among current commercial antibiotics, the substitution pattern of substituents around the core carbapenem scaffold has remained unaltered, excepting at C2, resulting in similar susceptibility to carbapenemase-mediated hydrolysis. We now report the synthesis and *in vitro* evaluation of a structurally modified meropenem (MEM) derivative, JDB-1-200, (i.e. 8-epi-meropenem, where the stereochemistry of the C8 hydroxyl is inverted), displaying enhanced activity, relative to MEM, against KPC-producing CRE. JDB-1-200 alone displayed superior activity (MICs 0.5 to 1 mg/L, compared to > 8 mg/L for MEM) against several clinically relevant Enterobacterales, including KPC-producing *K. pneumoniae* and *Citrobacter freundii.* Crystallographic analysis of JDB-1-200 complexes with the E166Q deacylation-deficient KPC-2 mutant, compared with an analogous MEM (8*R*-hydroxyl) complex, indicates improvement is from the JDB 8*S*-hydroxyl group acting as a hydrogen bond donor to the hydrolytic water, slowing acyl-enzyme hydrolysis with similar interactions observed in a CTX-M-15:JDB-1-200 complex.



SWRM 2026 SW538

Dual catalytic and convergent approach to δ- and γ-lactones via photo- and lutidinium-catalysis

***Parul Sharma**, parshar@okstate.edu, Avery Ethridge, Eric Rhoades, Spencer Pitre, Jimmie D. Weaver. Chemistry, Oklahoma State University, Stillwater, Oklahoma, United States*

Lactones represent key structural motifs in a wide range of natural products and pharmaceuticals; however, conventional synthetic strategies, such as intramolecular cyclizations or C–H activation strategies typically require multiple steps and extensive pre-functionalization to forge the necessary bonds. In contrast, our approach breaks this traditional synthetic sequence by enabling the construction of two key bonds in a single transformation, providing a fundamentally new disconnection strategy for lactone synthesis. This streamlined pathway not only simplifies access to these valuable heterocycles but also demonstrates remarkable substrate generality, proceeding efficiently across a wide range of leaving groups, substitution patterns, and sterically demanding architectures that often impede classical methods. Using Ir[p-F(t-Bu)-ppy]3 under visible light, we developed a mild photocatalytic carbo-lactonization that converts simple alkenes into γ- and δ-lactones with broad substrate generality, including bromo- and chloroacetamides and previously underutilized acetic acid derivatives. Through mechanistic analysis, it is revealed that the lutidinium alkyl iodide salt functions in dual capacities. It serves as a co-catalyst by promoting radical generation through nucleophilic exchange (i.e., a Finkelstein reaction) and subsequently facilitating halogen atom transfer with the iodide formed in situ via its reduced form. Critically, after the initial radical addition to the alkene, the resulting carbon-centered radical must undergo oxidation to form the corresponding cationic intermediate required for productive lactone closure. While the precise identity of the oxidant remains under investigation, our data are consistent with a pathway in which transient iodine-based species function as a net oxidant to turn over this radical intermediate. Taken together, these steps enable efficient atom-transfer-mediated radical addition and subsequent cyclization to the lactone. Together, these steps allow an efficient, sustainable route to value-added lactones with wide utility in synthesis and medicinal chemistry.

SWRM 2026 SW539

Enantioselective *N*-heteroaryl C–H functionalization for piperidine–azine conjugation via dearomative addition–hydrogen auto-transfer

***Seoyoung Lee**[1], sl55925@my.utexas.edu, Sarah Teoh[1], Pei-Pei Xie[2], Erin M. McManus[1], Brandon I. Gonzalez[1], Tate A. Claggett[1], Peng Liu[2], Michael J. Krische[1]. (1) The University of Texas at Austin*

College of Natural Sciences, Austin, Texas, United States(2) University of Pittsburgh, Pittsburgh, Pennsylvania, United States

Piperidines, azetidines, and azines are privileged heterocyclic motifs in pharmaceutical chemistry, yet direct asymmetric C–C bond formation between saturated nitrogen heterocycles and azines remains challenging, especially without premetalated reagents, directing groups, or Lewis acid activation. In contrast, hydrogen auto-transfer offers a catalytic strategy for C–C bond formation in which transient organometallic nucleophiles are generated in situ from π-unsaturated pronucleophiles, avoiding preformed organometallic reagents and stoichiometric metallic byproducts. This work describes the first enantioselective *N*-heteroaryl C–H functionalization via dearomative addition-hydrogen auto-transfer. In this process, alkynes serve as latent allylmetal pronucleophiles, undergoing dearomative azine addition followed by β-hydride elimination to furnish products of C–H allylation. This strategy enables direct asymmetric conjugation of saturated nitrogen heterocycles with electron-deficient azines, providing access to piperidine–azine and azetidine–azine conjugates with high levels of enantioselectivity. The broad azine scope and compatibility with both piperidine- and azetidine-containing alkynes highlight the utility of this platform for assembling heterocycle-rich molecules. Isolation of a dearomatized intermediate and DFT calculations support a dearomative pathway and show that the site of C–C bond formation is guided by the electronic structure of the *N*-heteroarene. Together, these studies establish alkynes as effective allylmetal pronucleophiles for enantioselective heteroaryl C–H functionalization.

SWRM 2026 SW540

Photophysical investigation of BODIPY molecular systems promoting aggregation-induced emission

Snigdha Dutta[1]*, snigdhadutta@my.unt.edu, Shahrzad Kazemi*[1]*, Amiy Krishna*[2]*, Rajneesh Misra*[2]*, Francis D'Souza*[1]*. (1) Chemistry, University of North Texas, Denton, Texas, United States(2) Chemistry, Indian Institute of Technology Indore, Indore, MP, India*

Conventional fluorophores, such as BF_2-chelated dipyrromethene (BODIPY), are known for their efficient emission in dilute solution. But they suffer from severe Aggregation-caused Quenching (ACQ) in the solid state or in aggregated form. This poses a serious application problem since fluorophores are expected to be functional in the solid/aggregated state in OLEDs and bioimaging. In this work, two series of compounds have been investigated to examine whether notoriously ACQ-prone chromophores can instead be engineered to exhibit Aggregation-induced Emission (AIE) and single-component white-light emission (WLE). Series 1 comprises bis-styryl BODIPY dyes bearing a pyridinium-naphthalene acceptor at the *meso*-position. Studies reveal AIE along with WLE in selected derivatives, owing to a proper balance of naphthyl emission, energy transfer, and charge transfer within these compounds. Series 2 compounds contain triphenylamine (TPA) at the BODIPY *meso*-position with varying peripheral units. AIE in these compounds suggests a charge-separation-driven, quenching-resisting mechanism distinct from the classical restriction-of-motion model. Together, these studies will provide insight into converting ACQ-susceptible chromophore families into AIEgens and tuning them into functional white-light emitters for bioimaging, sensing, and solid-state lighting applications.

SWRM 2026 SW541

Investigation of cobalt complexes for visible-light-driven radical reactions: Insights from axial and square planar ligand variation

***Subrata Pal**, supal@okstate.edu, Martin Pauze, Spencer Pitre. Chemistry, Oklahoma State University The College of Arts and Sciences, Stillwater, Oklahoma, United States*

Upon reduction to Co(I), macrocyclic four coordinate cobalt complexes exhibit high nucleophilicity, enabling S_N2-type transformation with almost any electrophile, like alkyl halides, to form a weak Co(III)—C bond. Visible light photolysis of this bond generates a nucleophilic C-centered radical, a reactivity pattern that has made these complexes a center of interest as photocatalysts in C—C bond-forming reactions. Vitamin B_{12} remains the most widely used photocatalyst of this type, but its high cost and limited solubility in aprotic solvents motivates the search for synthetic alternatives, as the investigation of new alternatives of cobalt complexes that can be used for nucleophilic cobalt photocatalysis remains limited. In this work, we discussed our progress towards the preparation of a series of cobalt complexes and their performance in different photochemical reactions. In particular, the effects of both the axial and square planar ligands on their catalytic activity and their efficiency in different photochemical reactions in comparison to Vitamin B_{12} will be discussed.

SWRM 2026 SW542

Radical and photochemical amination of polymers and small molecules

***Robert Comito**[1], rjcomito@central.uh.edu, Subrata Ghosh[2], Mengnan Hu[3], Lizhe He[1], Qingqing Dong[1], Adam Czader[1]. (1) University of Houston, Houston, Texas, United States(2) University of Michigan, Ann Arbor, Michigan, United States(3) Affinity Chemistry, Wilmington, Delaware, United States*

Amines are central to the bioactivity of small molecule medicines and polymers. This presentation will cover two synthetic methods developed by our laboratory that introduce basic amines in a single step. In the first method, simple amination of sp3 CH bonds gives primary amines (RNH2) in one pot, via CH imination. We use this process in the synthesis of small molecule amines and in the CH amination of polyolefins. The modification significantly increases the polarity of polystyrene even at a low loading (up to 0.5%), improving its potential biocompatibility. In our second method, we achieve the photoalkylation of imines using energy transfer photocatalysis. This process delivers complex alpha-tertiary primary amines, and is amenable to a wide range of functional groups and substrates. To avoid the potential side reactivity of imines, we also developed a cascade process that generates the imines in situ for alkylation. All of these reactions come with detailed physical organic analysis and computational modelling, providing a comprehensive mechanistic picture.

SWRM 2026 SW543

Highly stereoselective olefin cyclopropanation via enzyme-catalyzed reductive activation of *gem*-dibromoalkanes

***Aakash Pal**, aakash.pal@utdallas.edu, Shrivatsa Thulasiram, Z Jaron Tong, Bo M. Couture, Juan D. Villada, Rudi Fasan. The University of Texas at Dallas, Richardson, Texas, United States*

Over the past decade, engineered hemoproteins have emerged as powerful biocatalysts for asymmetric, new-to-nature carbene transfer reactions. Despite significant advances in biocatalytic cyclopropanation reactions, these transformations have been largely limited to diazo-based carbene precursors with electron-deficient substituents. Herein, we report a biocatalytic strategy for stereoselective cyclopropanation of olefins using gem-dibromoalkanes as carbene precursors. This method enables the asymmetric cyclopropanation of vinylarenes bearing both electron-donating and electron-withdrawing groups to afford *trans*-1,2- diarylcyclopropanes in up to >99% yield and with high diastereo- and enantiodivergent selectivity (>20:1 *d.r.*; up to >99% *ee*). This strategy could be further applied to the generation of a variety of complex, valuable, sp^3-rich spirocyclic scaffolds via cyclopropanation of exocyclic methylene-substituted benzofused carbo and heterocycle derivatives and extended to σ-bond (Si-H/S-H) carbene insertions. Mechanistic studies support the formation a α-halo radical intermediate via enzyme-mediated reduction of benzylic *gem*-dibromides as a key step for generation of the reactive heme-carbenoid species implicated in carbene transfer. This work expands the scope of biocatalytic carbene transfer reactions, and it paves the way to the exploitation of *gem*-dibromoalkanes and other non-diazo carbene precursors in enzyme-catalyzed new-to-nature transformations.

SWRM 2026 SW544 - Withdrawn

SWRM 2026 SW545

Synthesis of fluorosulfonyl aziridines and β-lactams from alkenes as multifunctional hubs

Varun Prabhakar[1]*, varunp18@tamu.edu, Quentin Michaudel*[1,2]*. (1) chemistry, Texas A&M University, College Station, Texas, United States(2) Material Science, Texas A&M University System, College Station, Texas, United States*

Sulfonyl fluorides (RSO_2F) have found applications in fields ranging from medicinal chemistry to materials science as a chemical handle for Sulfur (VI) Fluoride Exchange (SuFEx) click chemistry. However, despite their presence in bioactive compounds, synthetic methods for accessing sulfamoyl fluorides ($NR_1R_2SO_2F$), the nitrogen-containing counterparts of sulfonyl fluorides, remain scarce. Most reports to date rely on the installation of the $–SO_2F$ group onto amines, thereby limiting the scope of sulfamoyl fluorides. This presentation will discuss an alternative approach focused on the synthesis of sulfamoyl fluorides through C–N bond formation. First, a Rh-catalyzed synthesis of bifunctional fluorosulfonyl aziridine from alkenes using FSO_2NH_2 will be covered. A safe and practical method for the synthesis of FSO_2NH_2 was developed by the photodegradation of fluorosulfonyl azide (FSO_2N_3) in solution with UV light. Then, the synthetic utilities of bifunctional fluorosulfonyl aziridines will be highlighted with a variety of examples, including SuFEx couplings, ring-opening reactions of aziridines, cycloaddition reactions, and the formation of multi-click hubs.

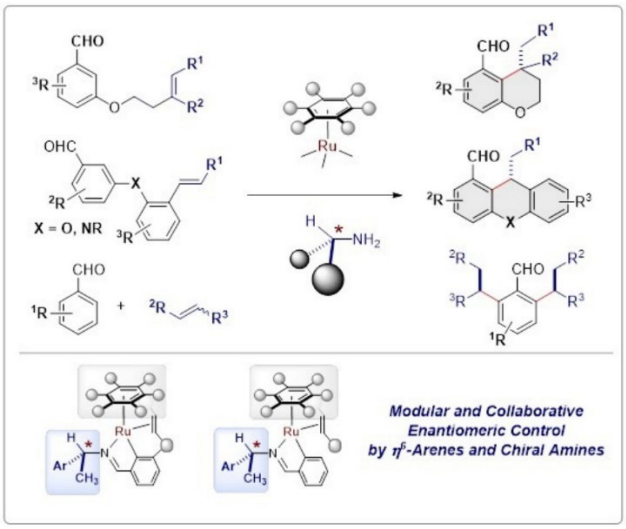
SWRM 2026 SW546 - Withdrawn

SWRM 2026 SW547

Cooperative non-covalent rigidification for enantioselective and regioselective C–H hydroarylation via chiral transient directing groups

***Weinan Tan**, wt411@msstate.edu, brian tran, Xin Cui. chemistry, University of North Texas, Denton, Texas, United States*

Enantioselective C–H functionalization provides a direct and atom-economical approach to chiral molecules from readily available substrates. Ruthenium is an attractive platform owing to its low cost and well-established C–H activation chemistry. Unlike palladium, which often favors Heck-type olefination, ruthenium can promote hydroarylation to directly construct saturated C–C bonds and stereogenic centers. Here, we report a Ru-catalyzed enantioselective hydroarylation employing α-branched amines as chiral transient directing groups (cTDGs). This strategy enables the direct synthesis of chiral benzofused heterocycles, including chromane and xanthene derivatives, from simple alkenes without preinstalled directing groups. The combination of tunable Ru(II)–arene complexes and chiral amines enables cooperative control of reactivity and enantioselectivity. Modification of the catalytic system further enables enantioselective intermolecular hydroarylation, demonstrating broad substrate scope and catalytic versatility. Mechanistic studies, including H/D scrambling, kinetic isotope effects, and DFT calculations, reveal a condition-dependent turnover-determining transition state and distinct rate-determining steps for the two enantiomeric pathways. These findings provide insight into asymmetric induction in d6 metal systems and the interplay between the cTDG and η6-arene ligand. The retained aldehyde functionality enables diverse downstream transformations, providing access to bio-relevant polycyclic scaffolds and previously unreported architectures. Overall, this work establishes a versatile platform for Ru-catalyzed enantioselective hydroarylation and expands the utility of cTDGs in asymmetric C–H functionalization.



SWRM 2026 SW548

Academic celebrations and digital portfolios: Alternative assessment strategies for scientific literacy in inorganic chemistry

***Julia Chan**, julia_chan@baylor.edu. Chemistry & Biochemistry, Baylor University, Waco, Texas, United States*

Developing students' ability to critically analyze and communicate primary literature is a central learning objective in upper-level inorganic chemistry courses. To support this goal, two

complementary assessment approaches were implemented: an oral examination reimagined as an "Academic Celebration" and a digital portfolio focused on student-selected journal articles. In the Academic Celebration format, students presented and discussed a research article with the instructor in a conversational, low-stakes environment designed to evaluate content mastery, scientific reasoning, and communication skills. The digital portfolio required students to curate and summarize a contemporary inorganic chemistry research paper, synthesize its key findings, connect the work to course concepts, and reflect on its broader scientific significance. This presentation will describe the design, implementation, and assessment of these activities and compare outcomes with those obtained using more traditional assessment methods, including written exams and article summaries. Assessment data, student performance metrics, and student feedback will be presented to evaluate the impact of these approaches on scientific literacy, engagement with the primary literature, and confidence in communicating chemistry. Lessons learned, challenges encountered, and recommendations for adapting these strategies to other chemistry courses will also be discussed. Results suggest that integrating oral assessment and reflective digital portfolios can promote deeper engagement with the chemical literature while providing opportunities for students to demonstrate learning in ways that extend beyond traditional examinations.

SWRM 2026 SW549

Bridging the gap between chemical education research and classroom practice

Stephen G. Prilliman*, sgprilliman@okcu.edu. Chemistry, Oklahoma City University, Oklahoma City, Oklahoma, United States*

Chemical education research of the last forty years has revealed the importance of inquiry, social learning, addressing misconceptions and particulate representations. Education, however, is an inherently conservative endeavor with teachers and instructors tending to teach the way they were taught. This tendency is exacerbated by structural issues like class sizes and, especially at the high school level, by high teacher turnover and ongoing shortages of teachers in STEM subjects. As such, the hard-won lessons of chemical education research often remain unadopted in chemistry classrooms. This work seeks to understand routes to communicate and facilitate adoption of these lessons in the context of the author’s experience writing a one-volume book on particulate representations.

SWRM 2026 SW550

Focus on successful students in general chemistry

Diana S. Mason*, diana.mason@unt.edu. Chemistry, University of North Texas, Denton, Texas, United States*

It is possible to identify the majority of the students who will be successful in general chemistry the first day of class. Their automaticity (what they can do without a calculating device) matters! The more arithmetic facts that can be correctly recalled without the use of a calculating device, the more successful on the average students will be. Basic arithmetic skills, when committed to memory, may be one of the most important skills all students have. This study has been in progress since 2016, involves over 9000 Texas students, and has expanded to several other states and at least one other country, Colombia, South America. What is interesting are the similarties in all studies to date.

SWRM 2026 SW551

Using language mindfully to effectively assess students' learning

Stephanie M. Taylor[1]*, stephaniem.taylor@utdallas.edu, Renee Davis*[2]*, Gregg R. Dieckmann*[3]*, Bill Hefley*[4]*, Carie King*[5]*, Md Mohedul Islam*[6]*, Christina Hailu*[4]*, Claire Phan*[2]*. (1) Science/Math Education, The University of Texas at Dallas School of Natural Sciences and Mathematics, Richardson, Texas, United States(2) The University of Texas at Dallas, Richardson, Texas, United States(3) Chemistry and Biochemistry, The University of Texas at Dallas School of Natural Sciences and Mathematics, Richardson, Texas, United States(5) The University of Texas at Dallas Harry W Bass Jr School of Arts Humanities and Technology, Richardson, Texas, United States(6) University of Pikeville, Pikeville, Kentucky, United States*

Exam questions are designed to assess students' understanding and mastery of concepts; however, an often overlooked second component for students' success involves their understanding of what is stated and asked in each question. To consider the construction of exam questions, we assembled an interdisciplinary team to investigate 20+ years of multiple-choice exam results for large enrollment (1000+) general chemistry courses to identify language in questions that best predicts student success. Additionally, Fall 2022 to Spring 2026, we incorporated one piloted question in each general chemistry I and II exam, with questions using various language constructs but identical data and answer palette. The team will present what we have learned—e.g., which question constructs best predict student success and what demographics help or hinder student success with these questions. Considering question format and language can affect students and is worth considering.

SWRM 2026 SW552

Teaching organic chemical nomenclature through an educational game

Celyna Rackov[1]*, crackov@tarleton.edu, Hiale Yane Silva de Souza*[2]*. (1) Chemistry, Tarleton State University, Stephenville, Texas, United States(2) Chemistry, Universidade Federal do Acre, Rio Branco, AC, Brazil*

Nowadays, didactic games are increasingly being incorporated into classrooms as a way to supplement traditional instructional methods and make learning more dynamic and interactive. Rather than serving only as a means of transmitting knowledge, these games encourage active participation and the collaborative construction of knowledge. It is important to emphasize that didactic games are not intended to replace traditional teaching methods but rather to serve as complementary instructional tools that support teachers and increase student motivation throughout the teaching–learning process. This study presents Organic Dice, an educational dice-based game designed to teach the nomenclature of organic compounds, and reports its implementation in a Brazilian high school classroom. The game uses multiple dice representing the organic functional group, the number of carbon atoms, and the type of carbon–carbon bond, allowing students to construct and name the resulting compounds according to the official IUPAC nomenclature. Following the classroom implementation, increased student motivation and interest in identifying and naming organic compounds were observed. These findings suggest that Organic Dice is an effective supplementary tool for teaching and learning organic chemical nomenclature.

SWRM 2026 SW553

Teaching thermodynamics; a journey of pedagogical partnership

***Mashhad Fahes**, mashhad.fahes@ou.edu, Layla Williams, Deborah Rufus, Kelvin Asamoah, Geneva Murray. The University of Oklahoma, Norman, Oklahoma, United States*

As STEM instructors, many of us resist the idea that education research is relevant to our experience and to our students' learning needs. Even those of us interested in improving are rarely motivated to transition from theoretical framing to actually trying things out. On one hand, academic incentive structures in research-intensive universities implicitly discourage investing time to improve teaching. On the other hand, trying something new carries risks: Will it work? How much time and effort will this take? These barriers can, even with the best of intentions, keep us relying heavily on lectures and a one-way delivery of information. Dr. Fahes' view of "what makes a good teacher" evolved many times over the past two decades. Each evolution brought her closer to understanding the process of learning. However, it was the Developing Understanding and Engagement Together (DUET) program at OU that put her on the path for a very different evolution. DUET is facilitated by Dr. Murray and pairs a faculty and a student fellow as pedagogical partners for a semester. Through weekly observations and discussions, the team worked through targeted classroom improvements that were grounded in pedagogical theory, were directly suited for the instructor's teaching preferences, and were responsive to the students' experience. Dr. Fahes, an Associate Professor in Petroleum Engineering, was paired with Layla Williams, a doctoral candidate in the Department of Philosophy as part of the DUET program, working with Graduate Teaching Assistant Deborah Rufus and Kelvin Asamoah. The instructor joined DUET due to problems with students' ability to fully comprehend concepts and apply it correctly to solve problems. In this talk, the team shares practical instructional experiences of how they tried to resolve these challenges pre- and post- participation in DUET. It covers ways in which the team worked on delegating some of the "cognitive load" to students during class time, ways in which addressing "metacognition" and building "self-efficacy" helped students gain more control of their learning experience, and some intentional practices that were introduced targeting an increase in student engagement in the classroom. The presentation will also address some best practices for STEM academic units on how they can encourage faculty to work on improving their teaching methods and reduce the heavy reliance on passive lecturing.

SWRM 2026 SW554

Memes, molecules, and mechanisms: Making organic chemistry click

***Roxane Jourdain**, roxanejourdain@gmail.com. Chemistry and Biochemistry, Baylor University, Waco, Texas, United States*

Organic Chemistry is a major hurdle for many undergraduate STEM students. Often described as a "weed-out" course, it can feel less like learning Chemistry and more like learning a new language. Students are expected to interpret unfamiliar symbolic representations, such as Newman and Fischer projections, understand what curved mechanistic arrows represent, and connect 2D drawings to 3D structures. These challenges can be especially pronounced for Gen Z learners, who often report lower engagement with traditional lecture-based instruction. This presentation explores creative approaches for making Organic Chemistry more accessible, engaging, and memorable through the use of memes, pet photos, and other forms of popular media.

SWRM 2026 SW555

Flesh-eating flies, fake tequila, radioactive rhinoceri, and conflict-affected critical minerals: Exploring new topics and ways to teach 21st century chemistry

***Scott J. Donnelly**, scott.donnelly@azwestern.edu. Arizona Western College, Yuma, Arizona, United States*

As a faculty what have I done (or am doing right now) to prepare the next generation to have the intellectual tools and analytical mindset to meet future, wicked problems head on with minimal trepidation and confidence? A first start is to try to connect what is being taught in the classroom to what is actually happening in the world. This presentation will describe certain active learning (AL)-based classroom activities that I have created that illustrate chemistry's direct or indirect connection to relevant, real-world phenomena and local, regional, or nationally-scaled societal, agricultural, and environmental problems. General chemistry 1 and organic chemistry 1 students engage with these AL classroom activities. Specifically, students are tasked with isotopic information to figure out how chemistry is used to: 1. combat the spread of the New World screwworm blowfly, 2. counteract the poaching of wild rhinoceri in Africa, 3. determine if tequila is fake, and 4. track critical minerals sourced from conflict-designated nations as defined in Section 1502 of the Frank-Dodd Act.

SWRM 2026 SW556

Cobalt tritolycarboxyl porphyrin-carbon black composite as a bifunctional electrocatalyst for NO_3RR and CO_2RR

***Kamal Dhakal**, kamaldhakal@my.unt.edu, Alankar Kafle, Swatej Sabbarwal, Diliraj Subedi, Mohammad K. Altafi, Alireza Hajiseyedjavadi, Thomas R. Cundari, Francis D'Souza. Chemistry, University of North Texas College of Science, Denton, Texas, United States*

Electrochemical nitrate reduction reaction (NO_3RR) and carbon dioxide reduction reactions (CO_2RR) can serve as environmental remediation tools for pollution control and thus help support a circular economy for sustainability. The electrochemical process relies heavily on electrode materials; thus, developing highly active and efficient electrocatalysts for these reactions in a green and cost-effective way is essential. In this study, we examined cobalt porphyrins with different modifications for electrochemical NO_3RR and CO_2RR to independently produce ammonia and acetic acid/formic acid. The carboxylic acid group-substituted cobalt tetrakis(p-tolyl) porphyrin showed a high Faradaic efficiency of 94% for ammonia, 33% for CH_3COOH, and 21% for HCOOH at various potentials in a neutral pH (~7) electrolyte. Computational results suggest that enhanced binding of key NO_3RR and CO_2RR intermediates to the -COOH group-substituted cobalt porphyrin during the electrocatalysis.

SWRM 2026 SW557

Selective ammonia synthesis via electrocatalytic nitrate reduction reaction using chalcogenide vacancy engineered transition metal dichalcogenides

***Piumi Kularathne**, piumikularathne@gmail.com, Alankar Kafle, Mojgan Gharaee, Renuka Rathnayake Mudiyanselage, Manan Guragain, Jeffry Kelber, Thomas R. Cundari, Francis D'Souza.*

Department of Chemistry, University of North Texas College of Science, Denton, Texas, United States

Electrochemical nitrate reduction reaction (NO_3RR) has emerged as a sustainable pathway for ammonia synthesis while enabling nitrate ion remediation in wastewater, offering a cost effective, low carbon alternative to the energy-intensive, traditional Haber-Bosch Process. However, developing highly efficient, selective electrocatalysts for electrochemical nitrate reduction to produce ammonia remains crucial. Given the circumstances, two-dimensional transition metal dichalcogenides (TMDCs) provide a versatile platform due to their interesting properties, such as tunable electronic structure and the ability to modify the material via defect engineering. In our work, chalcogen vacancy (sulfur and selenium) engineered TMDCs, specifically $MoSe_2$, WS_2, and WSe_2, are investigated for the selective electrocatalytic nitrate reduction to produce ammonia. Density Functional Theory (DFT) calculations reveal that sulfur and selenium vacancies are catalytically active sites that optimize nitrate adsorption and lower the reaction energy barriers. Based on these insights, chalcogen vacancy-rich exfoliated $MoSe_2$, WS_2, and WSe_2 were synthesized via chemical exfoliation and systematically evaluated using various characterization methods. Among those catalysts, the selenium-vacancy containing exfoliated $MoSe_2$ exhibits maximum ammonia production at -0.8 V vs Ag/AgCl with a Faradaic efficiency of 93.6 % with a yield rate of 4.9 mmol g_{cat}^{-1} h^{-1}. Sulfur vacancy-rich exfoliated WS_2 achieves a Faradaic efficiency of 71.8% at -0.55 V vs Ag/AgCl with a yield rate of 1.25 mmol g_{cat}^{-1} h^{-1}, while selenium vacancy-rich exfoliated WSe_2 achieved a high Faradaic efficiency of 95.6 % at -0.5 V vs Ag/AgCl with a yield rate of 1.79 mmol g_{cat}^{-1} h^{-1}. Overall, the findings of our study highlight that chalcogen vacancies in TMDCs significantly enhance NO_3RR performance, enabling efficient, selective and sustainable ammonia production, while supporting environmental remediation.

SWRM 2026 SW558 - Withdrawn

SWRM 2026 SW559

Computational study of pesticide capture by metal-organic frameworks

Lauryn Guzman[1,2]*, laguzman@smu.edu, Haoyuan Chen*[1,2]*. (1) Chemistry, Southern Methodist University, Dallas, Texas, United States(2) Physics, The University of Texas Rio Grande Valley, Edinburg, Texas, United States*

The issue of pesticide usage in agricultural settings remains prevalent as it can result in groundwater pollution, directly harming species and aqueous environments. Metal-organic frameworks (MOFs) are nanoporous materials that can be designed at atomic-level precision and can contribute to finding a solution to the matter of pesticide pollution by capturing them from water. In this work, we use computational chemistry methods to study the interactions between three representative MOFs (Cu-BTC, Fe-MIL-101, and NU-1000) and five chemically and structurally distinctive pesticides that contain a wide variety of functional groups: glyphosate ($C_3H_8NO_5P$), clopyralid ($C_6H_3Cl_2NO_2$), aldicarb ($C_7H_{14}N_2O_2S$), simazine ($C_7H_{12}ClN_5$), and imidacloprid ($C_9H_{10}ClN_5O_2$). Quantum chemical calculations were performed to determine the stability of each pesticide's combined structures with each MOF in various binding modes, establishing the preferred binding structure and their respective energies. Specifically, we carried out density functional theory (DFT) calculations to optimize each molecular structure. Two sets of single-point energy calculations were made to reinforce the previously established preferred binding mode of each combined structure in their respective

optimization. Each combined structure was calculated in the gas phase and in solution. We observed that each pesticide molecule and designated MOF structure can sometimes vary in its preferred binding mode between the gas phase and solvent environment, single-point energy calculations with different density functionals, and optimization in comparison to each single-point energy calculation. Both coordination bonding of the pesticide to the metal atom in its respective MOF and non-covalent interactions including hydrogen bonding and π-π stacking exist in many of these structures and may determine the most stable binding mode. The results of this work can serve as a benchmark dataset to assist in the design of new materials for efficient pesticide capture.

SWRM 2026 SW560

Fluorescent carbon dots sensing for PFAS and PFOS detection and removal through integrated membrane filtration

SUNITH BABU MADDURI*, sbmadduri@pvamu.edu, Raghava R. Kommalapati. CENTER FOR ENERGY & ENVIRONMENTAL SUSTAINABILITY, Prairie View A&M University Roy G Perry College of Engineering, Prairie View, Texas, United States*

Per and polyfluoroalkyl substances (PFAS), particularly perfluorooctanoic acid (PFOA) and perfluorooctanesulfonic acid (PFOS), represent one of the most challenging classes of emerging contaminants due to their chemical stability, bioaccumulation potential, and resistance to conventional water-treatment technologies. This study presents a hybrid remediation and sensing framework that integrates nanomaterial-based fluorescence sensing with polymeric ultrafiltration (UF) membranes for PFAS removal and quantification in aqueous environments. Nitrogen-doped carbon dots (CDs) were synthesized via a rapid, one-step microwave-assisted pyrolysis process using citric acid and ethylenediamine precursors. Initial optical characterization through UV–Vis absorption and steady-state fluorescence spectroscopy confirmed their high fluorescence yield and stability. Fourier-transform infrared spectroscopy (FTIR) revealed characteristic bands corresponding to hydroxyl, amine, and carboxyl surface groups, confirming successful nitrogen doping. The synthesized CDs were utilized as fluorescent probes for PFAS detection via a quenching-based mechanism. Incremental additions of PFAS solutions (0.1–10 µg/L) to CD suspensions led to progressive fluorescence quenching, following the Stern–Volmer relationship with excellent linear correlation ($R^2 > 0.99$). These results demonstrate the potential of CDs as fast, low-cost sensors for real-time PFAS monitoring in environmental waters. In parallel, a PVDF-based ultrafiltration membrane system was evaluated for PFAS removal efficiency. Using Triton X as a nonionic surfactant (0.5 ppm) to enhance wetting and dispersion, the membrane achieved 41 % removal of PFAS and 34 % removal of PFOS from 5 ppm feed solutions, confirming that polymeric UF membranes can partially mitigate PFAS loads through combined adsorption and size-exclusion mechanisms. This integrated approach, combining fluorescence nanoprobes for rapid PFAS detection with functionalized UF membranes for removal, offers a scalable, energy-efficient, and environmentally benign route toward mitigating PFAS contamination. The synergy between carbon-dot-based sensing and membrane filtration represents a significant advancement toward next-generation hybrid technologies for real-time monitoring and sustainable treatment of persistent, fluorinated pollutants in water systems.

SWRM 2026 SW561

Anaerobic digestion–assisted hybrid ceramic membrane filtration for microplastic and nanoplastic removal

***PRASHAN RODRIGO**, pmrodrigo@pvamu.edu, Raghava R. Kommalapati. CENTER FOR ENERGY & ENVIRONMENTAL SUSTAINABILITY, Prairie View A&M University Roy G Perry College of Engineering, Prairie View, Texas, United States*

Microplastics (MPs) and nanoplastics (NPs) are persistent pollutants that resist conventional wastewater treatment and raise concerns about ecological and human health. This study evaluates hybrid ceramic membrane filtration as a scalable approach for removing micro- and nanoplastics from wastewater, and it investigates anaerobic digestion (AD) as a biological pretreatment to enhance membrane performance and separation outcomes. Experiments were conducted using a flat-sheet ceramic membrane with a 1.4 μm pore size for MP removal and a tubular ceramic membrane with a 1 kDa molecular weight cut-off for NP retention. The influence of AD pretreatment was quantified by measuring changes in suspended solids, particle concentrations, and membrane flux behavior during filtration. Anaerobic digestion reduced suspended solids by 57–67%, demonstrating its potential to mitigate fouling drivers in complex wastewater matrices. Average microplastic concentrations decreased from approximately 1782 MP/L to 913 MP/L following AD pretreatment. In contrast, NP concentrations increased after AD, with values rising from about 4268 NP/L to 10,066 NP/L, indicating that biological pretreatment may promote fragmentation or mobilization processes that convert larger plastics into smaller nanoscale fractions. Filtration performance also depended on pretreatment: flux across the flat-sheet membrane declined from roughly 106.5 to 25 L m^{-2} h^{-1} as filtrate collection progressed, while AD improved flux by approximately threefold. For the tubular membrane, flux was ~6.1 L m^{-2} h^{-1} at 2.0 L/min, decreasing by 50% after membrane treatment. Overall, hybrid ceramic membranes offer efficient physical separation without secondary chemical pollution, and AD pretreatment can substantially improve operational performance while altering MP-to-NP partitioning.

SWRM 2026 SW562

Fluorescent NU-1000 metal–organic framework for sensitive PFAS detection and environmental water monitoring

***Nafees Iqbal**, nafees.iqbal@utdallas.edu, Mario Wriedt. Chemistry, The University of Texas at Dallas, Richardson, Texas, United States*

Access to clean drinking water remains a global challenge, with over 1.2 billion people consuming contaminated water daily. Among the most persistent and harmful pollutants are per- and polyfluoroalkyl substances (PFAS), a class of synthetic chemicals used in nonstick cookware, cosmetics, and water-repellent materials1,2. Short-chain PFAS are especially difficult to detect due to their high chemical stability and low concentrations in environmental samples3,4. To address this challenge, we investigate the synthesis and application of NU-1000, a zirconium-based metal-organic framework (MOF), as a sensing platform for long-chain PFAS in water. NU-1000 offers several advantageous properties: a very high surface area > 2000 m2/g, robust chemical stability, and a unique hierarchical pore structure consisting of microporous triangular channels (~12 Å) and mesoporous hexagonal channels (~30 Å) that promote efficient diffusion and adsorption of small contaminants1,3. Additionally, its highly conjugated linkers exhibit strong fluorescence that changes upon PFAS interaction4—enabling fast, visual detection. Our research highlights NU-1000's potential as a selective, regenerable, and field-deployable material for detecting long-chain PFAS, offering a practical alternative to instrumentation-heavy methods currently used in environmental monitoring.

SWRM 2026 SW563

Augmenting DNA nanotechnology using synthetic macrocycles

***Janarthanan Jayawickramarajah**, jananj@smu.edu, SOUMEN PRADHAN, Husain Kagalwala, Aunindya Jyoti. Chemistry, Southern Methodist University Dedman College of Humanities and Sciences, Dallas, Texas, United States*

The construction of controllable molecular- and nano-machines that function in aqueous/biological media is an important endeavor, with potential practical applications in biosensing, theranostics, and computing. In terms of well-controlled systems and assemblies that function in water, DNA nanotechnology has led the way due to the programmability of DNA architectures using simple base-pairing rules. In this talk, we describe how the judicious covalent linkage of various macrocycles, such as porphyrins, cyclodextrins, and cucurbiturils, with DNA can lead to the enhancement of DNA nanotechnology via the generation of novel systems with potential photonic, therapeutic, and diagnostic applications. This talk will also discuss some novel directions into the development of mechanically interlocked (bio) polymers.

SWRM 2026 SW564

Single-molecule DNA–peptide nanostructures for protease activity detection

***Imon K. Phukan**, ikphukan@utexas.edu, Shivudu Godhulayyagari, Dylan M. Snider, Devleena Samanta. Chemistry, The University of Texas at Austin, Austin, Texas, United States*

Proteases, which regulate diverse biological processes by selectively cleaving peptide substrates, are implicated in numerous diseases, including cancer, inflammatory disorders, and infectious diseases. However, direct detection of protease activity is challenging due to the limited signal generated by a single substrate-cleavage. To overcome this limitation, we developed a modular DNA–peptide molecular switch that amplifies protease-mediated cleavage into a readily detectable enzymatic response. The system comprises two thrombin-binding DNA aptamers connected by a protease-cleavable peptide linker. In the intact state, the linked aptamers inhibit thrombin activity. Upon proteolytic cleavage of the linker, the aptamers dissociate, relieving inhibition and restoring thrombin activity. Thrombin then serves as a reporting enzyme, generating a fibrin-based output that can be detected by turbidity measurements or directly by the naked eye. The platform demonstrated high sensitivity, with a limit of detection of approximately 7 nM, and high selectivity. Moreover, simple reprogramming of the peptide linker enabled detection of multiple cancer-associated proteases, including cathepsin B, from fewer than 5,000 colorectal cancer cells. These results establish this as a versatile modular platform for protease-mediated allosteric control of enzyme activity without modifying the target protein

SWRM 2026 SW565

Sequence encoded molecular interactions in peptide biomolecular condensates revealed by NMR, Raman and FT-IR spectroscopy

***Navneet Sahoo**, navneet.sahoo@uta.edu, Debdatta Das, Jenny Nguyen. Chemistry and Biochemistry, The University of Texas at Arlington, Arlington, Texas, United States*

Biomolecular condensates formed through liquid liquid phase separation are stabilized by networks of weak, multivalent interactions, yet resolving the molecular interactions that connect peptide sequence to condensate formation and dynamics remains challenging. Here we investigate a series of short Arginine and aromatic rich peptides as minimal models for elucidating sequence dependent peptide condensation. Multidimensional solution NMR spectroscopy was used to establish residue level spectral assignments and probe changes in local chemical environments associated with salt-induced condensation. Temperature and time-dependent measurements further revealed sequence dependent changes in aromatic and arginine resonances, including chemical-shift perturbations and linewidth variations that report on the evolving molecular dynamics of the peptide assemblies. Confocal Raman spectroscopy provides complementary spatially resolved information on the chemical environment of tryptophan- and tyrosine-rich regions within the condensed phase, while FTIR spectroscopy is used to evaluate changes in backbone secondary structure accompanying assembly. Together, these measurements indicate that peptide condensation cannot be attributed to a single interaction but instead emerge from the collective contributions of aromatic interactions, electrostatics, hydrogen bonding, and sequence-dependent molecular organization. Comparison of closely related peptide variants demonstrates how small changes in sequence and arginine valency alter intermolecular interactions and condensate dynamics. These results establish short peptides as experimentally tractable models for defining sequence–interaction–structure relationships governing biomolecular condensation.

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SWRM 2026 SW567 - Withdrawn

SWRM 2026 SW568

Non-covalent interactions in chemosensor design for molecular recognition

***Rashid Mia**, rashid.mia@sfasu.edu. Department of Chemistry and Biochemistry, Stephen F Austin State University, Nacogdoches, Texas, United States*

Non-covalent interaction, especially hydrogen bonding, is an attractive approach to design molecular sensors by introducing various fluorescence mechanisms. We have designed variety of molecular probes by incorporating hydrogen bonding, synthesized, and deployed to selectively bind with various analytes such as metals (Zn^{2+}, Cd^{2+}, Cu^{2+}, Ni^{2+}, Hg^{2+}, Co^{2+}, Pb^{2+}), and anions (CN^-, CH_3COO^-, F^-, PO_4^{3-}), and organophosphorus compounds. Hydrogen bonding interactions is a weak bond typically (4 – 120) kJ, however, four molecular probes have been designed such a way so that enamine-NH moiety is adjacent to coumarin keto (C=O) group (or imine moiety is adjacent to phenolic hydroxyl group) that allows to form a new six-membered ring system through resonance-assisted hydrogen bonding (RAHB) which is typically stronger bond and give rise to optical properties of the sensor due to the extended conjugation. Upon the addition of target analytes, RAHB perturbed which produced unique optical responses because of sensor-analyte interactions both in UV-Vis and fluorescence spectroscopy. Furthermore, we designed another coumarin-quinidine molecular probes having no RAHB, we found that this sensor can bind to metal cations (Cd^{2+} and Zn^{2+}) with high affinity *via* an excimer formation (*π-π interaction*) due to the quinaldine moiety adopting a *syn* arrangement when coordinated to the metal Zn^{2+} ions.

SWRM 2026 SW569

Design and application of porous porphyrin-derivative frameworks

***Shengqian Ma**, shengqian.ma@unt.edu. University of North Texas, Denton, Texas, United States*

Over the past two decades, the rapid growth has been witnessed in the fields of metal-organic framework (MOF) and covalent organic framework (COF) that feature tunable, designable, and functionalizable nanospace. The utilization of new types of organic ligands for the construction of MOFs/COFs has long been sought after, as evidenced by the success in porphyrin-based MOFs/COFs. Beyond porphyrins, we show how their derivatives of corroles and rosarins can be employed as new building blocks to construct porous framework materials, which interesting properties in catalysis and electronics.

SWRM 2026 SW570

Can porous structures be constructed without interactions between building blocks?

***Ognjen Miljanic**, miljanic@uh.edu. University of Houston System, Houston, Texas, United States*

Porous materials are transforming several areas of science and technology, and have been honored with the 2025 Nobel Prize in Chemistry. While the chemical identities of building blocks differ among e.g., metal-organic frameworks (MOFs) and covalent organic frameworks (COFs), the general principles of reticular chemistry apply to both: a porous structure is constructed by the connection of rigid building blocks through directional interactions that are reversible and allow for error correction. We have been interested in challenging the notion that directional interactions are necessary for the creation of persistent pores and have prepared a series of porous molecular crystals (PMCs) that are constructed from discrete molecular building blocks and held together by progressively weaker and less directional non-covalent interactions. Starting from fluorinated aromatic pyrazoles assembled into porous molecular crystals by a combination of hydrogen bonding and pi-pi stacking, through cyclobenzoin macrocycles held by "zippers" of hydrogen bonds, we have now reached saddle-shaped quinoxaline macrocycles that assemble into porous crystals and co-crystals solely through weakly directing dispersion and pi-pi interactions. This persistence of porosity across a wide structural landscape suggests that molecular shape alone can play a role in the assembly of a porous structure, without the need for any specific interactions between the individual building blocks. Our work on cyclotetrabenzoin esters appears to validate this hypothesis, as small molecules assemble into structures with BET surface areas exceeding 500 m2 g-1 without any covalent or non-covalent organizing interactions.

SWRM 2026 SW571

Directed hydrogen bonding for stabilizing mesoporous covalent organic frameworks

***Ronald Smaldone**, ronsmaldone@gmail.com. Chemistry and Biochemistry, The University of Texas at Dallas, Richardson, Texas, United States*

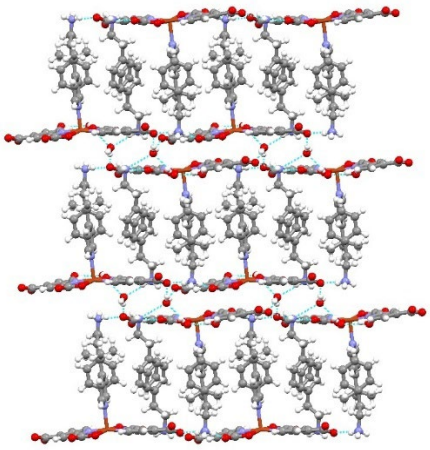
2D covalent organic frameworks (2D-COFs) are a class of crystalline, porous polymers with 2D layers that are constructed from rigid monomers connected through dynamic covalent bonds. These sheets are stacked in three dimensions through non-covalent interactions. The interplay between these interactions can determine the mechanism of polymerization, or even whether or not the final polymer is crystalline or amorphous. This results in a limited number of monomeric building blocks to make “crystalline” structures. In many cases, porous polymers can be obtained under conventional COF synthesis conditions, however, if not designed properly, the resulting polymers will be amorphous in structure. In several recent reports we have described a new class of two dimensional COFs, which we have called COFamides, that contain monomers that use out of plane amide groups to direct hydrogen bonding interactions between the stacked sheets. These hydrogen bond networks are extremely effective in improving crystallinity and making COFamides stable for extended periods of time in aqueous or even acidic solutions. The unique interlayer hydrogen bonding networks can be installed using either the node or linkers, with the location having a significant effect on the properties, as well as the orientation of the hydrogen bonding interactions. This talk will cover the design and applications of large pore COFamides such as hosting biomolecular guests and as high-capacity adsorbents for pollution remediation in aqueous environments.

SWRM 2026 SW572

Coordinative-inclusion of pyridine molecules within hydrogen-bonded metal-organic frameworks (HBMOFs)

Greg A. Hogan*, ghogan@tamut.edu. Chemistry, Texas AM University-Texarkana, Texarkana, Texas, United States*

Small-molecule inclusion and remediation are important areas of research due to their potential applications in waste cleanup, molecular storage and transport, and catalysis. Hydrogen-bonded metal-organic frameworks (HBMOFs) offer advantages over traditional metal-organic frameworks (MOFs) because their hydrogen-bonded layers provide greater structural flexibility. This flexibility allows the framework to accommodate guest molecules of varying sizes and shapes through structural adaptation. This investigation examines the inclusion of small molecules within HBMOFs through co-crystallization and dissolution processes. Subsequent studies will evaluate the ability of these flexible frameworks to function as molecular “sponges” for the uptake and retention of guest molecules. The resulting materials will be characterized using thermogravimetric analysis (TGA), powder X-ray diffraction (pXRD), and single-crystal X-ray diffraction (SCXRD) to evaluate their composition, thermal stability, and structural changes associated with guest inclusion.



SWRM 2026 SW573

Intrinsic chirality in organic-inorganic hybrid materials

Daniel B. Straus[1]*, dstraus@gmail.com, Zheng Zhang*[1]*, Jackson G. Smith*[1]*, Santu Biswas*[2]*, Matthew Montemore*[2]*. (1) Chemistry, Tulane University, New Orleans, Louisiana, United States(2) Chemical and Biomolecular Engineering, Tulane University, New Orleans, Louisiana, United States*

In most chiral organic–inorganic hybrid metal halides, chirality is extrinsically introduced by chiral organic cations because the inorganic framework is otherwise achiral. However, there are a few hybrid metal halides where chirality emerges spontaneously, i.e. in the absence of chiral molecules. Yet, the mechanisms that cause this intrinsic chirality to emerge are unclear. In this presentation, I report the discovery and investigation of the intrinsically chiral material pyrrolidinium palladium chloride ((C4H10N)PdCl3), which consists of bent edge-sharing square-planar palladium chloride dimers separated by [C4H10N]+ cations. Its crystal structure indicates that hydrogen bonding interactions between N-bound hydrogens and Cl anions induce chirality, and this hypothesis is supported by the achirality of the all-inorganic material CsPdCl3 as well as our density functional theory calculations. The situation is reversed for octahedrally coordinated copper(II) chlorides, where previous reports show that (C4H10N)CuCl3 is achiral while CsCuCl3 exhibits intrinsic chirality. This reversal is caused by the electronic degeneracy in octahedral Cu2+. In CsCuCl3, cooperative Jahn–Teller distortions cause Cu2+ ions to move off-center within their octahedra, inducing chirality, while hydrogen bonding interactions with (C4H10N)CuCl3 break symmetry, so the cooperative chiral distortion no longer occurs. I also will discuss our discovery of temperature-induced chirality in a similar organic-inorganic hybrid material that does not contain chiral molecules. At room temperature, an achiral crystal structure forms, but at elevated temperatures, we get nearly 100% yield of an intrinsically chiral material. Varying the ratio of organic to inorganic precursors in the crystal growth completely changes the phases we recover. Although the source of intrinsic chirality is usually unclear, our findings show that hydrogen bonding interactions, crystal growth temperature, and the ratio of organic to inorganic precursors can cause intrinsic chirality to emerge in organic–inorganic hybrid materials. They also highlight the importance of the metal's electron configuration and metal-halide coordination geometry on the emergence of intrinsic chirality, thereby providing guidance for the targeted synthesis of intrinsically chiral organic–inorganic hybrid materials.

SWRM 2026 SW574

MYC activation induces selective snRNP imbalance and coordinated splicing-polyadenylation remodeling

Ayesha Khan[1]*, axk2579@mavs.uta.edu, Sanat Myti*[1]*, Yuwei Miao*[2]*, Duc Ngu*[1]*, Aiswarya Balakrishnan*[3]*, Kai-Lieh Huang*[3]*, Arunprasath Duraisamy*[1]*, Armeen Nasir*[1]*, Morgan Gresky*[1]*, Junzhou Huang*[2]*, Eric Wagner*[3]*, Byung Ran So*[1]*. (1) Chemistry, The University of Texas at Arlington, Arlington, Texas, United States(2) Computer Science and Engineering, The University of Texas at Arlington, Arlington, Texas, United States(3) School Medicine and Dentistry, University of Rochester, Rochester, New York, United States*

Oncogenic activation of MYC increases RNA production, placing greater demands on pre-mRNA processing and making cells more dependent on efficient spliceosome function. While spliceosome vulnerability in MYC-driven cancers is well-established, how MYC-induced transcriptional stress alters

spliceosome homeostasis remains incompletely understood. Here, we show that MYC activation selectively alters the relative abundance of small nuclear ribonucleoprotein particles (snRNPs), core components of the spliceosome, and is accompanied by widespread changes in RNA processing. Using an inducible MYC–estrogen receptor system in human mammary epithelial cells, we found that activation of MYC by 4-hydroxytamoxifen selectively increased the abundance of U2, U4, and U5 snRNAs and their corresponding mature snRNPs, while U1 and U6 remained largely unchanged, thereby altering the relative imbalance of snRNPs. Transcriptome-wide and quantitative proteomic analyses revealed that MYC activation remodels alternative splicing and 3'-end processing, accompanied by differential expression of cleavage and polyadenylation factors. Furthermore, antisense morpholinos-mediated perturbation of U1 snRNP function increased MYC expression at both mRNA and protein levels without activating canonical MYC target genes. Together, these findings support a bidirectional model in which MYC-driven transcriptional amplification alters spliceosomal snRNP homeostasis, while perturbation of U1 snRNP function reciprocally affects MYC activity, linking oncogenic transcription with RNA processing.

SWRM 2026 SW575

Establishing cellular models of cancer-associated mutations of U1 snRNA to investigate snRNP biogenesis

Arunprasath Duraisamy*, axd8899@mavs.uta.edu, Sanat Myti, Ayesha Khan, Byung R. So. Department of Chemistry and Biochemistry, The University of Texas at Arlington, Arlington, Texas, United States*

U1 small nuclear ribonucleoprotein (U1 snRNP), a key component of the spliceosome, plays a critical role in pre-mRNA splicing and prevents premature cleavage and polyadenylation through telescripting. Recurrent mutations in non-coding U1 snRNA have been identified in several cancers; however, their functional consequences remain poorly understood. Studying these mutations has been challenging because of the multicopy nature of endogenous *RNU1* loci, which limits efficient and precise genomic manipulation. To address this challenge, we developed a system to introduce additional copies of U1 snRNA along with its native promoter and terminator at the AAVS1 safe-harbor locus. We used near-diploid HCT116 cells, in which targeting one or both AAVS1 alleles provides a system for generating heterozygous and homozygous targeted integrations, respectively, enabling dosage-dependent studies of mutant snRNA expression. HCT116 cells were co-transfected with an AAVS1 SA-2A-puro-pA donor vector containing a U1 snRNA expression cassette with its native promoter and terminator and PX330-AAVS1 T2, which expresses both Cas9 and a gRNA targeting the AAVS1 locus. The donor was designed such that correct integration at the AAVS1 locus enables transcription of the puromycin-resistance gene through the endogenous AAVS1 transcriptional context, thereby allowing selection of cells with targeted integration. These models will allow us to determine how mutant U1 snRNA affects snRNP biogenesis, alternative splicing, and polyadenylation, providing insight into U1 snRNA mutations may contribute to cancer development.

SWRM 2026 SW576

Protein engineering for precise control over organelle-organelle interaction

Ura Kang*, ura.kang@utdallas.edu, Tianqi Wang, Ziwen Jiang. Chemistry and Biochemistry, The University of Texas at Dallas, Richardson, Texas, United States*

Communication between organelles contributes to the exchange of metabolites and molecular signals. In recent years, aberrant inter-organelle interactions have been linked with several diseases. For example, TDP-43 protein has been shown to disrupt the endoplasmic reticulum (ER)-mitochondria associations and presented in amyotrophic lateral sclerosis. Moreover, increased contact between ER and mitochondria can result in increased Ca^{2+} level in mitochondria, inducing an increased mitochondrial permeability to signal apoptosis. However, the roles of inter-organelle communications in disease pathogenesis are less understood due to a lack of tools to precisely control the organelle interactions. Herein, we have developed a series of engineered protein constructs with tunable repeats of epitope tags (StarTAC), accurately controlling the distance between organelle membranes. We expect that the tool development for regulating inter-organelle communications will shed light on the fundamental understanding of cell signaling events.

SWRM 2026 SW577

Autophagy receptor-inspired antibody-fusion proteins for targeted intracellular degradation

Tianqi Wang*, tianqiwang992@gmail.com, Ziwen Jiang. Chemistry and Biochemistry, The University of Texas at Dallas, Richardson, Texas, United States*

Autophagy is responsible for the degradation of large intracellular contents, such as unwanted protein aggregates and organelles. Impaired autophagy can therefore lead to the accumulation of pathological aggregates, correlating with aging and neurodegenerative diseases. However, a broadly applicable methodology is not available for the targeted degradation of protein aggregates or organelles in mammalian cells. Herein, we developed a series of autophagy receptor-inspired targeting chimeras (AceTACs) that can induce the targeted degradation of aggregation-prone proteins and protein aggregates (e.g., huntingtin, TDP-43, and FUS mutants), as well as organelles (e.g., mitochondria, peroxisomes, and endoplasmic reticulum). These antibody-fusion-based AceTAC degraders were designed to mimic the function of autophagy receptors, simultaneously binding with the cellular targets and the LC3 proteins on the autophagosomal membrane, eventually transporting the target to the autophagy-lysosomal process for degradation. The AceTAC degradation system provides design principles for antibody-based degradation through autophagy, largely expanding the scope of intracellular targeted degradation technologies.

SWRM 2026 SW578

Investigating thymine DNA glycosylase-RNA interactions in the chromatin

Laura Ruemmele*, lr22@tamu.edu, Jonathan T. Sczepanski. Chemistry, Texas A&M University System, College Station, Texas, United States*

TDG (Thymine DNA Glycosylase) is a bifunctional member of the uracil DNA glycosylase superfamily that excises 5-formylcytosine (5fC) and 5-carboxycytosine (5caC) to initiate base-excision repair (BER) at G-T and G-U mismatches. TDG and associated proteins in the BER pathway demethylate 5mC, an important epigenetic modification, to an unmodified cytosine. Although TDG is essential for active DNA demethylation and the maintenance of appropriate DNA methylation patterns, the mechanisms that regulate its activity and substrate recognition remain incompletely understood. Emerging evidence suggests that RNA and RNA–DNA hybrid structures may influence the localization, interactions, and activity of DNA repair proteins, yet the role of RNA in regulating TDG

function remains poorly characterized. We aim to profile how TDG interacts with RNA in cells, and how these interactions influence its association with DNA and chromatin, may provide important insight into the mechanisms that coordinate DNA repair with epigenetic regulation.

SWRM 2026 SW579

Investigating the impact of CXCR4 S338X mutation on receptor internalization, signaling, and dimerization

***MOJEED A. ASHIRU**, mashiru@ttu.edu, Adam W. Smith. Chemistry & Biochemistry, Texas Tech University, Lubbock, Texas, United States*

Chemokine receptors are class A G protein-coupled receptors (GPCRs) that mediate cell migration, proliferation, and survival in response to the binding of chemokine ligands, such as stromal cell-derived factor 1 (SDF-1), also known as CXCL12. Mutations in the Ser/Thr-rich C-terminal tail of CXCR4 have been linked to Waldenström's macroglobulinemia (WM) and warts, hypogammaglobulinemia, infections, and myelokathexis (WHIM) syndrome. For example, earlier studies have characterized the functional consequences of the CXCR4 S338X mutation, including enhanced signaling and impaired receptor desensitization. However, the biophysical interactions between WT and mutant (MUT) CXCR4 receptors remain underexplored. Here, we combined biophysical and functional assays to investigate how the S338X mutation affects receptor organization at the plasma membrane and downstream signaling. PIE-FCCS analysis revealed a strong interaction between co-expressed CXCR4-WT and CXCR4-MUT receptors under basal conditions. Flow cytometry showed that the WM-associated CXCR4 mutant exhibited a delayed rate of ligand-induced internalization compared with the WT receptor following CXCL12 stimulation. In addition, cAMP functional assays showed that CXCR4-MUT cells displayed altered and reduced cAMP responses to CXCL12 relative to WT cells, which were effectively reversed by treatment with the CXCR4 antagonist plerixafor (AMD3100). Collectively, these findings demonstrate that the CXCR4 S338X mutation disrupts normal receptor trafficking and signaling, while retaining the capacity to associate with WT CXCR4. These results suggest that WT–MUT receptor interactions may contribute to CXCR4 dysregulation in WM.

SWRM 2026 SW580

Mechanisms of synergistic cellular toxicity between α-synuclein and zinc probed by systematic mutagenesis

***Meghana M. Nittala**, nittala.meghana@gmail.com, Rishob Dasgupta, Robert W. Newberry. Department of Chemistry, The University of Texas at Austin College of Natural Sciences, Austin, Texas, United States*

Parkinson's disease is strongly associated with α-synuclein, making mechanistic investigation of the protein central to understanding the disease. Disrupted metal homeostasis is a feature of Parkinson's disease, and elevated zinc ions have been shown to increase α-synuclein toxicity. However, the cellular mechanism underlying this toxicity phenotype remains unclear. Because zinc ions may alter α-synuclein toxicity by shifting the balance between its biological states rather than acting at a single residue, we used deep mutational scanning (DMS) in Saccharomyces cerevisiae to map the sequence determinants of α-synuclein toxicity in the presence and absence of zinc ions. We used this

cellular model as it offers a simple, tractable system that recapitulates key features of α-synuclein toxicity and conserved cellular pathways relevant to Parkinson's disease. The DMS data revealed mutations that enhance or suppress zinc ions' synergistic effect on α-synuclein toxicity. These cellular responses differ from those observed in vitro and do not support a simple, localized mechanism of zinc ions' action. Instead, these results suggest multiple possible mechanisms for how zinc ions may perturb the α-synuclein folding landscape and alter toxicity. Using representative enhancer and suppressor variants, we probed whether zinc ion-dependent toxicity arises from direct changes in α-synuclein membrane interactions or aggregation behavior, or indirectly through key proteostasis pathways. In this presentation, we will discuss how DMS, together with complementary in vivo and in vitro approaches, can be used to distinguish among potential mechanisms linking zinc ion exposure to changes in α-synuclein behavior and cellular toxicity.

SWRM 2026 SW581

Identifying protein targets of sulfated glycosaminoglycan mimetics using photoaffinity labeling

***Shakila M. Silva**, shakilasilva@my.unt.edu, Jabila Mary, Daniel Afosah. Chemistry, University of North Texas, Denton, Texas, United States*

Glycosaminoglycans (GAGs) are anionic linear polysaccharide biomolecules that interact with a wide range of proteins and, as a result, modulate several biological processes. Thus, they hold promise in the development of potential therapeutic agents. However, the therapeutic development of GAGs remains a significant challenge due to their structural complexity, heterogeneity, and difficulties in synthesis and characterization. Non-saccharide GAG mimetics are fully synthetic compounds that mimic the structure and function of GAGs. These molecules are much easier to synthesize and typically lack the heterogeneity found in natural GAGs. However, like GAGs, they can also interact with a wide variety of targets. Here, we report a photoaffinity labeling (PAL) strategy for identifying protein targets of a synthetic sulfated GAG mimetic. We designed and synthesized a diazirine-based photoaffinity-capable analog of our sulfated GAG mimetic that covalently captures interacting proteins upon UV irradiation. We then applied this approach to human plasma, zebrafish plasma, and zebrafish kidney cells to identify its protein interactome. We systematically optimized and refined key steps of a previously reported workflow, including optimization of probe concentration, selection of the most effective fluorophore from multiple candidates, and biotin affinity pulldown. SDS-PAGE analysis showed that labeling increased with probe concentrations, as indicated by greater band intensity. No detectable labeling was observed in the absence of UV irradiation, and competition was observed following addition of the parent compound, which supports specific probe-protein interactions. Consistent trends were observed in both human plasma and zebrafish kidney lysates. A biotin-affinity pulldown experiment further demonstrated selective isolation of probe-bound proteins. Overall, we established a robust experimental framework for PAL-based target identification of highly sulfated GAGs in complex biological environments. This study addresses key challenges in GAG-protein interactions and provides a foundation for future proteomics studies aimed at identifying high-affinity protein targets of GAG mimetics for drug discovery.

SWRM 2026 SW582

Identification of zoliflodacin as a potent inhibitor against tuberculosis DnaE1 polymerase through high throughput docking and scaffold hopping

Ragavishagan Rajasekar[1]*, ragavishagan@gmail.com, Kamlendra Singh*[1,2]*, Eiichi Ami*[1,2]*. (1) Bond Life Sciences Center, University of Missouri, Columbia, Missouri, United States(2) Department of Veterinary Pathobiology, University of Missouri System, Columbia, Missouri, United States*

Tuberculosis (TB), caused by Mycobacterium tuberculosis (Mtb), remains a major global health threat due to its high mortality and drug resistance. While all current treatments are highly effective, they are ineffective against multidrug-resistant (MDR-TB), ~16% of treated patients develop drug resistance (2), resulting in compromised therapies. Therefore, novel drugs directed to new targets are urgently needed (3). Replicative DNA polymerase DnaE1 of Mtb is required for bacillary survival and gene replication, as the loss of DnaE1 is lethal. Additionally, DnaE1 is a novel target, as all existing TB drugs are directed to cell wall synthesis or RNA transcription. Nucleic acid polymerases have been the most sought-after for drug development against many pathogens. Inhibition has been demonstrated to be a viable therapeutic approach against other pathogens (5). Here, we report the identification of an FDA-approved compound discovered using a two-step approach. First, we developed the Sbdock platform to streamline and accelerate the virtual screening workflow. We then used this workflow to identify compounds with high binding affinity to the Mtb DnaE1. More than 2.5 million compounds were filtered to 500,000 by excluding compounds failing Lipinski's Rule of Five, topological polar surface area (TPSA), and PAINS. The filtered compounds were then docked at the active site of DnaE1 using Sbdock through the Slurm Workflow Manager. By analyzing patterns among the top compounds, we discovered that the high binders contained the core scaffold of Zoliflodacin, namely the aromatic ring and spiro-barbituric acid. Scaffold hopping off this core scaffold, we identified a new class of compounds that possess extremely high binding affinities. We tested Zoliflodacin's effectiveness against DnaE1 in the primer extension assays. The discovery of compounds that can be repurposed aligns with one of the FDA's current goals: minimizing resources in drug discovery.

SWRM 2026 SW583 - Withdrawn

SWRM 2026 SW584

Biochemical blockade of the SARS-CoV-2 RBD-ACE2 interface by a mutation-tolerant DNA aptamer

Arnav Peram*, arnavperam1@gmail.com. Arizona College Preparatory, Chandler, Arizona, United States*

Spike receptor-binding domain (RBD) mutations have repeatedly eluded monoclonal antibody therapeutics against SARS-CoV-2, several of which lost activity within months. The ACE2-contacting residues are difficult to escape. Entry requires angiotensin-converting enzyme 2 (ACE2) recognition, so weakening substitutions carry a fitness cost, and that interface stays comparatively fixed while the epitopes around it drift. DNA aptamers suit this kind of target. They are made by solid-phase phosphoramidite synthesis, so redesigning one means resynthesizing a sequence rather than rebuilding an expression system. Almost every reported anti-spike aptamer, though, was selected against a single RBD background, and whether such ligands survive sequence drift has not been tested. We aligned broad spike sequences to find conserved ACE2-contacting residues (RBD 417-502), screened candidate 80-mers, and ranked them by HADDOCK docking. The selected aptamer buried about 2,085 A2 at the interface. Over 10 ns of molecular dynamics on the solvated ACE2-RBD-aptamer tri-complex the minimum ACE2-to-epitope distance remained above 8.8 A, exceeding

the 6 A cutoff for productive contact, and docking metrics persisted across escape-associated substitutions. Binding was measured by enzyme-linked oligonucleotide assay. Signal rose with RBD concentration from 0 to 300 nM and exceeded the no-aptamer, no-RBD, and blank controls by 11.3-, 8.8-, and 18.3-fold, with replicate variation under 3%. In competition assays, aptamer reduced recombinant ACE2-Fc binding to immobilized RBD with a mean IC50 of 71.08 +/- 8.20 nM, a Hill slope of 0.911, and 85-90% maximum inhibition. A slope this close to unity points to single site competition. Profiles for Wuhan-Hu-1, Alpha, Delta, Omicron B.1.1.529, and Omicron BA.5 were nearly indistinguishable. Chitosan nanoparticles made by ionic gelation encapsulated 76.9% of aptamer and 61% of the dose lingered in artificial nasal fluid, against 1% for free aptamer. These are recombinant protein measurements, showing receptor competition, not viral neutralization, and pseudovirus assays are needed.

SWRM 2026 SW585

Multiplex RNA sensor for accurate infectious disease biomarker detection

Sathya Samaraweera[1], *sdewara@okstate.edu, Rahul P. Kumarchinchole*[1], *Zia ul Quasim Syed*[1], *Joshua D Ramsey*[2], *Sadagopan Krishnan*[1]. *(1) Chemistry, Oklahoma State University The College of Arts and Sciences, Stillwater, Oklahoma, United States(2) School of Chemical Engineering, Oklahoma State University, Stillwater, Oklahoma, United States*

Accurate disease detection is essential for early diagnosis of infectious diseases and preventing outbreaks, ensuring timely patient treatments, avoiding complications, and reducing healthcare burdens. However, relying on a single biomarker increases the risk of false positives or false negatives, demanding sensors capable of detecting multiple analytes simultaneously. Colorimetric detection methods gain attraction due to their simplicity and real-time analysis ability, making them suitable for resource-limited environments. However, achieving multiplex detection with colorimetric platforms remains challenging, as it is limited by non-specific collateral cleavage in CRISPR-Cas systems and low sensitivity in enzyme-linked immunosorbent assay-based methods. To address these limitations, we introduce a magnetic-particle-based nucleotide multiplex sensor capable of detecting multiple SARS-CoV-2 variants in a single mixture through collective signal amplification. Specificity and sensitivity of the biosensor, which are crucial for early disease detection, are achieved by using nucleotide probes. The sensor utilizes streptavidin-modified, carboxylated magnetite particles to capture biotinylated capture nucleotide sequences, enhancing analytical sensitivity. Complementary detection nucleotide sequences that are complementary to the target sequences were hybridized upon introduction to the corresponding target RNA sequences. The target concentrations were determined based on the color intensity. The developed biosensor is capable of simultaneously detecting up to three RNA sequences in undiluted serum over the concentration range of 100 aM to 1 nM. The limit of detection (10^4 copies/mL) aligns with viral load observed at peak infection. Further, the hybridization mechanism of the multiplex biosensor was determined by analyzing the association of binding energies of probes, which were correlated with the sensor's performance. Therefore, this novel multiplex platform provides rapid, sensitive disease diagnostics by detecting multiple analytes in a single assay.

SWRM 2026 SW586

Microfluidic ultra-low cell separations: Towards urinary tract infection diagnostics

***Abigail Dowell**, abdowell@ttu.edu, Dimitri Pappas, Kitiara Griffin. Chemistry, Texas Tech University, Lubbock, Texas, United States*

Urinary tract infections (UTIs) are bacterial infections affecting the urinary system that impact a large portion of the population each year and can eventually lead to sepsis if not identified and treated. Women are more likely to be afflicted by a UTI but often only get diagnosed after reporting symptoms from the affliction. UTIs are also specifically more harmful to geriatric populations as their immune response declines with age, and recognizing the onset of symptoms can be difficult when dealing with dementia patients. With respect to these age-related impairments, rapidly identifying a UTI or other infections can become difficult for both the patient and their caregiver.
The goal of this research is to develop a microfluidic test that can be quickly applied on site to determine if a patient has a UTI without needing to wait for the incubation period that current tests require. Our microfluidic chip utilizes affinity-based capture to isolate white blood cells (WBCs) that are present in urine when a patient is affected by a UTI. A urine sample is taken from a patient and then stained with MitoTracker green to allow for fluorescent observation and identification of the WBCs. The urine sample is then run through the chip, allowing the WBCs to encounter antibodies that are conjugated onto the glass surface of the microfluidic chip. The WBCs bind to the antibodies allowing the rest of the liquid sample and non-target cells to leave the chip. Using a microscope, the bound cells can be viewed, imaged, and then counted, allowing for the UTI to be diagnosed. The chip design has been altered to allow for a quick run time, while still providing the cells proper time to interact and bind to the antibodies. This microfluidic chip design is capable of low concentration detection of target cells in urine which will enable future clinical diagnosis of UTIs.

SWRM 2026 SW587

Bioengineered virus like particles: A delivery platform for central nervous system

***Neelima Koti**, neelima.koti@utdallas.edu, Ikeda Trashi, Orikeda Trashi, Y Nhu Nguyen, Jeremiah Gassensmith. Chemistry& Biochemistry, The University of Texas at Dallas, Richardson, Texas, United States*

The blood–brain barrier (BBB) remains a major obstacle to the treatment of central nervous system (CNS) disorders, as its highly restrictive nature limits the brain penetration and intracellular delivery of therapeutic proteins and other biologics. Virus-like particles (VLPs) have emerged as versatile nanocarriers owing to their noninfectious nature, genetic programmability, and ability to simultaneously display targeting ligands and encapsulate therapeutic cargo. Here, we engineered bacteriophage Qβ VLPs displaying a neuronal targeting peptide (TP) to develop a platform for brain delivery. Cre recombinase (Cre), a site-specific DNA recombinase, was encapsulated within TP-functionalized Qβ VLPs through recombinant co-expression in *E.coli*. Recombinant Qβ VLPs were purified using ammonium sulfate precipitation followed by ultracentrifugation. Dynamic light scattering and SDS-PAGE confirmed intact particle assembly, TP display, and Cre encapsulation. Functional intracellular delivery of Cre was evaluated in HEK293 reporter cells using fluorescence microscopy and flow cytometry to assess Cre-mediated recombination. To investigate the *in vivo* potential of the platform, preliminary studies were initiated in Ai14 Cre-reporter mice following systemic administration of Cre@Qβ-TP VLPs to evaluate brain delivery and reporter activation. In addition to functional protein delivery, this platform is readily adaptable for the incorporation of imaging payloads, enabling the development of targeted, noninvasive imaging approaches for the central nervous system. Collectively, these results establish TP-functionalized Qβ VLPs as a modular protein delivery platform capable of encapsulating functional cargo and provide a foundation for the development of targeted protein therapeutics and gene-editing strategies for CNS applications.

SWRM 2026 SW588

Rational design of carbon dots through informed precursor selection for therapeutic and diagnostic purposes

***Luke Fourroux**, lfourrou@ttu.edu, Dimitri Pappas. Chemistry & Biochemistry, Texas Tech University, Lubbock, Texas, United States*

Carbon dots (CDs) are a branch of carbon based quasi-spherical nanomaterial that serve as a malleable base for the construction of nanoparticles with unique and expansive properties. Most types of CDs exhibit significant qualities, such as tunable fluorescence across the entire visible light spectrum, and can be further specified to a desired role through heteroatom doping or post-synthesis modification. While CDs modified in this way have been utilized to great effect, less attention has been drawn to the specific selection of precursors to inherit affinity from the precursor to the CD. As such, the development of model CDs that retain the properties of their precursor could simplify the route to crafting nanoparticles to virtually any aim. In our lab, we have previously shown that carbon dots derived from proteins such as transferrin or albumin retain their respective affinities for associated protein receptors. In our current work, we are aiming to extend this to other forms of materials, such as enzymes, to elucidate further options for the applications of CDs. We aim to compare the efficacy of these novel CDs with that of their precursor materials to identify applications where they could be implemented especially for various diagnostic, therapeutic, and/or optical imaging purposes.

SWRM 2026 SW589

Filter-resolved *in vivo* NIR-II imaging of the biodistribution and pharmacokinetics of CoMoCAT single-walled carbon nanotubes

***Pramita Sharma**, p.sharma@tcu.edu, Anton V Naumov. Department of Physics & Astronomy, Texas Christian University, Fort Worth, Texas, United States*

Semiconducting single-walled carbon nanotubes (SWCNTs) exhibit intrinsic, photostable fluorescence in the second near-infrared window (NIR-II), making them promising probes for deep-tissue imaging and image-guided biomedical applications. However, the potential of mixed-chirality SWCNT preparations for multiplex *in vivo* imaging remains insufficiently explored. Here, we investigate the optical performance, biodistribution, pharmacokinetics, and short-term biocompatibility of DSPE-mPEG-coated CoMoCAT SWCNTs in BALB/c mice. Band-pass filters centered at 1000, 1050, and 1100 nm resolve the emission contributions of the dominant (6,5) nanotubes and coexisting SWCNT chiralities. Longitudinal whole-body imaging following intraperitoneal administration demonstrates rapid systemic distribution and preferential accumulation in reticuloendothelial organs. *Ex vivo* analysis reveals the fluorescence-intensity hierarchy liver, spleen, lungs, heart, kidney, brain, and thymus across all three detection channels. The conserved organ-distribution pattern indicates that the detected SWCNT chiralities exhibit similar biodistribution under the investigated conditions. Control-subtracted serum fluorescence follows an apparent monoexponential decay, yielding an estimated elimination half-life of approximately 2.69 h. During a 21-day tolerability assessment, treated animals maintain stable body mass and normal behavior, while organ fluorescence returns to baseline. Histological examination of the liver, kidney, and lung reveals preserved tissue architecture without detectable inflammatory or fibrotic lesions. These

results establish practical dosing and filter-selection conditions for multiplex NIR-II imaging with CoMoCAT SWCNTs and support their continued development as nanoscale probes for biosensing, longitudinal biodistribution studies, and image-guided biomedical applications.

SWRM 2026 SW590

Improved *in vivo* transient tissue transparency

***Zoya U. Chaudhry**, dal347003@utdallas.edu, David Asante-Asare, Zihao Ou. The University of Texas at Dallas, Richardson, Texas, United States*

Light scattering in tissues prevents us from seeing through tissue. Transient tissue optical clearing has emerged as a promising strategy for increasing transparency in tissues. Absorbing molecules like Tartrazine are used to reduce refractive index mismatches of structures within the tissue making internal structures visible to the human eye. While this technique works excellently ex vivo, there is a limitation when trying to apply in vivo. Slow diffusion of dye molecules through the skin makes it difficult to achieve fast and consistent transparency over larger areas of tissue. In this study, we investigated the use of enhancers for accelerating in vivo tissue clearing. In vivo experiments demonstrated that enhancers significantly reduced the time required to achieve tissue transparency while enabling more rapid and consistent clearing across larger tissue areas. To quantitatively evaluate these improvements, enhancers were applied to mouse skin samples, and transmittance measurements were taken using a spectrophotometer. We found out that enhancers reduce clearing time by about 10-fold These findings show that enhancers are a promising strategy for accelerating in vivo topical optical tissue clearing, opening a bigger avenue for practical biological applications

SWRM 2026 SW591

Polymer mediated precipitate suppression to increase stability in optical clearing agents

***Kelsey I. Arze**[1], dal236442@utdallas.edu, Rohit Kajla[2], Zihao Ou[2]. (1) Psychology, The University of Texas at Dallas, Richardson, Texas, United States(2) Physics, The University of Texas at Dallas, Richardson, Texas, United States*

Biomedical imaging is often limited by the strong scattering of light in skin and other biological tissues, which makes them appear opaque. We chose a FDA-cleared food additive, that possesses unique optical properties to render tissues transparent under specific wavelengths of light. Since the optical properties of tissues vary among animal species, our laboratory optimizes the food additive to achieve effective refractive-index matching for each tissue type. If we increase the concentration of the food dye, the solution becomes unstable. This produces a growing precipitate, rather than a clear liquid, therefore disrupting the optical properties that allow for increase effective imaging time. To solve this problem, this study proposes the idea of introducing polymers to the dye solutions in hopes of making the solutions stable. After examining the molecular structure of the food additive, we chose each polymer based on the theorized effectiveness for preventing the precipitate formation of the additive's molecules. Here, we illustrate how different polymer concentrations interacted with our dye solutions, with some of the best polymers slowing precipitate growth up to ten times.

SWRM 2026 SW592

Miniaturized spectrophotometer for monitoring fluidic performance in a portable microsampling backpack

Esther Kalejaye[1]*, kalejaye@uark.edu, Olivia Enietan*[1]*, Sara R. Thomas*[2]*, Michael A. Johnson*[2]*, Patrick M. Pysz*[1]*, Julie A. Stenken*[1]*. (1) Chemistry and Biochemistry, University of Arkansas, Fayetteville, Arkansas, United States(2) Chemistry, The University of Kansas, Lawrence, Kansas, United States*

Direct chemical measurements using fluidic sampling methods such as microdialysis are difficult in freely moving animals because pumps, fluidic connections, and analytical instrumentation are typically external. A portable microsampling platform therefore requires miniaturization and integration of fluidic and analytical components while minimizing size, weight, power consumption, and dead volume. This work describes a small, low-cost, low-power spectrophotometer based on the ams OSRAM AS7341 multispectral sensor for integration into a portable microsampling backpack for rat studies. Rather than directly measuring neurochemicals, the sensor provides dynamic feedback during animal testing to assess pumping, dead volumes, and system response times. The spectrophotometer combines an AS7341 sensor, visible LED, and low-volume quartz flow cell in a custom 3D-printed housing. The flow cell uses a 6-mm quartz capillary with a 1 × 1 mm internal cross-section, providing a 1-mm optical path length and approximately 6 µL internal volume. Custom 3D-printed components align the optical and fluidic components while providing mechanical support and external-light isolation. The complete detector occupies 4.8 cm^3 and weighs less than 5 g. A custom RP2040-based circuit board provides sensor acquisition and control and operates an in-house fabricated 3D-printed microbore peristaltic pump capable of 0.1–20 µL/min flow rates. Characterization included repeated standards, concentration step changes, extended measurements, short-term noise, baseline stability, signal drift, and fluid-transport effects. Initial in vivo integration was evaluated using retrodialysis of methylene blue in the brain of an anesthetized rat. A 135 µM methylene blue solution in lactated Ringer's solution was perfused through an implanted CMA-12 (4 mm) probe at 2 µL/min while effluent absorbance was continuously monitored using the AS7341 red channel. Switching between solutions with and without methylene blue produced corresponding absorbance changes, including during operation with the 3D-printed pump. These results demonstrate initial integration of compact spectrophotometric detection with low-volume fluidics, custom electronics, and miniaturized pumping for real-time monitoring of a portable microsampling platform. NIH NS140877 is acknowledged for support. The views expressed here are our own and not those of NIH.

SWRM 2026 SW593

Programmable transport gating converts the apparent Michaelis-Menten constant into a design metric in a microneedle biosensor: The case of glucose oxidase

Rahul Pandit Kumarchinchole*, rahul.p_k@okstate.edu, Sathya Samaraweera, Sadagopan Krishnan. Department of Chemistry, Oklahoma State University, Stillwater, Oklahoma, United States*

The apparent Michaelis–Menten constant $K_{M,app}$ of an enzyme electrode is conventionally treated as an empirical, fixed figure of merit. In this work we show that the solid carbon-paste composite microneedle biosensor, $K_{M,app}$ is a dynamically controllable output governed by mass transport through the enzyme-entrapping hydrogel. An integrated, carbon-paste microneedle was functionalized as MN/CP/PB/GOx-CHI-PEG-PEGDE, combining a Prussian Blue (PB) transducer for

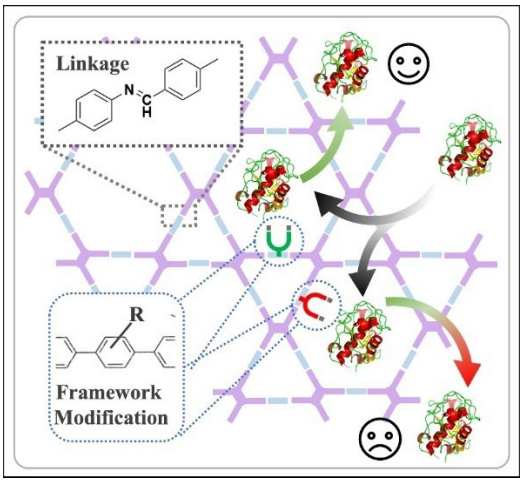
selective, low-potential hydrogen peroxide (H_2O_2) reduction with glucose oxidase (GOx) immobilized in a chitosan–poly(ethylene glycol) network cross-linked with poly(ethylene glycol) diglycidyl ether (PEGDE). By holding PEG constant while systematically varying PEGDE (0.5% to 4.0%), we modulated the hydrogel cross-link density, restricting substrate diffusion without altering intrinsic enzyme kinetics. Electrochemical characterization and mass-transport diagnostics revealed a 15-fold reduction in effective diffusivity (D_{app}) and a drop in partition coefficient (K_P), driving a shift in the dimensionless Thiele modulus (Φ = 0.77 to 3.00) and Damköhler number (Da = 0.60 to 9.00). Consequently, $K_{M,app}$ shifted predictably from 7.0 mM to 50.3 mM in phosphate-buffered saline (PBS) and from 8.2 mM to 58.8 mM in artificial interstitial fluid (AISF). A transport-coupled Fick–Michaelis–Menten model quantitative predicted every $K_{M,app}$ value from independently measured transport parameters (R^2 = 0.99), confirming that localized diffusional gating governs kinetic expansion. This work establishes transport gating as an a priori design lever to tune the linear range and sensitivity of wearable continuous monitoring platforms for target physiological regimes.

SWRM 2026 SW594

Tuning pore microenvironments in covalent-organic frameworks for controlled enzyme loading and release

Wenlu Fan[1]*, wenlufan@my.unt.edu, Joshua Phipps*[1]*, Kui Tan*[2]*, Thamraa AlShahrani*[3]*, Shengqian Ma*[1]*. (1) chemistry, University of North Texas, Denton, Texas, United States(2) The University of Texas at El Paso, El Paso, Texas, United States(3) Princess Nourah bint Abdulrahman University, Riyadh, Riyadh Province, Saudi Arabia*

Covalent-organic frameworks (COFs) with tunable pore environments provide a versatile platform for enzyme immobilization and delivery; however, the relationship between pore microenvironment, enzyme–framework interactions, and the resulting loading, release, and retained activity remains insufficiently understood. Here, we developed a series of TPE-based imine-linked COFs constructed from tetrakis(4-aminophenyl)ethene and structurally related dialdehyde linkers bearing —H, —CH_3, or N,S-containing heterocycles. These frameworks maintain comparable structural backbones while providing systematically varied pore polarity and hydrophilicity–hydrophobicity, enabling direct evaluation of microenvironment effects on enzyme behavior. Using papain as a model enzyme, we quantitatively investigated enzyme loading, release, and retained activity. The more hydrophilic N,S-functionalized framework exhibited enhanced papain loading but lower release and retained activity, consistent with stronger multipoint enzyme–framework interactions and confinement. In contrast, the more hydrophobic methyl-functionalized framework showed lower loading but facilitated enzyme release and better preserved enzymatic activity. In situ FTIR spectroscopy further provided molecular-level evidence for these interactions, revealing changes in hydrogen bonding and characteristic protein and framework vibrations during papain adsorption. These observations support a trade-off in which stronger enzyme–framework interactions favor uptake but can hinder release and compromise retained activity, whereas weaker interactions enhance enzyme mobility and release at the expense of loading. Overall, this study demonstrates that balancing interaction strength and pore microenvironment compatibility, rather than maximizing enzyme adsorption alone, is critical for the rational design of COF-based enzyme immobilization and delivery platforms.



SWRM 2026 SW595

Relating nanoscale film characteristics to electrochemical performance in cytochrome P450 membrane enzyme films

Silan Bhandari[1]*, silan.bhandari@okstate.edu, Matthew Dixon*[2]*, Charuksha T. Walgama*[3]*, Rajasekhara Nerimetla*[1]*, Sadagopan Krishnan*[1]*. (1) Chemistry, Oklahoma State University Department of Chemistry, Stillwater, Oklahoma, United States(2) Nanoscience Instruments Inc, Phoenix, Arizona, United States(3) Department of Physical & Applied Sciences University of Houston-Clear Lake, Houston, Texas, United States*

The membrane-bound human liver cytochrome P450 (CYP) enzymes are essential catalysts in drug metabolism. Large-scale in vitro assays and biosensor applications benefit from using bacterial expression systems (“bactosomes”) that offer a practical and abundant enzyme source. Effective sensor integration requires appropriate surface chemistry and an understanding of biofilm formation.We employed quartz crystal microbalance with dissipation (QCM-D) to evaluate the adsorption of bactosomal films carrying CYP3A4/CPR onto two distinct surfaces, cystamine self-assembled monolayers (SAMs) and polyethylenimine (PEI)-modified gold-coated crystals. We then examined a low-cost, efficient electrochemical strategy to assess direct electron transfer and electrocatalytic behavior of the same CYP3A4 + CPR bactosomal films when deposited on Au/cystamine and Au/PEI disk electrodes, which were designed to mimic the QCM-D gold crystal surface.QCM-D data captured the adsorption process and film development over time, yielding quantitative values for mass loading, thickness, and viscoelastic properties — both for the modified surfaces and after bactosome deposition. Following washing steps, bactosomes on SAM reached ~113 nm in thickness with a mass of 11.9 μg cm^{-2}, while bactosomes on PEI produced thinner films (~40 nm) with lower mass (4.2 μg cm^{-2}). Viscosity was comparable between the two systems (2.5 cP), but elastic modulus values diverged sharply: 2.0 × 10^4 Pa for SAM-based films versus 2.5 × 10^5 Pa for PEI-based films — pointing to a rigid film structure on PEI. Electrochemical study under argon and oxygen-saturated conditions revealed stronger faradaic signals from SAM-modified electrodes (I_p of 5.6 ± 0.6 μA under Ar; Ilimiting of 95.9 ± 3.9 μA under O_2) compared to PEI-modified electrodes (3.2 ± 1.0 μA under Ar; 72.6 ± 3.3 μA under O_2). This gap is due to the larger quantity of immobilized bactosomes on the SAM surface and correspondingly better electronic connectivity between the redox enzymes and the gold electrode, even though the SAM films were thicker overall. These findings offer comparative insights into designed surface chemistries for CYP bactosomes-based biocatalytic electrodes, where trade-offs between film thickness, immobilized mass, rigidity, and signal output may influence performance in drug metabolism studies, toxicity assessments, electrosynthesis, biosensors, and environmental monitoring.

SWRM 2026 SW596

Species-dependent myoglobin redox behavior: Linking electrochemical signatures to protein structural features in beef, pork, and chicken

Sachinthani Ayabadda Devage[1], *sayabad@okstate.edu, Minha Arankuny*[2], *Silan Bhandari*[1], *Greeshma Sreejesh*[2], *Ranjith Ramanathan*[2], *Sadagopan Krishnan*[1]. *(1) Department of Chemistry, Oklahoma State University, Stillwater, Oklahoma, United States(2) Department of Animal and Food Sciences, Oklahoma State University, Stillwater, Oklahoma, United States*

Redox properties of myoglobin (Mb) from beef, pork, and chicken using an electrochemical method at pH 5.6 (postmortem muscle pH), and correlated these properties with the protein structural features, particularly the exposed oxidation-protein amino acids, volume of the heme-ligand binding cavity (heme cavity), and the OxyMb (Oxymyoglobin)/MetMb (metmyoglobin) contents were investigated. The extracts were prepared from the specific muscle types for each species, and the average total myoglobin concentrations (n=4) were: beef, 394 μM (OxyMb =312 μM, MetMb =75 μM); pork, 183 μM (OxyMb= 103 μM, MetMb= 62 μM,); and chicken, 55 μM (OxyMb=18 μM, MetMb= 29 μM). These values reflect the naturally occurring proportions of OxyMb and MetMb in each muscle type per 10 g of meat extracted. This study focuses on the endogenous state of the studied muscle rather than intentionally prepared same starting myoglobin percentages. Structural modeling indicated variation in cavity volume across species, with chicken myoglobin cavity (505 $Å^3$), followed by beef (484 $Å^3$), and pork (466 $Å^3$). Kinetic analysis of oxygen affinity (K_M) further showed the species variation, demonstrating beef K_M=713 ±12 μM (P=0.003, P< 0.05), followed by chicken (K_M=559±64μM) and pork (K_M= 476 ± 13μM). The number of moles of myoglobin molecules adsorbed on the electrode for each species varies. It was 283 pmol cm^{-2} for beef, followed by pork 93 pmol cm^{-2}, and chicken 42 pmol cm^{-2} . Oxidation-prone residues in myoglobin and their exposure area to the environment contributes towards the oxidation of amino acids in the meat myoglobin samples.

SWRM 2026 SW597

Toward the three-dimensional structure of AprL: Crystallization and computational insights into a PLP-dependent sugar aminotransferase

Oluwaseun O. Ajayi*, oluwaseun.ajayi@uga.edu, Robert S. Phillips. Chemistry, University of Georgia, Athens, Georgia, United States*

Aminotransferases that act on sugar-nucleotide intermediates are key tailoring enzymes in antibiotic biosynthesis, yet their structures often remain undetermined due to difficulties producing stable, active enzyme. AprL, a pyridoxal 5′-phosphate (PLP)-dependent aminotransferase from the apramycin biosynthetic pathway of Streptoalloteichus hindustanus, exemplifies this challenge. AprL converts UDP-4-keto-4-deoxy-β-D-glucose to UDP-4-amino-4-deoxy-β-D-glucose, a step essential to building the apramycin scaffold, but no structural model of the enzyme currently exists.
Having resolved earlier expression bottlenecks to obtain purified, catalytically active AprL, we have advanced to high-throughput crystallization screening, which has produced initial crystal hits, and have collected preliminary X-ray diffraction data toward solving the structure. In parallel, we developed a computational workflow integrating molecular docking, molecular dynamics simulations, and MM/GBSA binding free energy calculations to model substrate positioning within the AprL active site ahead of structure determination. Together, the crystallographic and computational efforts are

converging on a structural picture of how AprL recognizes its UDP-sugar substrate, offering insight into substrate specificity among PLP-dependent aminotransferases and a foundation for structure-guided engineering of next-generation aminoglycoside antibiotics.

SWRM 2026 SW598

Integrating enzyme kinetics and NMR spectroscopy to elucidate the catalytic mechanism of an F_{420}-dependent sugar-6-phosphate dehydrogenase from *Nocardioidaceae brasiliensis*

***Md Sabid Ahamed**, mxa1554@mavs.uta.edu. Chemistry & Biochemistry, The University of Texas at Arlington, Arlington, Texas, United States*

F_{420}-dependent glucose-6-phosphate dehydrogenase (FGD), though first identified in *Nocardia*, has been extensively investigated in *Mycobacteria* due to its health relevance to tuberculosis (TB) treatment. FGD catalyzes the oxidation of glucose-6-phosphate (G6P) to 6-phosphogluconolactone using the oxidized F_{420} cofactor, which becomes reduced during turnover. Here, we investigate FGD from *Nocardioidaceae brasiliensis* (*Noca*-FGD), which utilizes a broader range of sugar-6-phosphate substrates, including glucose-6-phosphate (G6P), mannose-6-phosphate (M6P), fructose-6-phosphate (F6P), and glucose-1-phosphate (G1P). This diverges from the mycobacterial enzyme, which only uses G6P as a substrate. Our primary objective is to characterize *Noca*-FGD using binding, steady-state and pre steady-state kinetic approaches to gain detailed mechanistic insight. After expressing and purifying the wild-type *Noca*-FGD, we examined its hydride-transfer reaction mechanism. The enzyme displayed strong binding affinities for all tested substrates, and steady-state analysis indicated that G6P exhibits the highest catalytic efficiency. Notably, NMR experiments revealed that F6P is isomerized to G6P, demonstrating previously unrecognized isomerase activity. In contrast, M6P produced only spectral shifts without evidence of isomerization or 6-phosphogluconate formation. Together, these results show that *Noca*-FGD functions as both a dehydrogenase and an isomerase, uncovering a newly identified dual enzymatic role.

SWRM 2026 SW599

Kinetic characterization of AncD1, an ancestral F_{420}-dependent dehydrogenase

***Ana Ledesma**[1], all3048@mavs.uta.edu, Kaileigh Skidmore[1], Kayunta L. Johnson-Winters[1], Ghader Bashiri[2]. (1) Chemistry and Biochemistry, The University of Texas at Arlington, Arlington, Texas, United States(2) The University of Auckland, Auckland, Auckland, New Zealand*

F_{420}-dependent dehydrogenases are deazaflavoenzymes that play important roles in redox metabolism in Actinobacteria and other microbial lineages. By reducing the F_{420} cofactor to $F_{420}H_2$, these enzymes generate reducing equivalents that support a diverse range of F_{420}-dependent processes, including prodrug activation and reductive detoxification. Despite growing interest in this enzyme family, the relationships among sequence, catalytic function, and evolutionary diversification remain poorly understood. Recent phylogenetic reconstruction identified AncD1 as the resurrected common ancestor of F_{420}-dependent glucose-6-phosphate dehydrogenases (FGDs) and the recently characterized F_{420}-dependent sugar-6-phosphate dehydrogenases (FSDs). FGDs catalyze the F_{420}-dependent oxidation of glucose-6-phosphate to 6-phosphogluconolactone, with concomitant reduction of F_{420} to $F_{420}H_2$. In contrast to mycobacterial FGDs, which exhibit strong specificity for glucose-6-phosphate, AncD1 is catalytically promiscuous and accepts a broader range of phosphorylated sugar

substrates. Here, we report the expression and purification of AncD1 and its kinetic characterization across its substrate range using binding, steady-state, and pre-steady-state kinetic approaches. We also report initial crystallization conditions for AncD1, establishing a foundation for future structural studies aimed at identifying the molecular determinants of its catalytic promiscuity. In parallel, ancestral sequence reconstruction will be extended across the broader F_{420}-dependent dehydrogenase clade, incorporating computational and AI-assisted approaches to investigate how evolutionary sequence changes contribute to functional divergence. Together, these studies integrate evolutionary biochemistry, structural enzymology, and protein engineering to define the molecular basis for the diversification of F_{420}-dependent dehydrogenases and evaluate AncD1 as a robust and versatile scaffold for future biocatalytic applications.

SWRM 2026 SW600 - Withdrawn

SWRM 2026 SW601

Biocatalytic, enantioselective oxa-Pictet-Spengler reactions for the asymmetric synthesis of tetrahydropyranoindoles

William Jones[1]*, willralphj@gmail.com, Robert A. Myers*[1]*, Yashodha Aluth Gedara*[1]*, Nathan D. Woods*[1]*, Veniamin A. Borin*[2]*, David C. Miller*[1]*. (1) Chemistry, Oklahoma State University, Stillwater, Oklahoma, United States(2) Physiological Sciences, Oklahoma State University, Stillwater, Oklahoma, United States*

Tetrahydropyranoindoles (THPIs) are a class of biologically active compounds which are used for the treatment of inflammation, hepatitis C, and certain cancers. The synthesis of chiral THPIs is primarily achieved via asymmetric Oxa-Pictet-Spengler (OPS) reactions. Chiral acids have been widely employed for asymmetric OPS reactions, but these chiral acids often require lengthy synthesis, relatively high catalysis loading, and are non-trivial to recycle. Biocatalysts could provide an alternative platform for asymmetric OPS reactions by improving catalyst access, tunability, and the overall sustainability of these reactions. We report the first time an enzyme has catalyzed the synthesis of various THPIs using an engineered variant of Squalene-Hopene Cyclase (SHC) from *Zymomonas Mobilis* (*Zmo*SHC1). Through directed evolution, we can improve yields and stereoselectivity to provide high yields (up to 82%), high enantioselectivity (up to 99:1 e.r.), and high turnover numbers (up to 3370 TTN). Notably, measured TTNs represent the highest reported catalytic activity for an asymmetric OPS reaction to date. Molecular dynamic (MD) studies showcase that an oxocarbenium ion is formed as a discrete intermediate in this reaction, prior to 5-*endo* spirocyclization and carbocation rearrangement in the enzymatic active site. Our findings encourage future exploration of SHC's as a biocatalyst for the asymmetric synthesis of other classes of fused heterocycles with promising bioactivities.

SWRM 2026 SW602

Biocatalytic asymmetric oxa-Pictet Spengler cyclization for the synthesis of pyranopyrazole derivatives

***Yashodha Aluth Gedara**, yaluthg@okstate.edu, **Mackenzie Armstrong**, mackenzie.armstrong@okstate.edu, **David C. Miller**, david.c.miller@okstate.edu. Chemistry, Oklahoma State University, Stillwater, Oklahoma, United States*

Pyranopyrazoles are biologically active heterocyclic scaffolds that can act as σ-receptor ligands in the Central Nervous System (CNS). These molecules are useful in developing drugs targeting CNS-related disorders such as depression, schizophrenia, anxiety, neuropathic pain, and some neurodegenerative disorders. Pyranopyrazole derivatives can be synthesized through the oxa-Pictet Spengler (OPS) reaction. However, asymmetric OPS reactions with pyrazole-containing substrates are challenging because the heterocycle easily gets protonated by strong acidic conditions, leading to an unreactive aromatic nucleophile. Since most chiral acid organocatalysts are strong Brønsted acids (e.g., chiral BINOL-derived phosphoric acids), these are inherently challenging substrates. To date, there are no examples of asymmetric OPS reactions of pyrazole-derived substrates using organocatalytic protocols. To address this issue, we demonstrate a biocatalytic, asymmetric OPS reaction for the synthesis of pyranopyrazoles using a squalene hopene cyclase (SHC) enzyme from *Alicyclobacillus acidocaldarius* (*Aac*SHC), starting from vinyloxyethylpyrazole derivatives. Upon discovery of initial activity, site-saturation mutagenesis was used to engineer a high-yielding variant capable of achieving up to 99:1 er for this challenging substrate class. This work is the first example of an asymmetric OPS reaction for the synthesis of chiral pyranopyrazoles, expanding the catalytic activity beyond its native terpene cyclization chemistry. This work highlights the potential of SHCs as engineerable, confined Brønsted acid biocatalysts for expanding the scope of asymmetric cationic cyclization chemistry. This method could provide access to alternative fused heterocycles that contain Brønsted basic heterocycles, which are difficult to synthesize using traditional asymmetric catalysis.

SWRM 2026 SW603

Backbone nitrogen substitution to control the conformation and interactions of glycine residues in peptides

***Diana Thomas**, dianathomas0072014@gmail.com, Fengyi Gu, Robert W. Newberry. Department of Chemistry, The University of Texas at Austin College of Natural Sciences, Austin, Texas, United States*

Glycine's unique structure makes it essential to key protein structural motifs, including for example β-turns and transmembrane helix interfaces. However, the conformational flexibility and lack of modifiable side chain make it difficult to control the conformation and interactions of glycine residues for applications in peptide and protein engineering. Herein, we explore minimal substitutions of the peptide backbone that enable the control of glycine’s conformation and interactions in peptides. One such modification is the substitution of glycine's α-carbon with nitrogen (aza-glycine) which restricts backbone dihedral angles toward defined minima and introduces a stronger hydrogen-bond donor. We substituted key glycine residues with aza-glycine in two model systems: (1) β-hairpins with turns featuring distinct glycine conformations, to examine its effects on β-hairpin stability and (2) transmembrane helix interfaces, in which glycine C^{α}–H participates in hydrogen bonding, to examine its effects on helix–helix association. Together, the studies show that aza-glycine is more effective at disfavoring glycine conformations that are incompatible to that of its conformational minima than at reinforcing compatible ones, in both soluble and membrane protein contexts.

SWRM 2026 SW604

Role of gating and C-terminal regions in OfurPBP2

***Md. Ahad Khan**, ahad.khan@okstate.edu, **sanjana gautam**, sanjana.gautam@okstate.edu, **Smita Mohanty**, smita.mohanty@okstate.edu. Chemistry, Oklahoma State University, Stillwater, Oklahoma, United States*

Olfaction allows moths to detect chemical signals, enabling males to sense pheromones and locate mates. Disrupting this communication could provide an alternative to broad-spectrum insecticides, which raise health and environmental concerns. OfurPBP2, a pheromone-binding protein from the Asian corn borer, *Ostrinia furnacalis*, shows pH-dependent structural changes associated with ligand release. In *Antheraea polyphemus* PBP1 (ApolPBP1), the histidine gate and C-terminal region contribute to ligand binding and release. OfurPBP2 differs from ApolPBP1 at the histidine-gate position and in its C-terminal sequence. We generated a chimeric OfurPBP2 mutant containing the R70H substitution and ApolPBP1 C-terminal region to examine their structural contributions.
The mutant was expressed in *E. coli* and recovered from cell lysates, refolded over seven days using an established protocol, and purified by DEAE ion-exchange and size-exclusion chromatography. The purity of the proteins was confirmed by SDS-PAGE. CD spectroscopy analyzed with SELCON3 and 1H-15N HSQC HSQC NMR was used to characterize the mutant at pH 6.5, 5.5, and 4.5, followed by a return to pH 6.5. At pH 6.5, the mutant showed a well-dispersed HSQC spectrum consistent with a folded structure. At pH 4.5, substantial peak loss was observed. CD analysis showed that α-helical content decreased from 61.8% at pH 6.5 to 52.0% at pH 4.5, while β-sheet content increased from 2.7% to 6.1%. Near-UV CD changes between 250 and 320 nm suggested changes in the local environment and packing of aromatic residues. Compared with wild-type OfurPBP2, the mutant showed a less pronounced low-pH response while retaining substantial secondary and tertiary structure. This attenuated response suggests that the R70H substitution and C-terminal region replacement alter the protein's response to acidic pH. The HSQC spectrum recovered its well-dispersed pattern after returning to pH 6.5, demonstrating reversibility. These findings suggest that R70 and the C-terminal region contribute to the extent of the acidic-pH conformational transition in OfurPBP2. Defining OfurPBP2 structural features may help identify targets to disrupt pheromone detection. This work may support selective inhibitors that interfere with male moths' ability to locate females and provide an alternative to broad-spectrum insecticide control.

SWRM 2026 SW605

Experimental framework for assigning quenching mechanism in the dimethyl trisulfide–albumin system

***Md Sohanur Rahman**, mxr343@shsu.edu, Samuel Chirinos, Han Vo, Ilona Petrikovics, David E. Thompson. Chemistry, Sam Houston State University, Huntsville, Texas, United States*

Serum albumin presents hydrophobic binding sites and a free thiol at Cys-34, making it a plausible partner for poorly soluble sulfur species such as the cyanide antidotal candidate dimethyl trisulfide (DMTS). Changes in the native tryptophan emission of bovine serum albumin (BSA) upon addition of DMTS are, on their own, uninformative about mechanism: collisional quenching, ground-state complexation, and covalent modification by sulfane sulfur transfer are all consistent with a reduced signal, as are inner filter attenuation and variation in protein concentration across independently prepared samples. We present the experimental design developed to separate these possibilities. Emission is measured across a DMTS concentration series at multiple temperatures, with and without ethanol cosolvent. The magnitude of the apparent Stern–Volmer constant is evaluated first, against both the bimolecular quenching rate constant it implies and the aqueous solubility of DMTS, since

collisional quenching at accessible concentrations is bounded by each; the sign of its temperature dependence and the ground-state absorbance of the mixtures then discriminate residual collisional from static behavior. Sealed-cuvette controls address DMTS partitioning into the headspace, which varies with temperature and would otherwise mimic a static-quenching result. Preliminary measurements from the concentration series will be presented, together with the criteria by which each mechanism is assigned or excluded.

SWRM 2026 SW606

Mass spectrometry-guided discovery of a novel anabaenopeptin from benthic cyanobacterium *Floridanema evergladense* BLCC-F167

Mir M. Ali[1]*, maaz.ali2060@gmail.com, Terrance Meinardus*[2]*, Aaditi Chopade*[2]*, David E. Berthold*[3]*, Forrest Lefler*[3]*, H. Dale Laughinghouse*[3]*, Matthew Bertin*[2]*. (1) Saint Ignatius High School, Cleveland, Ohio, United States(2) Chemistry, Case Western Reserve University, Cleveland, Ohio, United States(3) Fort Lauderdale Research and Education Center, University of Florida Institute of Food and Agricultural Sciences, Gainesville, Florida, United States*

Benthic cyanobacterial mats are emerging contributors to water quality, however their chemistry remains understudied when compared to surface cyanobacterial harmful algal blooms (CyanoHABs). We explored the recently named genus, Floridanema, and employed metabologenomics, as well as analytical chemistry and structural characterization techniques to elucidate the chemistry of Floridanema evergladense BLCC-F167 Lyophilized F. evergladense BLCC-F167 biomass was extracted with methanol and components from the extract were purified via semi-preparative reversed-phase HPLC. Fractions were screened using high-resolution QTOF-MS, MS/MS, and 1D/2D NMR spectroscopy. The genome of the strain was analyzed with antiSMASH to identify non-ribosomal peptide synthetase (NRPS) biosynthetic gene clusters (BGC). The bioinformatics analysis revealed a putative NRPS BGC within the BLCC-F167 genome. Examination of adenylation domains predicted the incorporation of a tyrosine, D-Lysine, and an N-methyl alanine, suggesting that this pathway encoded for an anabaenopeptin-like molecule, though some residues were still unknown. Furthermore, HPLC analysis isolated the molecule, allowing for the accurate mass and molecular formula to be elucidated: 842.4453 m/z and C45H59N7O9. The MS/MS fragmentation data supported the presence of the unknown amino acids (homologated phenylalanine and phenylalanine and either leucine or isoleucine). Through proton NMR examination, key amino acid residues were then established, such as tyrosine, phenylalanine or homologated phenylalanine, and N-methyl alaninem; but the proton shifts for isoleucine and valine were too similar to differentiate in the 1H NMR spectrum. Using the HSQC NMR spectrum we confirmed the presence of the isoleucine residue through key carbon and proton correlations. The integration of genomic, spectroscopic, and spectrometric data - a metabologenomics approach - allowed for the proposal of the new anabaenopeptin 841. A new anabaenopeptin was elucidated through MS/MS and NMR, confirming that the metabologenomics approach is an effective way of characterizing new molecules. The discovery of new chemistry from this strain reveals the potential danger within these overlooked benthic mats, as they can be detrimental to public drinking water. Though anabaenopeptins are well-known toxins, they may also serve as potential therapeutic leads in biomedical research.

SWRM 2026 SW607

Comparative chemical characterization and bioactive properties of *Calotropis gigantea* and *Calotropis procera* latex

Saakshi Kumar[1]*, saakshikumar25@gmail.com, Manjula Verma*[2]*, Vishwa Nath Verma*[2]*. (1) Jordan High School, Fulshear, Texas, United States(2) University of Guyana, Georgetown, Demerara-Mahaica, Guyana*

Calotropis gigantea and *Calotropis procera* are medicinally important plant species that produce latex containing chemically diverse and biologically active constituents. This study investigated the physicochemical, spectroscopic, chromatographic, phytochemical, elemental, and biological properties of *Calotropis* latex and plant extracts. The two species exhibited distinct latex pH characteristics, with *C. procera* latex showing an acidic pH of 4.2 and *C. gigantea* latex showing a basic pH of 7.2 at 25 °C. Increasing temperature increased the pH of *C. gigantea* latex to 8.1, after which it remained constant. Because dried latex contains both polar and nonpolar constituents, a mixed-solvent system was developed for dissolution prior to further characterization. UV spectroscopic analysis demonstrated substantial absorption across the ultraviolet region, with maximum absorption observed near 315–320 nm. Thin-layer chromatography revealed multiple components whose separation and retention factors varied with mobile-phase composition. Phytochemical screening demonstrated the presence of tannins, saponins, flavonoids, terpenoids, and cardiac glycosides. Atomic absorption analysis further demonstrated the presence of several metal elements in latex, leaves, and bark. Biological evaluation of the latex demonstrated antifungal activity against *Aspergillus flavus*, with microscopic changes in fungal hyphal structure observed following exposure. Together, these findings demonstrate the chemical complexity and biological activity of *Calotropis* and support further investigation of its constituents as plant-derived sources of biologically functional compounds.

SWRM 2026 SW608

Antimicrobial effects of pulsed blue light on probiotic lactic acid bacteria

Ashley R. Chandler[1]*, chandlerar1@jacks.sfasu.edu, Haley Guillen*[1]*, Violet Bumah*[2]*. (1) Chemistry and Biochemistry, Stephen F Austin State University, Nacogdoches, Texas , United States Minor Outlying Islands(2) Chemistry and Biochemistry, Stephen F Austin State University, Nacogdoches, Texas, United States*

Pulsed blue light (PBL) has demonstrated antimicrobial activity against pathogenic bacteria and is being investigated as a potential non-antibiotic approach for bacterial control. However, relatively little is known about how PBL affects beneficial probiotic bacteria. This study investigated the effects of PBL on three lactic acid bacteria: *Lactiplantibacillus plantarum* (F201), *Pediococcus pentosaceus* (K18F), and *Pediococcus acidilactici* (K19D). Bacterial cultures were exposed to 405, 410, 425, and 450 nm PBL at an irradiance of 10 mW/cm^2, radiant exposure of 36 J/cm^2. Following irradiation, cultures were incubated for 48 hours, and bacterial survival was determined by colony-forming unit enumeration. Growth was also monitored using optical density measurements. Preliminary results demonstrated wavelength-dependent responses among all three strains. Relative to the untreated control, F201 survival was 19.6%, 41.1%, 74.1%, and 83.3% at 405, 410, 425, and 450 nm, respectively. K18F survival was 10.6%, 58.0%, 41.1%, and 65.7%, respectively, while K19D survival was 4.0%, 15.2%, 37.0%, and 49.5%, respectively. Thus, 405 nm produced substantial reductions in survival across all three strains, with K19D showing the greatest reduction. K19D also demonstrated relatively low survival at 410 nm, followed by progressively greater survival at 425 and 450 nm. K18F showed greater variability across wavelengths, with the lowest survival observed at 405 nm.

Furthermore, 405 nm produced the greatest reduction in bacterial survival, while survival progressively increased at longer wavelengths. Growth-curve measurements further demonstrated differences in growth patterns among the three strains over the 48-hour observation period. These findings provide preliminary evidence that PBL can inhibit probiotic lactic acid bacteria and that its effectiveness varies according to wavelength and bacterial species. Further investigation is needed to determine whether wavelength-specific PBL treatments can selectively target pathogenic bacteria while minimizing effects on beneficial probiotics.

SWRM 2026 SW609

Wavelength and growth phase-dependent susceptibility of *Lactobacillus* co-cultures to pulsed blue light

***Ezequiel Mora**, morae1@jacks.sfasu.edu, Jemimah Iliyasu, Violet Bumah. Chemistry and Biochemistry, Stephen F Austin State University, Nacogdoches, Texas, United States*

Bacterial interactions within mixed microbial populations may influence susceptibility to antimicrobial treatments. This study evaluated the effects of pulsed blue light (PBL) on co-cultures of *Lactiplantibacillus plantarum* (F201), *Pediococcus pentosaceus* (K18F), and *Pediococcus acidilactici* (K19D). Co-cultures were exposed to 405, 410, 425, and 450 nm PBL at an irradiance of 10 mW/cm^2, radiant exposure of 36 J/cm^2 and incubated for 48 hours before bacterial survival was determined by colony-forming unit enumeration. Results demonstrated substantial differences among bacterial combinations and growth phases. At stationary phase, F201 + K19D exhibited particularly strong sensitivity to PBL, with survival of 6.5%, 8.7%, 16.4%, and 21.5% following exposure to 405, 410, 425, and 450 nm, respectively. At exponential phase, survival was 17.2%, 10.1%, 16.0%, and 36.6%, respectively. F201 + K18F also demonstrated wavelength-dependent responses, with stationary-phase survival ranging from approximately 25.8% to 41.9%. K19D + K18F showed higher survival in one stationary-phase analysis, ranging from 66.0% to 85.9%. Tri-culture experiments containing all three strains also demonstrated reduced survival following PBL exposure, with survival ranging from 28.9% to 43.3% across the tested wavelengths. The greater susceptibility observed in the stationary-phase F201 + K19D co-culture may be associated with growth-phase-dependent changes in bacterial physiology, including alterations in metabolic activity, cell-envelope properties, or stress-response mechanisms. However, these mechanisms were not directly investigated in the present study. Overall, the findings suggest that bacterial growth phase, species composition, and physiological interactions influence susceptibility to PBL. Further studies are needed to determine the mechanisms underlying these differences and to evaluate PBL efficacy in complex microbial communities.

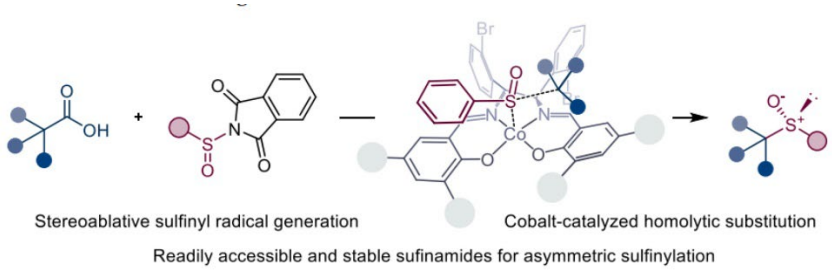
SWRM 2026 SW610

Asymmetric radical sulfinylation via stereoablative sulfinyl radical generation

***Jacob Sanchez**, sancjac04@gmail.com. Chemistry, The University of Texas at San Antonio, San Antonio, Texas, United States*

Stereogenic sulfur functional groups constitute an important class of chiral motifs with broad utility in medicinal chemistry, asymmetric synthesis, and catalysis, yet catalytic strategies for their enantioselective construction from simple and abundant precursors remain limited. We report herein a previously unexplored enantioconvergent decarboxylative sulfinylation of carboxylic acids enabled

by a merger of acridine photocatalysis and cobalt catalyzed asymmetric carbon sulfur bond formation. This catalytic platform leverages stable Ns ulfinylphthalimides as sulfinyl group transfer reagents and proceeds through a stereoablative S N bond cleavage process that generates a sulfinyl radical under mild conditions. The method provides efficient access to chiral sulfoxides with high enantioselectivity. Mechanistic studies revealed that acridinyl radical mediated PCET activation of the sulfinamide reagent, followed by selective cobalt catalyzed sulfinyl radical trapping and coupling of the resulting sulfinylcobalt intermediate with an alkyl radical collectively underpin the observed stereocontrol and efficiency. Together, these findings establish a mechanistically distinct blueprint for asymmetric radical sulfoxide synthesis and open new avenues for catalytic strategies that leverage stereoablative radical processes to access sulfur centered stereogenic motifs.



SWRM 2026 SW611 - Withdrawn

SWRM 2026 SW612

Investigation of the stability of amyloid-β (Aβ) fibrils upon interaction with SARS-CoV-2 protein fragment FI10: A molecular dynamics study

***Al Amin**, alaminchem40.ju@gmail.com, Ulrich H.E. Hansmann. Chemistry and Biochemistry, The University of Oklahoma, Norman, Oklahoma, United States*

Amyloid-β (Aβ) fibrils formation is considered one of the main reasons for the development and progression of Alzheimer's disease (AD). Recently, several studies have suggested that people who were previously infected with SARS-CoV-2 may have a higher risk of accelerating the progression of AD. However, the exact molecular level mechanism of how this acceleration caused by SARS-CoV-2 infection remains poorly studied. Possible reasons include the stabilization of mature Aβ fibrils - the final products of amyloidogenesis and formed from aggregates of Aβ peptides - by viral protein fragments. In previous work it was shown that the spike protein fragment FI10 preferentially stabilizes fibril structures that are found in patients with Alzheimer's Disease. However, this previous study looked only into a single patient-derived fibril model comparing it with one that was synthesized in vitro. Given the large polymorphism of Aβ-fibrils more work is needed to establish whether disease relevant geometries are indeed preferentially stabilized by the viral protein fragments, and whether such differential stabilization is due to a common mechanism. For this purpose, we have used molecular dynamics simulations to study the effect of FI10 on the stability of two additional patient-derived $A\beta_{1\text{-}42}$ and $A\beta_{1\text{-}40}$ fibrils, comparing our results with that of the earlier study of a patient-derived $A\beta_{1\text{-}42}$ fibril and a synthetic fibril model.

SWRM 2026 SW613

Thermodynamic and mechanical stability of hydrogen-bonded organic frameworks: Insights from density functional theory

***Muthukumar Devarasu**, mdevarasu@smu.edu, Haoyuan Chen. Chemistry, Southern Methodist University, Dallas, Texas, United States*

Hydrogen-bonded organic frameworks (HOFs) are an emerging class of porous crystalline materials assembled through directional, reversible hydrogen bonding. This assembly mode offers synthetic advantages, including mild reaction conditions and facile recrystallization, but the weak nature of hydrogen bonds raises concerns about mechanical robustness during guest activation and processing. Despite growing interest in HOFs, their mechanical stability remains largely unexplored computationally. Here, we investigate the thermodynamic and mechanical stability of approximately 50 HOF structures using Density Functional Theory (DFT) calculations performed with CP2K within the Gaussian and Plane-Wave (GPW) formalism. The structures are categorized into four hydrogen-bonding motifs: diaminotriazine (DAT), carboxylic acid, nitrile, and sulfonic acid-based connectivity. For each parent structure, single-point energy at the equilibrium geometry establishes a 0 K thermodynamic baseline, while the lattice energy quantifies the favorability of crystal packing across the library. Further the mechanical stability is evaluated through energy-volume (E-V), uniaxial, and shear distortion analyses using a relaxed-ion approach, in which internal atomic coordinates relax under imposed strain. E-V data, which is obtained by isotropically scaling lattice vectors with full geometry optimization at each scaled configuration, are fitted to the third-order Birch-Murnaghan equation of state to extract the bulk modulus and its pressure derivative. Uniaxial and shear distortions probe directional and angular stiffness respectively, capturing anisotropic mechanical behavior. Relaxed-ion calculations capture molecular rearrangement under strain, avoiding the stiffness overestimation of clamped-ion treatments and providing a more physically representative measure of mechanical response. To our knowledge, this is the first library-scale relaxed-ion computational assessment of HOF stability, linking hydrogen-bonding chemistry to mechanical robustness and guiding future synthesis.

SWRM 2026 SW614

Computational characterization of mesothelin-navenibody complexes using AI-driven structural prediction and molecular docking for targeted small cell lung cancer therapy

***Geetash Muddara**[2,1], Geetash.muddara@gmail.com, Gaurav Sharma[1]. (1) Eigen Sciences, Apex, North Carolina, United States(2) Emerson High School, Geetash.muddara@gmail.com, Texas, United States*

Small Cell Lung Cancer (SCLC) remains one of the most aggressive and fatal lung cancer subtypes, often associated with poor prognosis and limited therapeutic options. Mesothelin, a cell-surface glycoprotein overexpressed in SCLC, has emerged as a promising target for antibody-based immunotherapy. In this study, we performed computational modeling and molecular docking to characterize the interactions between mesothelin and Navenibodies—novel antibody candidates designed for selective tumor targeting. The amino acid sequence of mesothelin was retrieved from UniProt and structurally modeled using AlphaFold 3, while antibody structures were obtained and analyzed using ChimeraX. Machine learning tools such as P2Rank and ScanNet accurately predicted the mesothelin binding pocket, enabling high-precision docking with multiple Navenibody candidates through GRAMM and PRODIGY. Among the tested complexes, Navenibody 3BE9 demonstrated the most favorable combination of binding energy (−33.5 kcal/mol) and geometric stability, supported by extensive hydrogen bonding and hydrophobic interactions identified via PLIP analysis. These results

indicate that Navenibodies exhibit high affinity and structural complementarity toward mesothelin, suggesting strong potential for SCLC-specific targeting. Overall, this AI-driven computational framework highlights how machine learning–based modeling and docking pipelines can accelerate antibody discovery and design, offering a rational foundation for developing mesothelin-directed immunotherapies in small cell lung cancer.

SWRM 2026 SW615

Many-body second order Green's function theory for *ab initio* molecular quantum electrodynamics

Amir Amini[1]*, amiramini@tamu.edu, Leopoldo Mejía*[2]*, Arkajit Mandal*[1]*. (1) Chemistry, Texas A&M University, College Station, Texas, United States(2) Facultad de Ciencias Exactas, Universidad Andres Bello, Santiago, Santiago Metropolitan Region, Chile*

We develop a quantum-electrodynamical electronic-structure theory that describes the correlated ground state of molecules coupled to quantized electromagnetic fields inside optical cavities. Specifically, we combine finite-temperature second-order Green's-function theory (GF2) with coherent-state and Lang–Firsov approaches to describe electron–boson interactions. We find that the coherent-state GF2 approach produces accurate results, while the Lang–Firsov approach yields marginally better accuracy at a substantially higher computational cost. We apply these approaches to a wide range of chemical systems coupled to confined radiation.

SWRM 2026 SW616

Early steps of virus-induced TTR amyloid formation

Malinda B. Premathilaka*, malinda7066@ou.edu, Ulrich H.E. Hansmann. Chemistry and Biochemistry, The University of Oklahoma, Norman, Oklahoma, United States*

A growing body of studies suggests that people who were previously affected with SARS-CoV-2 have a higher risk of developing transthyretin (TTR) amyloidosis, an illness often affecting the elderly. However, a comprehensive molecular level explanation has not been established so far to explain how SARS-CoV-2 infections is correlated with TTR amyloidosis. We have previously demonstrated the ability of small protein fragments derived from SARS-CoV-2 to promote the amyloid formation of amyloid-β, α-synuclein and serum amyloid A, by shifting the ensemble of monomers towards aggregation-prone conformations or by stabilizing the resulting fibrils. In the case of TTR there may be an additional effect. We hypothesize that SARS-CoV-2 derived viral fragments can destabilize the native TTR tetramer, and as the released monomers are known to be unstable and to misfold easily into aggregation-prone chains, trigger the early stages of TTR amyloid formation. To test this hypothesis, we use all-atom molecular dynamics simulations to explore how TTR tetramer stability is affected in the presence of three viral fragments, FI10, SK9, and HV11. Our simulations demonstrate that SARS-CoV-2 viral fragments preferentially interact with B and C β-strands of TTR, destabilizing the monomer-monomer interface by disrupting a hydrogen bonding network that stabilizes this region. This pattern of destabilization is consistent with features previously reported for the amyloidogenic L55P and V30M mutations. Our findings reveal information on how SARS-CoV-2 viral fragments interact with TTR and establish a possible molecular-level mechanism for how SARS-CoV-2 infection destabilize the TTR tetramer.

SWRM 2026 SW617

Ligand-dependent inter-site coupling in human glutathione synthetase

***Matthew Stankus**, mjs736@cornell.edu, Mary E. Anderson. Texas Woman's University College of Arts & Sciences, Denton, Texas, United States*

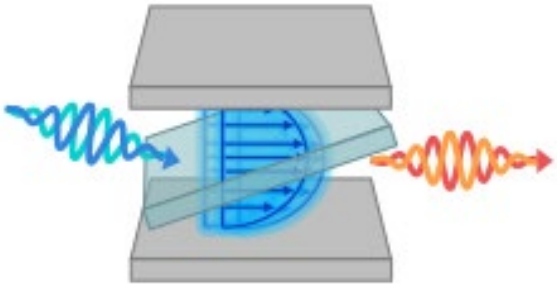
Human glutathione synthetase (hGS) is an obligate homodimer that catalyzes the final step of glutathione synthesis and displays negative cooperativity towards its gamma-glutamylcysteine substrate. In hGS, substrate binding at one subunit alters substrate affinity at the other active site, yet the structural basis for this coupling remains poorly understood. Here we used an aggregate of 6 microseconds of molecular dynamics simulations, pocket volume analysis, and dynamical network analysis to investigate inter-site coupling in two asymmetric states with either products or reactants in one active site while the partner site remained empty. We found that ligand identity substantially remodels the empty partner site and redistributes interactions across the dimer interface. In the product-bound state, the empty partner site has a 32.6% larger pocket volume but is 41.7% less hydrated than in the reactant-bound state. WISP dynamical network analysis identified a largely shared communication scaffold linking the two active sites, where 64.1% of transmission residues are shared between the product- and reactant-bound states. Our results support a model in which ligand-dependent remodeling of a distributed inter-subunit network that couples the distant active sites gives rise to negative cooperativity in hGS.

SWRM 2026 SW618

Tilted material in an optical cavity: Light-matter moiré effect and coherent frequency conversion

***Arshath Manjalingal**, avmanjalingal@tamu.edu, Saeed Koshkaki, Logan P. Blackham, Arkajit Mandal. Chemistry, Texas A&M University, College Station, Texas, United States*

Excitons in an optical cavity hybridize with confined photon modes to form quasiparticles known as polaritons, producing distinct upper and lower polariton branches in the dispersion relation and enabling a variety of new quantum phenomena. In two-dimensional bilayers, twisting one layer relative to the other can generate moiré periodicity, resulting in the formation of two distinct Dirac cones. Here, we introduce and theoretically characterize a light-matter moiré effect (LMME) that arises when a single-layer two-dimensional material is tilted within a planar optical cavity. We show that this geometric tilt produces an emergent periodic modulation of the light-matter coupling, resulting in displaced replicas of the polariton dispersion and flat polariton bands near the Brillouin-zone center. Using time-dependent quantum dynamical simulations, we further demonstrate that the LMME enables coherent frequency conversion and remains robust against phonon-induced decoherence. These findings establish the LMME as a new platform for engineering polariton band structures, generating flat bands, and realizing coherent frequency conversion for potential applications in polariton-based quantum devices.



SWRM 2026 SW619

ProPrep: Making biomolecular simulations accessible to experimental biochemists

Matthew J. Guberman-Pfeffer[1]*, mjgp@nmsu.edu, Adara Walker*[1]*, Padraic Nielsen*[1]*, John Cairns*[2]*. (1) Chemistry and Biochemistry, New Mexico State University, Las Cruces, New Mexico, United States(2) Independent Researcher, Naperville, Illinois, United States*

Dynamical and quantum mechanical/molecular mechanical simulations of biomedically relevant processes largely remain inaccessible to experimentalists studying those systems. Feature-rich preparation programs offer customization at the expense of extensive training, simplified tools favor usability in exchange for hidden or unchangeable defaults, and often several tools need to be daisy-chained into inefficient and difficult-to-reproduce workflows for specific research questions. Here, we describe and demonstrate ProPrep, a prompt-driven preparation platform distributed with AmberTools26, that helps users ACE-IT by providing Access to a Cohesive set of Educationally annotated Interactive tools with Traceable output. ProPrep orchestrates structure retrieval, assembly, alignment, curation, repair, simulation, and analysis for both soluble and membrane-embedded (metallo)proteins by interfacing with 15 programs in AmberTools, 4 online bioinformatics databases, and 2 quantum chemistry packages. An extensible framework detects, parameterizes, and transforms specialized residues such as metal sites, modified amino acids, and organic cofactors into force field-compatible forms, and deposits the parameters into a user library for reuse. At every step, ProPrep keeps users informed and in control while shouldering the labor of implementing their decisions. Each action is preserved in a session log that can be shared for reproducibility, replayed to regenerate results, or adapted as a template for batch work. In doing so, ProPrep serves both the newcomer learning the field and the expert working at scale.



SWRM 2026 SW620

Electronic structure insights into composition-dependent magnetism in alloyed two-dimensional transition-metal compounds

***Puja Rijal**, prijalschool@gmail.com, Kevin L. Shuford. Chemistry and Biochemistry, Baylor University, Waco, Texas, United States*

Two-dimensional transition-metal compounds belonging to the anti-MXene family have emerged as promising candidates for spintronic applications because their electronic and magnetic properties can be systematically tailored through chemical composition. Pristine anti-MXenes have the general composition M_2X_2, where M is a transition metal and X is a nonmetal. Alloying one of the transition-metal sites produces compounds of the form $M_1M_1'X_2$, where M′ is a second transition metal, providing a versatile platform for understanding how chemical substitution governs intrinsic magnetism. In this work, first-principles density functional theory and high-throughput computational screening are used to investigate how transition-metal alloying modifies the electronic structure and magnetic behavior of alloyed anti-MXenes. Following identification of thermodynamically, dynamically, and mechanically stable compounds, competing ferro- and antiferromagnetic configurations are examined to determine the magnetic ground state. Analysis of the electronic structure, magnetic moments, exchange interactions, magnetic anisotropy, and Curie temperatures reveals how the second transition metal modifies orbital hybridization, spin polarization, and magnetic exchange, leading to distinct magnetic ordering across the alloyed series. These results establish structure–property relationships that explain the electronic origin of intrinsic magnetism and provide general design principles for engineering magnetic behavior in two-dimensional transition-metal compounds for next-generation spintronic applications.

SWRM 2026 SW621

Transient magnesium is an essential cofactor for phosphoryl transfer in CDK2

***Muhammed Shameem**, kpm.shameem@gmail.com. chemistry and biochemistry, University of Texas at Arlington Research Institute, Arlington, Texas, United States*

Protein kinases comprise a family of more than 500 enzymes that regulate diverse cellular processes, including signal transduction and cell-cycle progression. Despite substantial structural similarity in their active sites, protein kinases exhibit considerable diversity in their requirements for divalent metal cofactors during phosphoryl transfer. While at least one Mg ion (MgN) is generally considered essential for catalysis, several kinases utilize a second, transiently bound Mg ion (MgT). Cyclin-dependent kinase 2 (CDK2) has traditionally been described as a single-Mg kinase. However, recent crystallographic and biochemical studies suggest that CDK2 can bind a second Mg ion upon formation of the ternary enzyme–ATP–substrate complex, with MgT dissociating following phosphoryl transfer. The physiological relevance of MgT in CDK2 remains unclear because the structural evidence for its binding was obtained at Mg concentrations exceeding 25 mM, substantially higher than the estimated freely available intracellular Mg concentration (~1 mM). Furthermore, CDK2 exhibits maximal catalytic activity at approximately 5 mM Mg, raising the possibility that MgT binding may be a consequence of nonphysiological Mg concentrations rather than an intrinsic requirement for catalysis. Here, we investigate the thermodynamic and structural basis of MgT binding in CDK2 using a combination of molecular dynamics simulations, electrostatic potential calculations, and relative binding free-energy calculations. Our results demonstrate that MgT binding is energetically favorable under catalytically relevant conditions and that MgT plays an essential role in organizing the CDK2 active site for efficient phosphoryl transfer. In particular, MgT stabilizes key electrostatic and structural interactions within the active site and promotes an ATP–substrate configuration conducive to

phosphoryl transfer. These findings support a mechanistic role for the transient second Mg ion in CDK2 catalysis and provide insight into how metal-ion coordination contributes to the catalytic strategies employed by protein kinases.

SWRM 2026 SW622

Quantifying the strength of acid/base functional groups in metal-organic frameworks

***Alitza Gracia**, agracia@smu.edu, Haoyuan Chen. Southern Methodist University, Dallas, Texas, United States*

Metal-organic frameworks (MOFs) are crystalline, nanoporous materials that have great potential as catalysts due to their structural tunability. The metal sites in MOFs can act as Lewis acids, and the organic linkers in MOFs can be functionalized with acid/base groups to act as Bronsted acids/bases, providing a synergistic environment that is critical in the catalysis of many organic reactions. The pK_a/pK_b of the functionalized MOFs is key in determining its catalytic power, however, it remains unknown for many of these MOFs. One of the most popular MOFs used for catalysis is UiO-66. Quantum chemical calculations have been performed on UiO-66 that is functionalized with various acid/base groups to determine the pK_a/pK_b shifts. The search for cluster geometries is done with ABCluster using extended tight-binding (xTB), and the resulting structures are then optimized with density functional theory (DFT). The pK_a/pK_b shifts are determined by comparing the pK_a/pK_b of the functionalized MOF to the pK_a/pK_b of the linker groups. Several candidate structures have been identified for the COOH- functionalized UiO-66 with four explicit waters. Its pK_a shift has been identified by using the average values of the pK_a of the functionalized MOF and linker groups, respectively.

SWRM 2026 SW623

Mapping neutral and autocatalytic mechanisms in polyester hydrolysis using bis(2-hydroxyethyl) terephthalate

***Amir O. Egberongbe**[1], aoegbero@cougarnet.uh.edu, SriBala Gorugantu[1], Alexander Shaw[2], Linda J. Broadbelt[2], Apoorva Ranjekar[3], Ana Rita C. Morais[3]. (1) Chemical and Biomolecular Engineering, University of Houston System, Houston, Texas, United States(2) Chemical and Biological Engineering, Northwestern University, Evanston, Illinois, United States(3) Wonderful Institute for Sustainable Engineering, Department of Chemical and Petroleum Engineering, University of Kansas Shared Print, Lawrence, Kansas, United States*

Hydrolysis of polyesters such as poly(ethylene terephthalate) (PET) for monomer recovery underpins complex chemistry governed by solvent interaction, proton activity, and polymer morphology. These interactions involve neutral, proton-driven and reverse esterification mechanisms operating in parallel. Resolving each contribution would inform catalyst design targeted at monomer recovery. Existing kinetic models do not explicitly treat solvent effects and rely on apparent kinetics fitted to experimental conversion data. This work combines density functional theory (DFT) that incorporates an explicit solvent with a mechanistic model based on mass-action kinetics of elementary steps of bis(2-hydroxyethyl) terephthalate (BHET) hydrolysis as a reactant leading to terephthalic acid (TPA) and mono-(2-hydroxyethyl) terephthalate (MHET) as major products. BHET retains the ester functionality of PET repeat unit while isolating hydrolysis chemistry from transport and morphology

effects. The competing neutral and acid-catalyzed pathways were incorporated into a continuum model validated against BHET, MHET, and TPA concentration profiles measured in-house at 20 bar of N_2 at room temperatureand 180-200 ^oC. This study reveals that the neutral hydrolysis of the ester linkage in BHET is the critical first step with an intrinsic barrier of 25 kcal/mol, while the acid-catalyzed route with its lower barrier (13 kcal/mol) begins to dominate as the pH decreases. The released MHET and TPA products deprotonate and raise the system acidity, accelerating TPA yields up to 16%, 31% and 61% at 180 – 200^oC, respectively, at around 160 min. Raising the temperature from 180 to 200 ^oC shortens the induction period preceding this acceleration while TPA solubility plays an important role in the extent of autocatalysis. In contrast to global models which are limited in their ability to be extrapolated, our mechanistic model offers a basis for tuning solvent, pH and temperature.

SWRM 2026 SW624

Optoelectronic properties and charge transfer mechanisms of naphthopyrone-based dyes on TiO_2 and ZnO

Thatcher Bentley*, trbentley1000@gmail.com, Juganta K. Roy. Chemistry and Physics, West Texas A&M University, Canyon, Texas, United States*

Dye-sensitized solar cells (DSCs) are not only cost-effective, but also customizable photovoltaic technologies capable of achieving energy efficiency exceeding 14%. DSCs possess a unique ability to be fabricated as a semi-transparent, multicolored modules, enabling their use in architecture as windows or roofs. Photochromic DSCs (or semitransparent DSCs, ST-DSCs) allow the pass-through of visible wavelengths that utilize their self-adaptive optical properties, dynamically adjusting the light in response to wavelength intensity and functionally adding comfort to any user by eliminating the harshness of the sunlight, alongside energy production. However, there are some trade-offs with this technology between optical transparency and conversion efficiency. Approaching this trade-off with naphthopyran (NPB) derivatives, that are a class of photochromic dyes that change color upon exposure to ultraviolet and near infrared wavelengths. Using this molecular engineering approach, the electronic structure, photochromic behavior, and the interfacial charge transfer of the NPB dyes can be controlled. This study investigates the interfacial photophysics of NPB dyes absorbed onto the surfaces of anatase TiO_2 and ZnO. Altering the five-membered and six-membered -spacers rings adjacent to the anchoring group of the NPB dyes, the DFT+U calculations predict the absorption stability, electronic structure of the interface, charge transfer, and electron injection rate for different dye semiconductor binding modes. Our results revealed that the bridge-bidentate mode is the most energetically favorable binding configuration compared with the other tested binding modes. This stability stemmed from the electronic effects of the heteroatoms, S, O, N, and Se, which alter the electronic coupling between the dye and the semiconductor. Providing an understanding of the dye/semiconductor interface on the molecular level, which can be used to design the next generation of ST-DSCs.

SWRM 2026 SW625

AI-accelerated *ab initio* bottom-up polymer structure prediction (AI2-BPSP) framework via hybrid DFT-based machine-learning force fields

***Bharatha Kaushalya Gunawardana**, bharathagunawardana@my.unt.edu, Teresa Shah, Deepa Ranabhat, Yizhi Song, Juliana Trejo, Srinjoy Ghose, Hsin-Yu Ko. Chemistry, University of North Texas, Denton, Texas, United States*

Polymers are an important class of materials ubiquitous in our lives. While the synthesis and processing protocols of many polymers are well established, experimental assignment of their microscopic structures at the atomistic resolution remains largely limited to highly crystalline systems. This gap is typically addressed via computer simulations by melting and quenching pre-folded macromolecular chains using empirical interatomic potentials, which can introduce uncontrolled uncertainties due to the long conformational relaxation time for high polymers. In this work, we develop a bottom-up polymer structure prediction framework to simulate chain-growth processes that mirror experimental syntheses and to address these difficulties by using efficient deep potential (DP) machine-learning force fields trained with the reliable van der Waals-corrected hybrid DFT. As a proof of concept, we apply this framework to predict one of the amorphous structures of one of the simplest but most commonly used synthetic polymers: polyethylene (PE).

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Comparison of computational modelling techniques for structure prediction of c-type cytochromes from *Yersinia enterocolitica*

***Newton Hilliard**, nhilliard@atu.edu. Mathematics and Physical Sciences, Arkansas Tech University, Russellville, Arkansas, United States*

Yersinia enterocolitica is a food borne pathogen causing abdominal pain and diarrhea. Chronic issues associated with infection can result in high mortality rates. Using the Integrated Microbial Genomes and Microbiomes database, it was found that *Y. enterocolitica* maintains genes for two separate and distinct low molecular weight mono-heme, c-type cytochromes which we designate as YEcyt1 and YEcyt2 based on their location in the genome. While OMEGA alignment identified the c-type heme binding site for each, only 21 identical residues and an additional 11 highly similar residues were found. Unique amongst these was a conserved LTDDDI sequence. Homology modelling using the SWISS Model site resulted in structures containing visible c-type heme binding clefts. In YEcyt2, a His/Met iron ligation was easily discernable as was a low level of charged residue on the protein surface. YEcyt1 displayed a high level of surface positive charge with unclear iron ligation of His/Arg or His/Lys. Sequences were also sent to both the DI-TASSER and AlphaFold 3 sites for modelling using *ab initio* techniques. DI-TASSER results clearly indicate both similarities and differences in the peptide backbone conformations but is not definitive with respect to potential differences in heme ligation. AlphaFold 3 results are more definitive with respect to both differences in surface charge and heme ligation. YEcyt2 maintains a slightly overall positive surface charge with His/Met heme iron ligation. YEcyt1 displays the highly positive surface charge identified during homology modeling. It also displays a very clear His/Lys heme iron ligation. While not a common occurrence, the His/Lys ligand pair is known for c-type cytochromes and may be associated with pH dependent activities. In both cytochromes, the aspartic acid triplet identified in the OMEGA alignment is easily discernable. These results support a model for two separate and distinct electron transfer pathways in *Y. enterocolitica*.

SWRM 2026 SW627

Enabling high-throughput training of machine-learning force fields with long-range electrostatic interactions with robust orbital localization methods

***Teresa Shah**, teresashah@my.unt.edu, Yizhi Song, Hsin-Yu Ko. Chemistry, University of North Texas, Denton, Texas, United States*

Machine-learning force fields (MLFFs), e.g., deep-potential (DP) models, achieve 106-108x speedups in *ab initio* molecular dynamics simulations without loss of DFT accuracy. Standard short-range formulations fail to capture long-range interactions, which are essential for ionic and polar systems. The Deep Potential Long-Range (DPLR) framework resolves this by combining a short-range DP model with a long-range Gaussian charge model built from localized orbital centroids. However, DPLR relies on Maximally Localized Wannier Functions (MLWFs) to determine these centroids, therefore requiring system-dependent optimizations that impede automated high-throughput workflows. Here, we demonstrate that more robust DPLR models can be obtained using more robust alternative localization schemes: Selected Columns of the Density Matrix (SCDM) or Truncated Density Convolution (TDC), both of which provide localized orbital centroids indistinguishable from those obtained using MLWFs. By eliminating system-dependent MLWF optimizations, this approach enables high-throughput MLFF pipelines capable of treating short-range quantum interactions and long-range electrostatics with equal rigor.

SWRM 2026 SW628

Robust parameter estimation of microkinetic models for heterogeneous catalysis

*M G Toufik Ahmed, **M M Faruque Hasan**, hasan@tamu.edu. Texas A&M University, College Station, Texas, United States*

Microkinetic models (MKMs) are models consisting of elementary reactions that connects molecular-scale chemistry to reactor-scale behavior. By explicitly describing the elementary reaction steps and surface intermediates involved in a heterogeneous catalytic system, MKM allows to predict reaction rates, selectivity, surface coverage, dominant pathways, and rate-determining steps. However, estimating their kinetic parameters remains challenging. The MKM parameter-estimation problems are often stiff and ill-conditioned, which make conventional nalgorithms sensitive to initialization and lead to numerical failure. In this work, we present the parameter estimation task as a nonlinear programming (NLP) problem that can combine experimental measurements, computational data, atomistic calculations, and semiempirical relationships within a common framework. We further develop a solution strategy based on adaptive feasibility restoration to improve convergence for difficult MKM problems. A minimum-norm least-squares direction addresses ill-conditioning in the reaction network, while a projected backtracking line search maintains physical parameter bounds without introducing additional inequality multipliers. We demonstrate the approach using experimental data for several reaction systems. The proposed approach improves convergence reliability, solution quality, and computational efficiency, providing a practical framework for parameter estimation in heterogeneous catalytic microkinetic models. The implementation and codes are available at https://github.com/SOULS-TAMU/MKMParameterEstimation.git.

SWRM 2026 SW629

AI-accelerated *ab initio* bottom-up polymer structure prediction of amorphous polyethylenimine

***Priya N. Limbu**, priyalimbu@my.unt.edu, Bharatha K. Gunawardana, Teresa Shah, Deepa Ranabhat, Kriti Alam, Yizhi Song, Hsin-Yu Ko. Physical Chemistry, University of North Texas, Denton, Texas, United States*

Polyethylenimine (PEI) is a highly versatile polymer with applications in gene delivery, CO_2 capture, and metal chelation. For instance, PEI acts as a non-viral vector in gene delivery due to a dense network of protonatable amine groups that buffer across a broad pH range and enable DNA release via the “proton sponge” effect. However, the amorphous nature of PEI makes the characterization of its atomistic structures an open challenge. In order to obtain an atomistic understanding of PEI and enable rational design of this important polymer, we applied a recently developed ab initio bottom-up polymer structure prediction (AI^2-BPSP) framework. Using this framework, we trained reactive machine-learning force fields based on first-principles data at the reliable hybrid density functional theory (PBE0+D3). weAs a proof-of-concept case study, we simulated the cationic ring-opening polymerization of PEI under experimental conditions to generate atomistically resolved condensed-phase structural ensembles of this macromolecule as a function of its chain length.

SWRM 2026 SW630

Benchmarking force fields and water models for MDM2–p53 unbinding kinetics

***Aloka Patabendi Mudiyanselage**, alokapatabendimudiyanselage@my.unt.edu, Omar Valsson. Chemistry, University of North Texas, Denton, Texas, United States*

Protein-protein and protein-peptide interactions are essential in many biological processes, often forming stable complexes with slow dissociation rates. A well-known example is the interaction between the tumor suppressor p53 peptide to the oncoprotein MDM2, which has an unbinding time of around 0.5 seconds. Employing atomistic simulation to obtain the dissociation times of protein-peptide complexes is important as dissociation kinetics strongly influence drug–target effectiveness. Although several enhanced sampling techniques have been applied to study these unbinding processes, the impact of factors such as the choice of protein force field on dissociation dynamics has not been thoroughly explored. Here, we present a comprehensive benchmark of the effects of different protein force fields and water models on the unbinding kinetics of the MDM2–p53 complex. We investigate multiple force fields from the Amber family in combination with several commonly used water models using Infrequent Metadynamics (InMetaD), an enhanced sampling approach designed to obtain kinetics of rare events. The reliability of the calculated unbinding times is assessed using statistical validation tests appropriate for rare-event kinetics. In addition, we investigate the effect of peptide capping on the unbinding kinetics of the MDM2–p53 system using the Amber99SB-ILDN force field with the TIP3P water model. Our results demonstrate that the choice of force field significantly influences the unbinding times of the MDM2–p53 complex, with differences across force fields and water models of around one to two orders of magnitude. This underscores the critical importance of carefully selecting force fields when comparing simulation outcomes with experimental data or across different computational approaches.

SWRM 2026 SW631

Infrequent metadynamics study of SH3-peptide dissociation kinetics: Effects of terminal capping

***Jaya Pathak**, jayapathak@my.unt.edu. Chemistry, University of North Texas System, Denton, Texas, United States*

Peptide-based therapeutics offer a powerful strategy for modulating protein-protein interactions by engaging extended, structurally diverse protein surfaces. An important consideration in developing such molecules is not only how strongly they bind, but also how long they remain associated with their target. The dissociation rate (k_{off}) is a key kinetic parameter that governs target residence time (tau), which describes how long a peptide remains associated with its target protein. Although molecular interactions play a critical role in protein-peptide unbinding, the specific interactions that determine k_{off} remain largely unexplored. Atomistic simulations provide a powerful framework for investigating protein–peptide binding and dissociation kinetics at the molecular level. Enhanced-sampling methods, such as infrequent metadynamics, has been successfully used in characterization of rare dissociation events. Here, we employ infrequent metadynamics method to investigate the effect of terminal capping (ACE and NME) group on the dissociation of the Src homology 3 (SH3) domain bound to a Sos proline-rich peptide as a model system. By comparing capped and uncapped forms of the peptide, we examine how terminal modification affects peptide interactions within the SH3 binding pocket and influences the stability and kinetics of the bound state. Our simulation results show that the capped Sos peptide exhibits a longer unbinding time than the uncapped peptide, indicating a longer residence within the SH3 binding pocket. To understand the molecular basis of this difference, we analyze specific residue-peptide interactions within the binding pocket and characterize how they evolve during dissociation. These findings highlight how terminal capping can modulate protein-peptide residence time and provide molecular-level insights into the design of SH3-targeting peptides with tunable binding kinetics.

SWRM 2026 SW632

Conformational equilibrium of geldanamycin and its reduced hydroquinone form in aqueous solution: A DFT and MD study

***Yubo Fan**, yubofan@hotmail.com. Mathematics and Sciences, Brazosport College, Lake Jackson, Texas, United States*

Two distinct conformations of geldanamycin (GM) have been identified: a *cis*-amide form when bound to Hsp90 and a *trans*-amide form in the solid state. The reduced hydroquinone derivative, GMH_2 is known to bind Hsp90 with approximately 40-fold higher affinity. To understand this enhancement, we assessed the conformational stability of GM and GMH_2 using various DFT methods and explored their free energy landscapes in aqueous solution via enhanced-sampling molecular dynamics. Our simulations show that the *trans*-conformer is the most abundant GM species in water, matching the solid-state geometry, while both *cis*- and *trans*-conformations reported in crystal structures were accessible during sampling. In terms of relative stability, the *cis*-conformer of GM is 2.1 kcal/mol higher in energy than the *trans*, whereas the difference narrows to 1.0 kcal/mol for GMH_2. DFT calculations further support these trends, with *trans*-GM favored by 1.2–2.5 kcal/mol, while the *cis*-form of GMH_2 becomes slightly favorable, with free energies ranging from 0.15 to –1.03 kcal/mol. Consequently, the equilibrium population of the *cis*-conformer rises significantly upon reduction: from just 1.4–11.1% for GM to 15.4–85.0% for GMH_2, representing a 6.1- to 80.6-fold increase in Keq. Interestingly, umbrella sampling simulations of ligand unbinding from Hsp90 indicated similar free energy barriers for both GM and GMH_2. Taken together, our findings suggest that the enhanced

binding affinity of GMH_2 is not due to a difference in the binding pathway, but rather to the thermodynamic stabilization and increased population of its bioactive *cis*-conformer under reducing cellular conditions.

SWRM 2026 SW633

Unraveling mutation-driven changes in barnase-barstar dissociation kinetics through full atomistic simulations

***Dipesh Shrestha**, dipeshshrestha@my.unt.edu, Omar Valsson. Chemistry, University of North Texas, Denton, Texas, United States*

Protein-protein interactions are essential for normal cellular functions; however, small disruptions in these interactions, which are often caused by mutations, may lead to the progression of several diseases including cancer and neurodegenerative diseases. Understanding how these interactions behave and how mutations alter them is therefore critical for uncovering disease mechanisms and for guiding the design of protein-based therapeutics. Studies show that the residence time $\tau = 1/ koff$, which reflects how long a complex remains bound before dissociation, is a more reliable predictor of pharmacological activity than binding affinity alone. Barnase-Barstar is among the most tightly bound protein-protein complex, exhibiting the wild-type residence time of ~2.4-75 hours. Remarkably, a single mutation at the binding interface can shorten this hour-long residence time to seconds. Accurately predicting how a single mutation alters the koff remains a major challenge using atomistic simulations. Here, we employ atomistic simulations in conjunction with metadynamics to study the dissociation kinetics of the Barnase-Barstar complex and its mutants, and we validate our findings by comparing with available experimental results. Our simulations show excellent agreement with experimental results, demonstrating that the combination of atomistic simulations with enhanced sampling methods can reliably capture the effects of mutations on dissociation kinetics in complex biomolecular systems. In addition, we also aim to see the effects of force-field and water model in this protein-protein complex. Our findings on the Barnase-Barstar complex and its mutants provide insights that extend beyond this specific protein-protein complex. The development of protein-based therapies such as antibodies that bind strongly to their target, is becoming more common. Understanding the dissociation kinetics is therefore crucial and evaluating the effects of mutation on dissociation kinetics helps in the design of effective therapeutics.

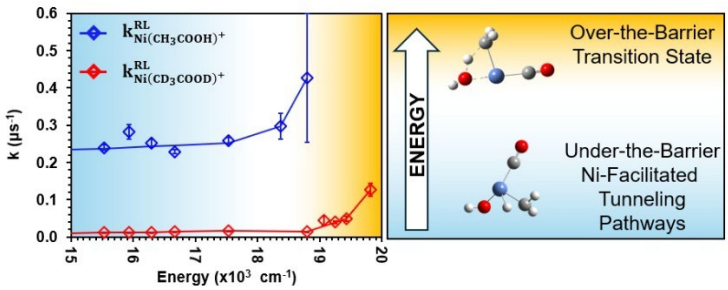
SWRM 2026 SW634

Unusual deep tunneling properties promoted by the Ni^+ cation in the dissociative rearrangement reaction of CH_3COOH and its deuterium labeled isomers

***Darrin J. Bellert**, darrin_bellert@baylor.edu. Chemistry, Baylor University, Waco, Texas, United States*

Quantum mechanical tunneling (QMT) is the penetration of a transition barrier by a reacting population. Here, the single photon initiated dissociative rearrangement reaction (SPIDRR) technique, developed at Baylor University, is used to measure energy-resolved reaction rate constants in the bare $Ni^+ + CH_3COOH$ gas-phase reaction. Hydrogen QMT (H -QMT) is identified in two ways in this study: (i) through measurements of a large hydrogen / deuterium kinetic isotope effect (H/D KIE = 19.0 ± 3.2) and (ii) by monitoring the reaction kinetics over an energy range where the controlling

dynamics change from under barrier (H-QMT) to over-barrier (RRKM statistics). The potential energy surface for this reaction is calculated using B3LYP with the def2-tzvp basis set. Most structures are single point energy corrected at the CASSCF/CASPT2 (9,8) level and used to guide interpretations. There are several surprising reaction properties measured in this study and presented here. (i) There is a near energy independence in the rate constants measured at energies where H/D -QMT dominates the reaction. And (ii), both C-H and O-H bond activation occurs in this low-energy reaction. These observations are discussed.



Reaction rate constants plotted against their measured energies in the Ni^+ promoted decomposition of CH_3COOH.

SWRM 2026 SW635

From lipid composition to reactivity: Molecular simulation of olefin accessibility in wastewater-grown *Yarrowia lipolytica*

***Esau Obuong**, c00543930@louisiana.edu. Chemical Engineering, University of Louisiana at Lafayette, Lafayette, Louisiana, United States*

Wastewater-grown oleaginous yeasts provide renewable unsaturated lipids for production of value-added chemicals through oxidative cleavage. However, precursor abundance may not directly translate into product formation when unsaturated acyl chains are embedded within complex microbial lipid environments. This study integrates experimental lipid characterization and molecular modeling to investigate whether molecular accessibility of C18:1 olefinic sites helps explain nonanoic-acid formation from wastewater-grown *Yarrowia lipolytica*. Across two wastewater-based cultivation conditions, mean total C18:1 concentrations increased from 63.2 to 198.8 μg/mL, approximately 3.1-fold, whereas mean nonanoic-acid concentrations following direct ozonolysis increased only from 8.65 to 10.39 mg/L. This non-proportional response suggests that bulk precursor abundance alone may not fully describe reactive availability within the microbial lipid phase. Experimentally determined fatty-acid profiles were therefore used to reconstruct condition-specific triacylglycerol ensembles representative of intracellular lipid composition. Molecular simulations are used to quantify olefin exposure, local molecular organization, and accessibility of unsaturated acyl chains. These accessibility descriptors are compared with experimentally measured nonanoic-acid formation to determine whether lipid organization provides predictive information beyond C18:1 concentration alone. This integrated experimental-computational framework provides a mechanistic basis for understanding oxidative conversion of microbial lipids and guiding renewable feedstock design for sustainable nonanoic-acid production.

SWRM 2026 SW636

First-principles investigation of surface functionalization in MXenes

Michelle Becerra[1]*, miquimouse@icloud.com, Cormac Toher*[2,1]*. (1) Department of Chemistry and Biochemistry, The University of Texas at Dallas School of Natural Sciences and Mathematics, Richardson, Texas, United States(2) Department of Materials Science and Engineering, The University of Texas at Dallas Erik Jonsson School of Engineering and Computer Science, Richardson, Texas, United States*

Ever-increasing amounts of carbon dioxide (CO_2) are being expelled into the atmosphere with potentially dire environmental consequences. One method to reduce atmospheric CO_2 is carbon capture, specifically post-combustion adsorption, which captures CO_2 from a single source, removing it from the air. In order to capture efficiently, an adsorption material with properties like preferential adsorption of CO_2 and non-activated charge transfer is required. 2D early transition metal carbides and nitrides known as MXenes are investigated as an effective sorbent material thanks to their diverse composition, chemically active surface functionalizations and overall versatile and tunable nature. The computational characterization of MXene surface functionalizations are being systematically explored through calculated adsorption energies from density functional theory (DFT) as well as material optimization via machine learning (ML) methods. Molecules and surfaces being modeled so far are: pristine surfaces (Ti_3C_2, Mo_3C_2), native surface functional groups (F, O, OH, Cl and H) and the interactions between them. Initial characterizations have shown that when adsorbing to a pristine Ti_3C_2 surface, single ions of F, O, OH, Cl and H all preferred binding to hollow sites. Pristine Mo_3C_2 with single ion adsorbates F, O and H also favored hollow sites, but OH and Cl preferred bridge sites. The characterizations and MXene designs generated by this research will not only fill in the divide between MXenes and carbon capture, but also unite industries and our environment through more accessible carbon capture methods.

SWRM 2026 SW637

Diagnosing and remediating failure modes of machine-learned interatomic potentials in reactive nitromethane decomposition

Cary Darwin*, cxd190027@utdallas.edu, Jan Dunal, Steve O. Nielsen. Chemistry and Biochemistry, The University of Texas at Dallas, Richardson, Texas, United States*

Machine-learned interatomic potentials (MLIPs) reproduce quantum-mechanical forces at a fraction of the cost, but their failure modes in reactive chemistry remain uncharacterized. Herein, we describe a diagnostic benchmark of five MLIPs; MACE-OFF23, MACE-Osaka24, MACE-OMOL, UMA-S-1P1, and ANI-1xnr on the thermal decomposition of condensed-phase nitromethane, emulating the protocol of a published reactive force-field study (Han et al.) and combining model-neutral starting structures, rigid bond-pull scans, and coupled-cluster reference energies. Our results demonstrate that each model fails for a distinct, localizable reason, and that this attribution determines what repair, if any, is possible: ANI-1xnr under-binds dissociation by as much as 50 kcal/mol, an error corrected by retraining against quantum-chemical dissociation curves; MACE-Osaka24's instability is gated by screened nuclear repulsion; and the spurious 27 kcal/mol rise shared by MACE-OMOL and UMA-S-1P1, traced by systematic ablation to a single per-system spin label, cannot be repaired by additional data. These findings provide a general strategy for evaluating reactive potentials in which failures are attributed to model components rather than ranked by error.

SWRM 2026 SW638

How well do classical water models capture orientation-dependent hydrogen bonding? A HEALPix benchmark against quantum mechanics

***Laxmi Pandey**, lakshupandey20@gmail.com. Chemistry, Oklahoma State University, Stillwater, Oklahoma, United States*

Classical water models are fit to reproduce bulk properties; density, diffusion, dielectric constant but not the orientation-dependent interaction energy that actually governs how two water molecules approach and hydrogen-bond. We test that gap directly. Fixing a rigid water dimer at an O–O separation of 2.8 Å, we sample 192 orientations uniformly over the sphere using a HEALPix grid and compute the interaction energy at every orientation with five classical water models (SPC/E, TIP3P, TIP4P/2005, TIP4P/Ice, TIP5P) and, as quantum references spanning a range of theoretical accuracy, AM1, HF, B3LYP, MP2, and CCSD(T). Rather than comparing only the hydrogen-bonded minimum, we score each classical model against the full orientational surface at every level of theory. Across the quantum mechanical model CCSD(T), TIP5P consistently reproduces the orientational interaction surface most closely, while the other classical models show larger and more orientation-dependent deviations. These results give a direct, quantitative framework for identifying which widely classical water model best captures quantum mechanical hydrogen-bonding behavior across orientations, and where each model's approximations break down.

SWRM 2026 SW639

Molecular docking and dynamic simulation analysis of NADH binding to bovine myoglobin at pH 5.6

***Greeshma Sreejesh**[1], greeshma.sreejesh@okstate.edu, Prabir Kumar Gharai[1], Surendranath Suman[2], morgan Pfeiffer[1], Gretchen G Mafi[1], Ranjith Ramanathan[1]. (1) Department of Animal and food Sciences, Oklahoma State University Division of Agricultural Sciences and Natural Resources, Stillwater, Oklahoma, United States(2) Department of Animal and food Sciences, University of Kentucky Martin Gatton College of Agriculture Food and Environment, Lexington, Kentucky, United States*

The US beef industry loses approximately $3.7 billion annually due to beef discoloration. Postmortem muscle is biochemically active, and pathways related to myoglobin redox state remain functional. Myoglobin can exist in three different forms, such as oxy-, deoxy-, and metmyoglobin forms, with each form imparting unique color to beef. Nicotinamide adenine dinucleotide in its reduced form (NADH) plays important roles in the biochemical processes occurring in postmortem muscle. NADH contributes to meat color stability by providing reducing power for the conversion of metmyoglobin, in which heme iron is in the ferric (Fe^{3+}) state, to deoxy- or oxymyoglobin containing ferrous (Fe^{2+}) iron through enzymatic and cofactor-mediated pathways. Despite its established importance in these processes, the molecular interaction between NADH and myoglobin remains poorly characterized. Computational molecular docking provides an approach to predict potential ligand–protein interactions and identify energetically favorable binding regions within the myoglobin structure. Therefore, the objective of this study was to use molecular docking to characterize the interaction of NADH with a homology-modeled bovine myoglobin structure at pH 5.6 and to identify potential NADH-binding regions within or near the heme pocket. Oxymyoglobin structures at pH 5.6 were prepared by protonation of the protein using the APBS web server. The heme group (HEM) and bound oxygen molecule (OXY) were incorporated into the protonated protein structures and

converted from PDB to PDBQT format using Meeko. Non-polar hydrogens were merged, partial charges assigned, and the prepared structures were used as rigid receptors for docking. Molecular dynamics simulations were performed using GROMACS to evaluate complex stability. PLIP analysis showed that NADH binding was stabilized by hydrogen-bonding and hydrophobic interactions with residues near the heme pocket, including LYS63, ASN66, THR67, THR70, LEU89, and SER92. During the 10 ns simulation, the protein remained stable, and NADH stayed associated with the heme-adjacent region. These findings support the suitability of the selected complex for further structural analysis of the trajectory and subsequent longer-timescale (200 ns) molecular dynamics simulations to evaluate the persistence of protein–ligand interactions and long-term conformational stability.

SWRM 2026 SW640

Molecular drivers of asphaltene aggregation: Evaluating the role of persistent radicals and molecular architecture through computed dimerization energies

Gretel A. Stokes*, gretel.jordan@tcu.edu, Benjamin G. Janesko. Chemistry and Biochemistry, Texas Christian University, Fort Worth, Texas, United States*

Asphaltenes, the heavy aromatic fraction of crude oil, readily aggregate and contribute to equipment fouling during petroleum production and refining. Although asphaltenes contain a small population of persistent organic radicals, whether these species drive aggregation remains unresolved. Recently, single-molecule atomic force microscopy (AFM) measurements have provided molecular structures of individual asphaltenes, enabling this hypothesis to be tested directly through computational dimerization studies. Here, we examine the initial step of aggregation by evaluating dimerization across a library of AFM-derived asphaltene structures from steam-cracked tar, coal-derived asphaltene, and petroleum pitch. Conformational sampling and dimerization energies were computed for 903 unique dimers using CREST with the GFN2-xTB method, with selected structures further evaluated using dispersion-corrected, spin-symmetry-broken density functional theory. Open-shell—open-shell dimers formed a small population of exceptionally strongly bound complexes, in some cases exhibiting covalent-like interactions with approximately twice the dimerization energy of closed-shell dimers. In contrast, open-shell—closed-shell interactions were not systematically stronger than closed-shell dimers. Because persistent radical species constitute only ~1-2% of asphaltenes, radical-radical encounters are intrinsically rare, limiting their contribution to bulk association despite their enhanced stabilization. Across the broader library, similar energy distributions were observed among the three feedstocks, while molecular architecture—so-called island, archipelago, and aryl-linked motifs—significantly influenced stabilization. Island-island dimers exhibited the strongest average interactions among closed-shell systems, consistent with favorable aromatic surface complementarity. Furthermore, homodimers exhibited modestly higher dimerization energies than heterodimers, whereas no systematic relationship was observed between molecular weight and mass-normalized dimerization energy. Together, these results refine the role of radical species in asphaltene aggregation: exceptionally strong radical-radical interactions may contribute to nucleation, but the broader initial association of asphaltenes is dominated by molecular architecture and geometric complementarity rather than radical character alone.

SWRM 2026 SW641

Electronic stopping power and nonlinear lattice response in Sr-doped halide perovskites

***Mario Borunda**, mario.borunda@okstate.edu. Physics, Oklahoma State Regents for Higher Education, Stillwater, Oklahoma, United States*

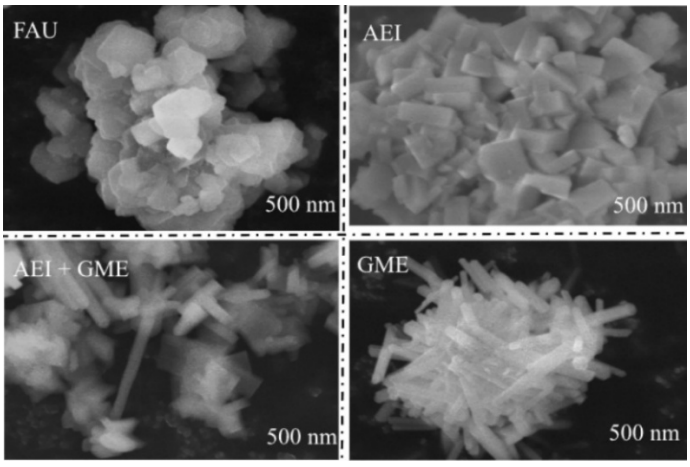
Evaluating the radiation tolerance of hybrid halide perovskites requires accurate models of electronic stopping power (S_e) and non-adiabatic energy dissipation. Using time-dependent density functional theory (TD-DFT) alongside empirical SRIM calculations, we investigated the S_e of hydrogen projectiles traversing pristine $FAPbI_3$ and Sr-doped$FA(Pb_{0.875}Sr_{0.125})I_3$. For unchanneled trajectories, both methodologies confirm that 12.5% Sr substitution preserves the bulk S_e. However, simulations on channeled trajectories reveal a complex, localized radiation-response that is obscured by the bulk averaging. By evaluating atomic forces, we demonstrate that structural buckling intrinsic to the Sr-doped lattice modulates localized energy transfer.

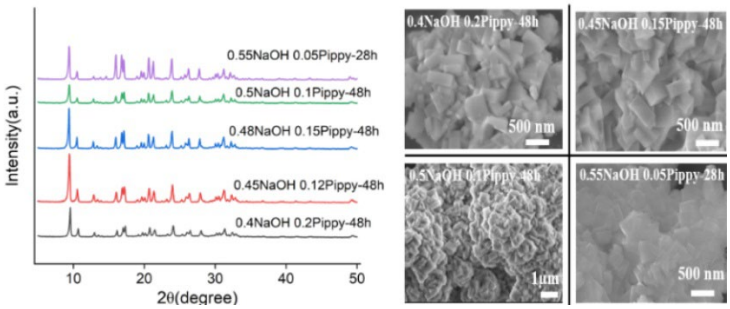
SWRM 2026 SW642

Expanding the synthetic scope of AEI zeolite by rational control of organic-inorganic structure directing agents

***Ivan Garcia**, garcia.ivan4214@gmail.com. University of Houston, American Chemical Society, Houston, Texas, United States*

The synthesis of AEI zeolite was investigated through rational control of the structure-directing agent and synthesis composition. AEI zeolite was prepared from two structurally similar but chemically distinct organic molecules, and the influence of NaOH content on phase selectivity and material properties was examined. The results showed that NaOH content strongly affects phase formation, while pH also plays a significant role in determining selectivity. A clear relationship was observed between textural properties, including total BET surface area and micropore volume, and the relative amount of structure-directing agent in the gel. In addition, AEI zeolite was successfully synthesized with a very low amount of organic material and a shortened crystallization time. Overall, these findings demonstrate that the total and relative amount of NaOH are critical parameters for controlling the crystallization of AEI zeolite and expanding its synthetic scope.





SWRM 2026 SW643

Quasi-reversible sodium insertion into a copper benzenehexathiol framework

***Ovie Soman**, oviesoman@utexas.edu, Michael L. Aubrey. Chemistry, The University of Texas at Austin, Austin, Texas, United States*

Copper benzenehexathiol ($Cu_3C_6S_6$) has garnered attention among π-d conjugated extended solids for its room-temperature metallicity, superconductivity, and non-van der Waals structure and has been investigated for its Li^+ storage properties. Consequently, it has been proposed as a candidate for lithium-ion battery cathodes due to its considerable reversible capacity and high cycling stability. However, due to the lower geographical abundance and higher costs of raw materials for lithium-ion batteries, sodium-ion batteries are fast emerging as a more sustainable long-term energy storage alternative. This work aims to shed light on the potential use of $Cu_3C_6S_6$ in sodium-ion batteries and to lead to the discovery of new metastable sodiated phases with diverse electronic properties. The theoretical specific capacity of this framework is on par with that of Prussian blue analogues and layered oxides, which are leading sodium-ion cathode candidates. 3 Na^+ per formula unit can theoretically be inserted into $Cu_3C_6S_6$, and we achieved near-stoichiometric insertion electrochemically. The reversibility of electron transfer was probed through galvanostatic cycling; the first equivalent of Na^+ inserted was not fully reversible. However, the reversibility increased from 0.5 inserted equivalents to 2.2 inserted equivalents. We attribute the overall poorer reversibility observed for Na^+ compared to Li^+ to its larger ionic radius, which exerts greater strain on the host lattice. The first inserted equivalent thus compels more extensive framework expansion, potentially causing a phase change in the host framework. Consequently, the newly widened channels for ion diffusion into the lattice would enable higher reversibility up to 2.2 inserted equivalents. A still greater insertion extent sees a drop in reversibility, indicating another potential phase transformation. Insertion was also performed chemically using sodium naphthalenide as the reductant. Elemental mapping confirmed the prevalence of sodium throughout the material, with approximately 2.34 Na^+ per formula unit. These results demonstrate Na^+ insertion into the $Cu_3C_6S_6$ framework and lay a foundation for investigations into the use of conjugated thiolate coordination solids for sodium-based charge storage.

SWRM 2026 SW644

Microcanonical kinetics reveal competing reaction pathways and hydrogen tunneling in cobalt mediated activation of acetic acid

***Simon Okafor**, simon_okafor1@baylor.edu. Chemistry & Biochemistry, Baylor University, Waco, Texas, United States*

Understanding how transition-metal catalysts activate strong chemical bonds is essential for developing more efficient catalytic processes for energy conversion and sustainable chemical manufacturing. Here, we investigate the gas-phase reaction of cobalt with acetic acid using State-Prepared Ion Dissociation Dynamics by Delayed Radiative Recombination (SPIDRR), which enables direct measurements of microcanonical unimolecular kinetics over a well-defined range of internal energies. Time-dependent product formation was analyzed using a reduced kinetic model that accounts for competing reaction pathways and branching between the cobalt methanol and cobalt ketene product channels. The measured energy-dependent rate constants reveal distinct kinetic behavior that cannot be explained by a single classical reaction pathway. Comparison of hydrogen and deuterium isotopologues shows a small kinetic isotope effect consistent with efficient hydrogen transfer despite isotopic substitution. The observed kinetics are discussed in terms of competing reactive populations, nonclassical hydrogen-transfer dynamics, and possible contributions from hydrogen tunneling and two-state reactivity. These results provide new mechanistic insight into transition-metal-mediated C-H and O-H bond activation and demonstrate the capability of SPIDRR to probe complex gas-phase catalytic reaction dynamics with high energy resolution.

SWRM 2026 SW645

Rational molecular engineering of mixed alkynyl-phosphine interfaces in atomically precise Au and Au-Cu nanoclusters

***Ayomide Oladele**, aoladele@smu.edu, Anindita Das. Chemistry, Southern Methodist University, Dallas, Texas, United States*

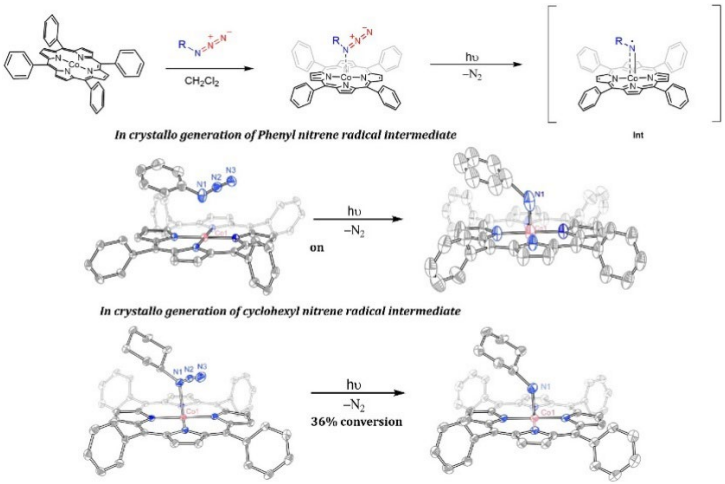
Size-dependent polydispersity of metal nanoparticles has long made it difficult to establish a clear picture of how their structure relates to their properties. Atomically precise metal nanoclusters, a well-defined system with definite number of metal atoms and protective ligands, has opened a way to study these relationships at a much finer resolution. Gold Nanoclusters have become very important as model systems due to their stability, well defined geometries, and tunable optical and electronic properties. Most work around this area has been focused on clusters protected by a single class of ligands, such as thiolates, phosphines, or alkynyls. Clusters protected by two different ligand types on the same metal surface, particularly alkynyls and phosphines, remain less studied. The inclusion of two chemically distinct coordination environments on a single cluster surface opens the possibility of cooperative ligand effects that could reshape electronic structure, redox behavior, and catalytic selectivity. In the poster, we present our efforts toward the rational design and synthesis of gold and gold-copper nanoclusters featuring mixed alkynyl-phosphine protecting shells. Using well-defined molecular precursors as building blocks, we explore how ligand identity and reaction conditions influence cluster nucleation, composition, and stability. Preliminary spectroscopic characterization suggests the formation of discrete cluster species distinct from previously reported all-alkynyl or all-phosphine analogues. Ongoing work aims to establish design principles for controlling the stability, electronic structure, and reactivity of these mixed-shell nanoclusters, with an eye toward their potential application in electrocatalysis and beyond.

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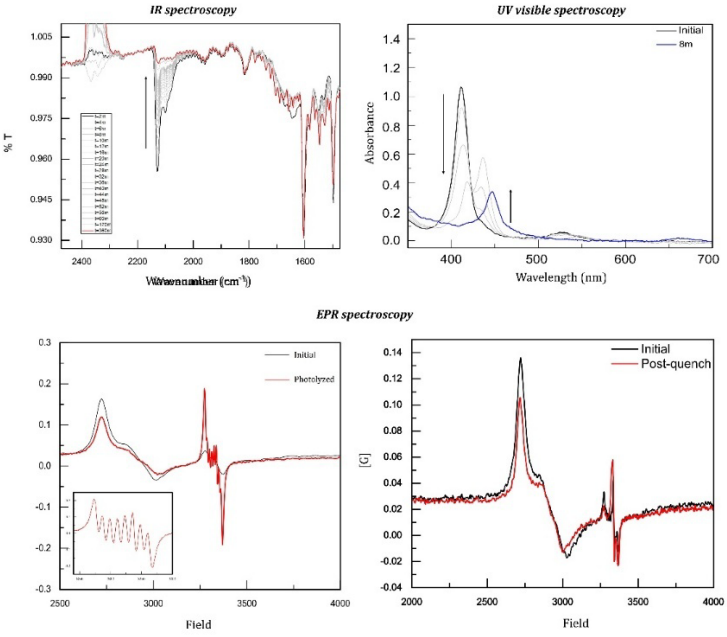
***In-crystallo* and matrix-isolated spectroscopic observations of catalytically relevant Co(III) porphyrin-nitrene intermediates**

***Subham Sarkar**, sarkarsubhu98@gmail.com. Chemistry, Texas A&M University System, College Station, Texas, United States*

Azides are ubiquitous nitrene precursors in C–H amination chemistry and are often used in conjunction with metal porphyrin catalysts. In particular, Co(II)-porphyrins are widely used catalysts for C–H amination, which is proposed to proceed via a reactive nitrene-radical intermediate. The existence of this intermediate has been shown through spectroscopic techniques, however the characterization of the nitrene intermediate has eluded crystallography. Part of the problem lies with the binding of weak donor azides on weak onto the metallo-porphyrin system, as well redox non-innocence of the metallo-porphyrins that can cause unwanted side-reactions with the azides. We show that when phenyl-azide-bound crystals of Co-porphyrin are photolyzed, extrusion of dinitrogen is observed along with the generation of phenyl nitrene-radical type intermediate. Formation of this intermediate is accompanied by the oxidation of Co(II) to Co(III). This observation is further supported by further spectroscopic studies including IR, UV-vis and EPR, confirming the photo-generation of the nitrene intermediate.



In crystallo observation of nitrene intermediate



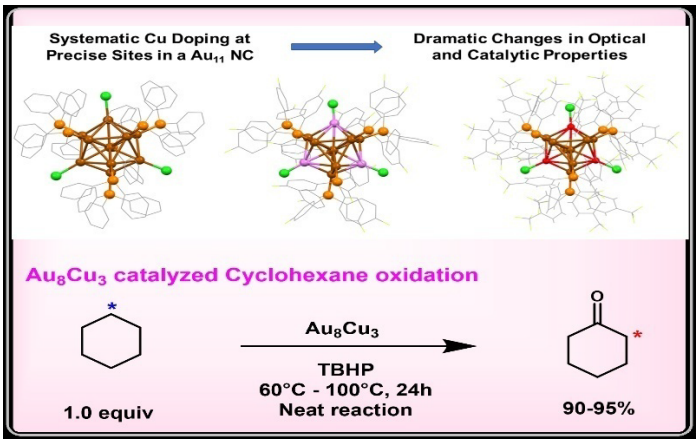
Spectroscopic observation of intermediate

SWRM 2026 SW647

Site-selective Cu doping of Au nanoclusters: Tunable optical properties and mechanistic insights into Au-Cu catalysis

Nagaraju Vodnala, *nagaraj.chem1@gmail.com, Anindita Das. Chemistry, Southern Methodist University, Dallas, Texas, United States*

Atomically precise alloy nanoclusters are good functional models for investigating multimetallic cooperativity in catalytic studies. In this study, a well-studied phosphine-protected Au_{11} nanocluster system was chosen to systematically incorporate up to 3 Cu atom dopants yielding atomically precise $Au_8Cu_3((p\text{-}CF_3Ph)_3P)_7Cl_3$ (Au_8Cu_3) and $Au_{9.4}Cu_{1.6}((p\text{-}FPh)_3P)_7Cl_3$ ($Au_{9.4}Cu_{1.6}$) alloy nanoclusters. Single-crystal X-ray crystallography reveals these nanoclusters to be structurally akin to the previously reported monometallic $Au_{11}(PPh_3)_7Cl_3$ (Au_{11}) nanocluster. Herein, the nanoclusters exhibit an incomplete icosahedral metal core where the surface Au atoms are protected by phosphines while the Cu atoms exclusively bind with chloride ligands. While the optical properties of the $Au_{9.4}Cu_{1.6}$ are found to be like the parent Au_{11} nanocluster, the absorption spectrum of the Au_8Cu_3 is drastically different as three Cu atoms are precisely exchanged for Au at three equivalent positions in the nanocluster core that are interchanged by a C_3 rotation. In this specific motif, Cu-doped nanoclusters are further found to efficiently catalyse the challenging oxidation of cyclohexane with high selectivity to form cyclohexanone. Interestingly, the monometallic Au_{11} nanocluster is found to exhibit greatly reduced catalytic activity in this reaction, further underscoring the significance of catalytically active Cu sites on the nanocluster surface. This is further corroborated by the fact that the Au_8Cu_3 nanocluster exhibits higher catalytic efficiency (up to ~95% conversion) as a solvent-free solid catalyst than the $Au_{9.4}Cu_{1.6}$ nanocluster with less Cu content.



SWRM 2026 SW648

Synthesis of gold-copper alloy nanocluster frameworks

Joshua T. Plank, *jplank@mail.smu.edu. Chemistry, Southern Methodist University, Dallas, Texas, United States*

Atomically precise metallic nanoclusters present a wide range of applications, including bioimaging, catalysis, and energy storage; however, with careful choices of ligands, it is possible to create larger nanostructures from nanoclusters. Ligands such as 4-(diphenylphosphino)benzoic acid and tris(2-carboxyethyl)phosphine can coordinate nanoclusters while maintaining free functionality for producing

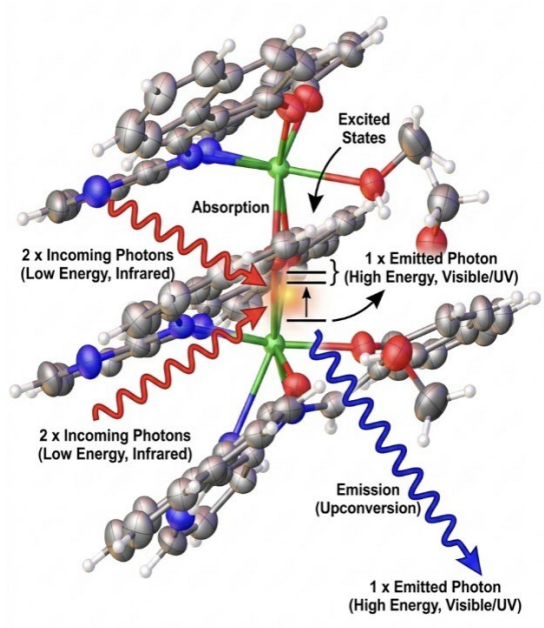
larger assemblies. We herein present novel framework materials consisting of gold/copper alloyed nanoclusters linked via the coordination of free carboxylate groups with metal ions. Said frameworks present an exciting new platform for both catalysis and storage of hydrogen gas.

SWRM 2026 SW649

Pyridyl and naphthylpyrasal lanthanide(III) complexes and their upconversion

Pooja Dogra[1], *pooja.dogra@ttu.edu, Jessica Q. Wallace*[2], *John Gorden*[1], *Jorge Monteiro*[3], *Ana de Bettencourt-Dias*[2], *Anne E. Gorden*[1]. *(1) Chemistry, Texas Tech University, Lubbock, Texas, United States(2) Chemistry, University of Nevada Reno, Reno, Nevada, United States(3) Chemistry, California State Polytechnic University Humboldt Bookstore, Arcata, California, United States*

Pyridyl and naphthylpyrasal tetradentate Schiff base ligands and their 3:2 ligand-to-metal ratio Ln(III) complexes exhibiting strong two-photon upconversion in solid state and solution have been synthesized and characterized. The isolated metal complexes include homobimetallic, heterobimetallic sandwich type complexes and their sulfonate incorporated water-soluble analogs, containing Er(III), Yb(III), Y(III) ions or their combination. Structural characterization was performed using FT-IR, high-resolution mass spectrometry, elemental analysis, and X-ray diffraction to confirm the formation of these complexes. Photophysical characterization through 980 nm laser excitation revealed Er(III)-centered upconversion in both solid-state and aqueous solution. The effect of ligand donor structure on the lanthanide emission and upconversion behavior of these complexes was analyzed. The π-π ligand interactions and shorter M-M bond distances in these complexes were observed to facilitate the energy transfer between Ln(III) ions through antenna effect. The incorporation of sulfonate groups in the complexes enhanced their solubility in water and other organic solvents, making them suitable for biological applications particularly for diagnosing diseases like cancer in living organisms. This study has laid the foundation of new lanthanide-based molecular systems which can be further improvised by controlling the coordination chemistry, and physical properties through ligand design and synthesis.



Two-photon upconversion in pyridyl naphthylsalophen Ln(III) complex

SWRM 2026 SW650

Synthesis and spectroscopic characterization of mono-ruthenium complexes with chiral thione ligands

Carla Hyppolite[1]*, carla.hyppolite@tsu.edu,* ***Vivian Tran***[1]*, v.tran5849@student.tsu.edu,* ***Phaith Harris***[1]*, p.harris3378@student.tsu.edu,* ***Bukuo Ni***[2]*, Bukuo.Ni@etamu.edu,* ***Tuan Phan***[1]*, tuan.phan@tsu.edu. (1) Chemistry, Texas Southern University College of Science Engineering and Technology, Houston, Texas, United States(2) Chemistry, East Texas A&M University, Commerce, Texas, United States*

Ruthenium complexes bearing chiral ligands have attracted considerable interest because of their potential applications in catalysis, medicinal chemistry, and asymmetric synthesis. In this study, mono-ruthenium complexes containing the chiral thione ligands (R)-4-benzylthiazolidine-2-thione (RBOT) and (S)-4-benzyloxazolidine-2-thione (SBOT) were synthesized through ligand substitution reactions. Reactions were conducted under different solvent conditions, with and without dichloromethane, to investigate the effects of solvent on reactant solubility, reaction efficiency, and product formation. The synthesized complexes were characterized using attenuated total reflectance Fourier-transform infrared (ATR-FTIR) spectroscopy, UV–Visible spectroscopy, mass spectrometry, melting-point analysis, and solubility studies. ATR-FTIR and UV–Visible spectra showed characteristic changes consistent with coordination of the chiral thione ligands to the ruthenium center, while mass spectrometric analysis supported the formation of the $Ru(PPh_3)_2(RBOT)_2$ complex. Ongoing work focuses on optimizing synthetic conditions, improving product isolation and purification, and further elucidating the structural and coordination properties of these ruthenium complexes. This research was supported by the National Science Foundation under Award No. 2400179.

SWRM 2026 SW651

Design and synthesis of symmetric β-oxo-δ-diimine (BODDI) ligands with tunable steric and electronic properties for aluminum and zinc catalysts

Bhawana Khatri*, bhawana.khatri@ttu.edu, Azmain Talukder, Anastacio Pando, John Gorden. Chemistry and Biochemistry, Texas Tech University, Lubbock, Texas, United States*

Ligand design plays a central role in controlling the stability and reactivity of main-group complexes. We report a modular library of β-oxo-δ-diimine (BODDI) ligands featuring systematic functionalization of ancillary N-substituents to tune electronic donation and steric environment around the (N,O,N) donor framework. This approach enables targeted variation of inductive and conformational effects, providing a platform for evaluating how these changes influence the coordination behavior, stability, and catalytic potential of aluminum and zinc BODDI complexes. The presentation will discuss representative Al and Zn systems, highlighting how ligand-based electronic and steric tuning shapes reactivity patterns and supports the development of new main-group catalytic transformations.

SWRM 2026 SW652

Beyond the primary coordination sphere: Tellurium–metal interactions in Cu(I) and Au(I) complexes

***Nishita Deb**, nxd3516@mavs.uta.edu, Gyeongjin Park. Chemistry & Biochemistry, The University of Texas at Arlington, Arlington, Texas, United States*

Secondary interactions are increasingly recognized as powerful tools for controlling the structure, reactivity, and excited-state behavior of transition-metal complexes. Among these, interactions involving heavy chalcogens are particularly attractive because their high polarizability, variable oxidation states, and strong spin–orbit coupling can introduce electronic effects. Herein, we exploit these features through N-heterocyclic carbene (NHC)-functionalized tellurium ligands designed to position tellurium near Cu(I) and Au(I) centers without disrupting their primary coordination environments. Structural, spectroscopic, and computational studies reveal distinct modes of Te-M electronic communication in the Cu(I) and Au(I) complexes, highlighting the ability of tellurium to engage coinage-metal centers through different secondary interactions. These interactions are also associated with enhanced catalytic performance in Au(I)-catalyzed alkyne hydroamination. Moreover, incorporation of tellurium into carbene–metal–amide complexes substantially alters their excited-state behavior, demonstrating the broader influence of secondary Te-M interactions on photophysical properties. This work highlights the potential of heavy-chalcogen interactions as a design strategy for controlling transition-metal chemistry beyond the primary coordination sphere.

SWRM 2026 SW653

Separation of molybdenum from other fission fragments by using a phase transfer agent

***Ashirafu "Ash" Tuyishime**, axt21l@acu.edu, Diego F. Zometa Paniagua. NEXT Lab, Abilene Christian University, Abilene, Texas, United States*

The Nuclear Energy eXperimental Testing Laboratory (NEXT Lab) mission is to provide solutions to the world’s need for energy, water, and medical isotopes by advancing the technology of Molten Salt Research Reactors while educating future leaders in nuclear science and engineering. In order to do so, NEXT Lab is assembling a Molten Salt Research Reactor (MSRR). NEXT Lab seeks to study chemical methods to identify and purify useful radioisotopes, such as molybdenum-99, that are products of fission reactions. NEXT Lab will collect gaseous and solid samples from the reactor. The samples produced from the reactor will hold hundreds of fission fragments; therefore, a critical step is to develop a technique to selectively capture elements of interest. The focus of this project is on molybdenum isolation, which is achieved with the utilization of a phase transfer agent. The agent is dissolved in an organic solvent of choice that is immiscible with water, which is then added to an aqueous solution containing molybdate, resulting in the formation of a bilayer. In this bilayer system, the agent interacts with molybdate, forming a complex and pulling the organic phase. Each phase is characterized using an Inductively Coupled Plasma-Mass Spectrometer (ICP-MS) and a UV-Visible (UV-Vis) spectrometer, confirming the migration of molybdate into the organic phase and evidence of a complex formed. To recover molybdenum to an aqueous phase, the organic solution is treated with a stripping agent of choice, thereby returning molybdate to an aqueous solution. Confirmation using ICP-MS and UV-Vis requires the solution to be in an aqueous solution. The molybdate-containing organic solution was treated with a stripping agent. This reduced the solubility of Mo in the organic phase, recovering it in the aqueous phase. Characterization of the recovered aqueous phase with ICP-MS and UV-Visible spectroscopy

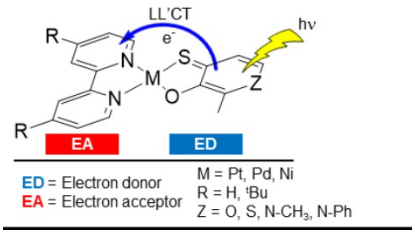
confirmed the movement of molybdate from the organic phase to the aqueous phase. The molybdate is then concentrated and carried in an acidic alumina column.

SWRM 2026 SW654

Ligand-to-ligand charge transfer (LL'CT) transitions in square-planar metal-bipyridyl complexes of heteroatom-substituted maltol derivatives

Muhammad Ahsan Usman[1]*, muhammadahsan_usman1@baylor.edu, Patrick J. Farmer*[1]*, Mohammad A. Omary*[2]*, Kevin L. Shuford*[1]*. (1) Chemistry and Biochemistry, Baylor University, Waco, Texas, United States(2) Chemistry, University of North Texas System, Denton, Texas, United States*

A series of square-planar d^8-metal complexes that exhibit ligand-to-ligand' charge-transfers (LL'CT) is reported, featuring bipyridines as acceptors and α-hydroxy-thiopyrone (i.e., thiomaltol) derivatives as donors. Eleven complexes of the general formula $[M(bpy)L]^+$ were synthesized, where M = Ni(II), Pd(II), or Pt(II); bpy = 2,2′-bipyridine or 4,4′-bis(tert-butyl)-2,2′-bipyridine; and L = 3-hydroxy-2-methyl-4H-pyran-4-thione, 3-hydroxy-2-methyl-4H-thiopyran-4-thione, 3-hydroxy-1,2-dimethylpyridine-4(1H)-thione, and 3-hydroxy-2-methyl-1-phenylpyridine-4(1H)-thione. Structural characterizations include nuclear magnetic resonance (NMR) spectroscopy, electron spray ionization mass spectrometry (ESI-MS), and single-crystal X-ray diffraction. Photophysical properties were investigated via electronic absorption and photoluminescence (PL) spectroscopies, and density-functional theory (DFT) computations compared the Frontier Molecular Orbitals (FMOs) for the ground states and Natural Transition Orbitals (NTOs) for CT excited states. All complexes exhibit donor-to-acceptor LL'CT bands, admixed with metal-to-ligand (bpy) charge transfer (ML'CT). For Pt complexes, excitation into the LL'CT band results in emissions in the yellow-to-red region, attributed to ligand-centered (^{3}LC or ^{3}LL'CT) phosphorescence. In the hydroxypyridine-thione complexes, multi-exponential decays suggest that these transitions are admixed with thermally activated delayed fluorescence (^{1}TADF). Excited-state lifetimes fall within the nanosecond regime, with longer-lived components emerging at 77 K, consistent with temperature-suppressed TADF accompanying significant luminescence rigidochromism demonstrated by ~1700 cm^{-1} blue-shifted I_{max} and ~5-10-fold sensitized quantum yields in cryogen-cooled rigid-glassy media vs fluid solutions.



SWRM 2026 SW655

Accessing rare Cu(I)–Bi bonding with tris(pyrazolyl)borate scorpionates

Brandon T. Watson, ***Khadijatul Kobra Meem****, kxm8360@mavs.uta.edu, Vo Quang Huy Phan, Owen Dong, Alvaro Muñoz-Castro, Rasika Dias. Department of Chemistry and Biochemistry, University of Texas at Arlington Research Institute, Fort Worth, Texas, United States*

Heavier group 15 donors such as $SbPh_3$ and $BiPh_3$ rarely form stable adducts with copper(I), owing to their weak donor ability and correspondingly weak metal–ligand interactions. Accessing and stabilizing such systems is key to expanding the scope of coordination chemistry into underexplored regions of the periodic table. In this work, fluorinated poly(pyrazolyl)borate (scorpionate) ligands are employed to support a series of copper(I)–pnictogen complexes (E = As, Sb, Bi). Two complementary ligand frameworks, $[HB(3,5\text{-}(CF_3)_2Pz)_3]^-$ and $[H_2B(3,5\text{-}(CF_3)_2Pz)_2]^-$, provide access to valence-isoelectronic complexes, enabling direct comparison across the group 15 series. This strategy affords a family of copper–pnictogen complexes, including a rare example featuring a direct, unsupported Cu–Bi bond. The difficulty encountered in isolating the bismuth analogue reflects the pronounced decrease in donor strength down the group. Computational studies reveal a progressive weakening of Cu–E interactions from P to Bi, driven by relativistic effects and diminished Lewis basicity, with bonding analysis showing these interactions to be predominantly electrostatic and dominated by pnictogen-to-copper σ-donation with minimal π-backbonding. Together, these results establish fluorinated scorpionate ligands as an effective platform for accessing weak and otherwise inaccessible metal–main group interactions, providing new insight into copper–pnictogen chemistry.

SWRM 2026 SW656

Stabilization of classical coinage metal carbonyl complexes using a sterically encumbered tris(pyridyl)borate ligand

***Achala Rajathunga**, amw1053@mavs.uta.edu, Mukundam Vanga, Israel Fernandez, Rasika Dias. Chemistry and Biochemistry, The University of Texas at Arlington, Arlington, Texas, United States*

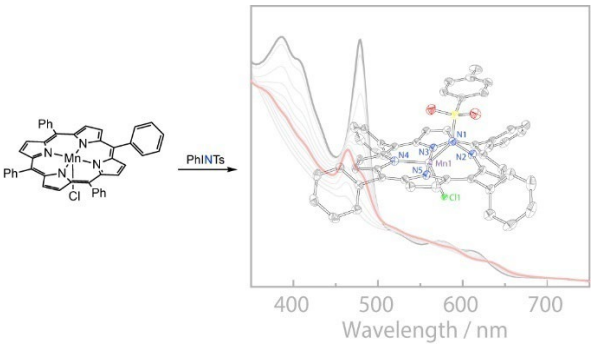
Classical coinage metal carbonyl complexes provide valuable platforms for understanding the nature of metal-carbonyl bonding, particularly the interplay between CO σ-donation and metal-to-CO π-backbonding. Despite their importance, electron-rich coinage metal carbonyl complexes remain uncommon because of the inherently weak affinity of Cu(I), Ag(I), and Au(I) for carbon monoxide and their susceptibility to reduction. In this study, the sterically demanding tris(pyridyl)borate ligand $[MeB(6\text{-}(Mes)Py)_3]^-$was employed to stabilize a series of copper(I), silver(I), and gold(I) carbonyl complexes. The strong donor ability and steric protection imparted by the ligand facilitate the isolation of classical carbonyl species, including uncommon gold(I) complexes that exhibit nonlinear coordination geometries. The complexes were characterized by multinuclear NMR, infrared spectroscopy, and single-crystal X-ray diffraction. Infrared spectra display markedly reduced ν(CO) stretching frequencies, indicative of substantial metal-to-CO π-backbonding, while crystallographic analysis reveals distinct structural features across the coinage metal series. Comparison of the Cu(I), Ag(I), and Au(I) complexes demonstrates the combined influence of metal identity and ligand architecture on metal-CO bonding and coordination geometry. These results highlight the effectiveness of sterically encumbered tris(pyridyl)borate ligands in stabilizing electron-rich classical coinage metal carbonyl complexes and provide further insight into the factors governing bonding and structure in late transition metal carbonyl chemistry.

SWRM 2026 SW657

Chemical non-innocence of porphyrin ligands in Mn-catalyzed nitrene transfer chemistry

***Arka Sinha**, arkas23@tamu.edu, Ryan X. Gruen, Matthew T. Figgins, David C. Powers. Chemistry, Texas A&M University System, College Station, Texas, United States*

Manganese porphyrins have been widely employed to catalyze nitrogen-group transfer (NGT) and oxygen-atom transfer (OAT) reactions of olefins and C–H bonds through high-valent manganese nitrenoid and oxo intermediates, respectively. While redox non-innocence of the porphyrin ligand is commonly invoked as operative in such transformations, much less appreciated is the potential of chemical non-innocence, in which the pyrrolide nitrogen of the porphyrin scaffold can insert into the M–L bond to afford “tuck-in” complexes. Here, we demonstrate that treatment of Mn(tpp)Cl with excess iminoiodinanes (PhINR) affords tucked-in Mn porphyrins. The formation of tucked-in porphyrins is supported by *in situ* UV-vis experiments and ESI-MS analysis and comparison with independently synthesized, crystallographically characterized authentic complexes, in which the iminoiodinane-derived nitrene fragment has inserted into one of the Mn–N bonds of Mn(tpp)Cl. Further mechanistic studies on Mn(tpp)Cl-catalyzed styrene aziridination revealed that the “tucking-in” of the porphyrin ring is slow relative to olefin functionalization, thereby establishing it as a chemically accessible — yet kinetically less preferred — pathway in Mn porphyrin-catalyzed NGT reactions.



In situ UV-vis monitoring demonstrating the formation of the tucked-in Mn porphyrin from Mn(tpp)Cl, with the crystal structure of the resulting complex shown

SWRM 2026 SW658

Synthesis and characterization of (^{Dipp}CCC)Mn-carbonyl complexes

***Aishee De**, aishee1999@tamu.edu. Chemistry, Texas A&M University, College Station, Texas, United States*

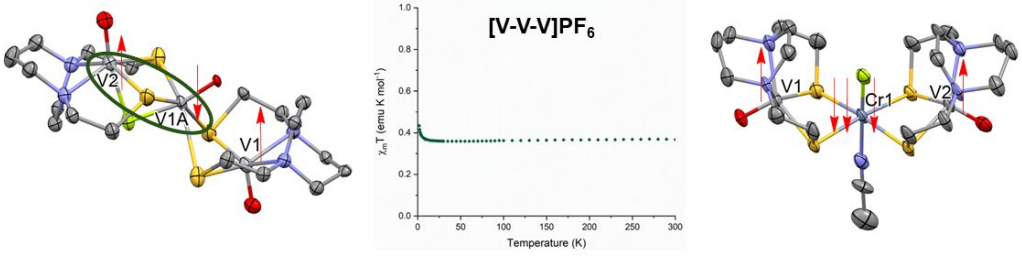
The development of catalysts based on earth-abundant first-row transition metals represents an important strategy toward sustainable organometallic chemistry and catalysis.[1] In this context, manganese is particularly attractive because of its high natural abundance, low cost, and comparatively low toxicity.[2] Despite the extensive development of manganese complexes supported by phosphine- and nitrogen-donor pincer ligands, manganese chemistry supported by strongly σ-donating *N*-heterocyclic carbene (NHC)-based CCC pincer ligands remains comparatively underexplored.[3-5] Herein, we report the synthesis and characterization of a series of manganese carbonyl complexes supported by the rigid ^{Dipp}CCC pincer scaffold [^{Dipp}CCC = bis(diisopropylphenyl-imidazol-2-ylidene)phenyl]. To the best of our knowledge, only a single structurally characterized CCC-supported manganese carbonyl complex has previously been reported,[6] highlighting the limited development of this class of compounds. Through reactivity studies we have isolated a tris-carbonyl (^{Dipp}CCC)Mn(CO)3 complex, a bimetallic terminal manganese hydride, (^{Dipp}CCC)Mn2(CO)8H, and a bridging-hydride, (^{Dipp}CCC)[Mn(CO)3]2(μ-H). These results establish NHC-based CCC pincer ligands as a versatile platform for stabilizing structurally diverse manganese carbonyl and hydride complexes and provide a foundation for investigating their reactivity and potential applications in manganese-mediated catalytic transformations.

SWRM 2026 SW659

Metallodithiolates as ligands to various transition metal ions: Coordination geometries and magnetic properties

Dakota Jones[1]*, djonesymail@gmail.com, Akhil Singh*[1]*, Manuel Quiroz*[1]*, Aruzhan Abdikaiym*[2]*, Naushad Ahmed*[1]*, Sourav Deb*[1]*, Brad Pierce*[2]*, Joseph Reibenspies*[1]*, Michael Hall*[1]*, Marcetta Y. Darensbourg*[1]*, Kim Dunbar*[1]*. (1) Texas A&M University System, College Station, Texas, United States(2) University of Alabama College Store, Tuscaloosa, Alabama, United States*

Thiolate ligands open up new directions for research in molecular magnetism because of their soft, diffuse character and ability to delocalize electron and spin density between metals. In 2023, Quiroz *et al.* reported trimetallic stair-step complexes [FeNO(bme-dach)-M-FeNO(bme-dach)]$(BF_4)_2$ (M = Ni, Pd or Pt). More recently, compositionally similar stair-step complexes, [V'NiV']$(BF_4)_2$, [VPdV]$(BF_4)_2$ and [VPtV]$(BF_4)_2$ were prepared and characterized by SQUID magnetometry and EPR spectroscopy. Magnetic measurements indicate that the two V centers are weakly ferromagnetically coupled and that the strength of the coupling increases moving from Ni (J = 0.282 cm^{-1}) to Pd (0.954 cm^{-1}) to Pt (1.37 cm^{-1}). This result, together with results from DFT and EPR, showed that, as was the case with the Fe-M-Fe series, the more diffuse orbitals of heavier transition metals more effectively mediate magnetic coupling. When Cu was added to the $M(N_2S_2)$ metalloligands in place of a group 10 metal, a tetrahedral geometry resulted around the Cu(I) center and weak ferromagnetic coupling was observed both in the case of FeNO-Cu-FeNO and VO-Cu-VO complexes. Magnetic studies show that the coupling between the two FeNO units through Cu, while weak, is greater than that between the vanadyl centers and suggest an intermolecular interaction through NO groups on adjacent [FeCuFe]BF_4 molecules. Finally, reactions of VO(bme-dach) with paramagnetic, early transition metal species, including VO^{2+} and Cr^{3+}, led to new molecular geometries including fluoride ligands, derived from BF_4^-, that are coordinated to the central metal. When VO^{2+} was used, the fluoride formed a bridge between the central vanadyl and one terminal vanadyl, leading to an asymmetric, distorted stair-step geometry as these two metal centers were drawn together. With Cr^{3+} as bridge, the final result was a basket-shaped geometry with the two VO(bme-dach) ligands in a cisoid configuration and the abstracted fluoride ligand oriented inside the basket. Both [V-V-V]PF_6 and [V-Cr-V]$(BF_4)_2$ exhibit antiferromagnetic coupling between the terminal VO^{2+} spin centers, strong enough that $[V\text{-}V\text{-}V]^+$ acts as a S = 1/2 system up to room temperature.



SWRM 2026 SW660

Synthesis and characterization of Cu(I) complexes bearing 2-picolyl-substituted mono-NHC ligands: Effect of NHC wingtips on coordination geometry

***Janet Sanwo-Olu**, janet.sanwo-olu@okstate.edu, Nick Back, Laleh Tahsini. Chemistry, Oklahoma State University, Stillwater, Oklahoma, United States*

N-Heterocyclic carbene (NHC) ligands have gained significant interest in transition-metal chemistry due to their strong σ-donating ability and highly tunable steric and electronic properties. Modification of the NHC wingtip substituents provides a useful approach for controlling the coordination environment of the metal center. Cu(I), with its d^{10} electronic configuration, is particularly sensitive to the steric and electronic environment imposed by its supporting ligands and can readily adopt coordination numbers ranging from two to four with geometries including linear, T-shaped, seesaw, and tetrahedral. While Cu(I) complexes bearing monodentate and polydentate NHC ligands have been widely studied, examples containing bidentate C^N ligands remain comparatively limited. We have developed a family of Cu(I) complexes supported by bidentate methylene-linked pyridyl-NHC ligands to investigate how modification of the NHC wingtip influences the coordination number and geometry of the Cu(I) center. A series of complexes bearing isopropyl (^{i}Pr), tert-butyl (*t*Bu), cyclohexyl (Cy), benzyl (Bz), diisopropylphenyl (Dipp), mesityl (Mes), para-trifluoromethylphenyl (p-CF_3Ph), and para-tolyl (p-CH_3Ph) wingtips have been synthesized and characterized by ^{1}H NMR and ^{13}C NMR spectroscopy, elemental analysis, and single-crystal X-ray diffraction. Crystallographic characterization reveals a remarkable variation in coordination geometry across the series, with the Dipp- and Mes-substituted complexes adopting a linear geometry, the p-CF_3Ph, p-CH_3Ph, and Bz complexes displaying T-shaped geometries, and the ^{i}Pr, *t*Bu, and Cy derivatives exhibiting a seesaw geometry. These structural differences demonstrate the significant influence of wingtip modification on the coordination environment of Cu(I) and provide insight into the steric and electronic factors governing the structures of these complexes.

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Metal–ligand cooperation in lutidine-linked bis-NHC Cu(I)–CNC complexes for the tandem carboxylation–esterification of terminal alkynes

***Nick Back**, nback@okstate.edu. Chemistry, Oklahoma State University, Stillwater, Oklahoma, United States*

Lutidine-based bis(imidazolium) C^N^C N-heterocyclic carbene transition-metal complexes, or pincer-NHCs, are emerging as highly efficient catalysts for a broad range of transformations. These complexes exhibit metal–ligand cooperativity through a distinctive dearomatization–aromatization mechanism. Under basic conditions, deprotonation of a methylene linker generates a highly reactive dearomatized complex capable of engaging substrates through the ligand framework. Reported reactions include nucleophilic attack at electrophilic substrates such as CO2 and phenyl acetylene, as well as deuterium incorporation from deuterated solvents. Our group has previously reported the synthesis and catalytic activity of Cu(I) pincer-NHC complexes bearing alkyl wingtips in C–C, C–N, and C–O cross-coupling reactions. We have also investigated the influence of aryl wingtip substituents, including electron-donating and electron-withdrawing groups, on the structures and properties of these complexes. By exploiting the reactivity of the dearomatized Cu(I) pincer-NHC, we developed a tandem carboxylation–esterification of terminal alkynes with a broad substrate scope encompassing aryl, alkyl, and pyridyl-substituted alkynes. Mechanistic investigations indicate that this transformation proceeds through a pathway distinct from previously reported Cu(I)–NHC-catalyzed carboxylation reactions. NMR spectroscopic and single-crystal X-ray diffraction data support the proposed mechanism and the involvement of ligand-based reactivity.

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Thermodynamic and electrocatalytic studies of M(triphosphine)(monophosphine) complexes containing group 10 metals and a bifunctional monophosphine ligand containing an organic hydride donor

***Clifford Alewine**, cja014@shsu.edu, Rachel Johnston, Christopher Zall. Chemistry, Sam Houston State University, Huntsville, Texas, United States*

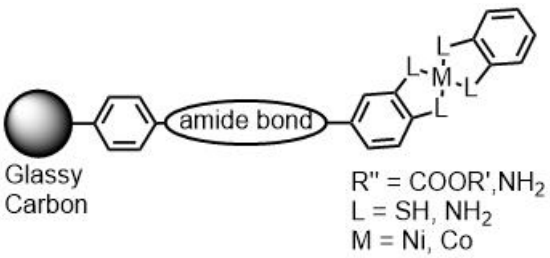
Metal-phosphine complexes are widely used as electrocatalysts for a variety of reactions, including H2 oxidation, proton reduction, and CO2 reduction. The design of these catalysts has been greatly aided by thermodynamic characterization, such as their reduction potentials and measurements of the acidity and hydricity of metal-hydride intermediates. In particular, thermodynamic studies of complexes of Group 10 metals with two diphosphine ligands were valuable in successfully developing Ni(diphosphine)22+ electrocatalysts for hydrogen oxidation and production. This presentation will describe electrochemical and thermodynamic studies of Group 10 complexes with an analogous M(triphosphine)(monophosphine) ligand set (M = Ni and Pd; monophosphine = PMe3, PEt3, PPh3). The nickel complexes with bulkier monophosphine ligands, PEt3 and PPh3, show reversible dissociation due to steric hindrance. This framework was extended to electrocatalytic studies of proton reduction using bifunctional palladium complexes, [Pd(triphosphine)(LH)]2+ and [Pd(triphosphine)(L+)]3+, in which LH and L+ are a novel monophosphine ligand containing an organic hydride donor in its reduced and oxidized forms, respectively.

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Covalent modification of glassy carbon electrodes with transition metal complexes for hydrogen production

***Olbelina A. Ulloa**, ulloa@stthom.edu. Chemistry and Biochemistry, University of Saint Thomas, Houston, Texas, United States*

The need to decrease carbon dioxide in our atmosphere and reduce our reliance on carbon-based fuels is one of the most pressing challenges of our time. Our approach to address this challenge is the improvement of catalytic activity and longevity of first-row transition metal complexes that catalyze production of hydrogen from acids. Our procedure builds on the modification of electrodes *via* electrochemical reduction of aryldiazonium salts by adding a linker that can chelate various metal complexes. All modifications and chelation of Ni, NiFe, Co or Fe complex are done in-situ at the electrode surface without the need for purification. Hydrogen production from acids by the immobilized complexes were studied in water and acetonitrile.



SWRM 2026 SW664

Fluorinated B-phenylated scorpionates as tunable platforms for stabilizing silver(I)–ethylene complexes

Vo Quang Huy Phan[1], *voquanghuy.phan@mavs.uta.edu, Anurag Noonikara Poyil*[1], *Mukundam Vanga*[1], *Pavel Mykhailiuk*[2], *Rasika Dias*[1]. *(1) Chemistry and Biochemistry, The University of Texas at Arlington, Arlington, Texas, United States(2) Enamine Ltd, Kyiv, Kyiv City, Ukraine*

Fluorinated and B-phenylated bis(pyrazolyl)borate and bis(pyridyl)borate ligands have been utilized in silver(I)–ethylene chemistry. These ligands contain electron-withdrawing trifluoromethyl or pentafluorosulfanyl groups that create a chemically inert half-rim and, together with a flanking phenyl group, provide steric protection around the metal center. The steric effects of these fluorinated supporting ligands were evaluated to understand their influence on the selectivity of alkane C–H functionalization *via* silver-catalyzed carbene insertion. Overall, these findings illustrate how fluorinated substituents and N-heterocyclic donor arms influence metal–ligand bonding, the stability of coinage-metal π-complexes, and the catalytic efficiency and selectivity of alkane C–H functionalization.

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Selective binding and oxidation of cannabinoids mediated by copper complexes

Brianna K. Neilan[1], *bkn006@shsu.edu, Alleigh N. Couch*[2], *Emma Fitzgibbons*[2], *J. T. Davidson*[2], *Christopher Zall*[1]. *(1) Chemistry, Sam Houston State University, Huntsville, Texas, United States(2) Forensic Science, Sam Houston State University, Huntsville, Texas, United States*

Δ^9-Tetrahydrocannabinol (Δ^9-THC) and cannabidiol (CBD) are the primary active compounds found in cannabis plants. These compounds, along with numerous other structural isomers such as Δ^8-THC, possess identical molecular weights and are consequently difficult to distinguish based on their mass spectra alone. Metal-ion complexation, an emerging alternative to traditional GC-MS, uses transition metals such as silver and copper to reversibly bind to these cannabinoid compounds; differences in their binding abilities can produce distinguishable mass spectra using soft ionization methods such as electrospray ionization (ESI). Incorporation of phosphine ligands to the metal centers can provide increased stability and solubility, facilitating differentiation. Intriguingly, the ESI-mass spectra using copper complexes show selective oxidation of Δ^9-THC and Δ^8-THC, but not CBD, which enables their differentiation without requiring tandem mass spectrometry (MS/MS). These reactions are attributed to the activation of O_2 at the copper center; however, the outcomes are complex and highly dependent on the solvent, cannabinoid, presence of a phosphine ligand, and the instrumental configuration. This presentation will describe studies of the copper-cannabinoid binding and oxidation reactions, using $[Cu(NCCH_3)_4]^+$ and a copper bis-phosphine complex, $[Cu(PPh_3)_2(NCCH_3)_2]^+$, in the presence of CBD and a THC analogue, tetrahydrocannabivarin, or THCv. The aerobic oxidation of cannabinoids was studied by NMR, cyclic voltammetry, FTIR, and ESI-MS methods. Electrochemical studies show that the Cu(I/II) oxidation potential is strongly solvent dependent, with the Cu(I) ions strongly stabilized in acetonitrile. The electrochemistry is strongly affected by the presence of the cannabinoid, indicating an interaction between the THCv and $[Cu(NCCH_3)_4]^+$ complex. The data provides insight into the complex interactions between the binding of cannabinoid, phosphine, and oxygen, and the effect of solvents on these reactions. The implications for cannabinoid differentiation by mass spectrometry will be discussed.

SWRM 2026 SW666

Müller versus Gutmann–Beckett for assessing the Lewis acidity of boranes

***Sameera Ranasinghe**, sameera_ranasinghe1@baylor.edu, Yijie Li, Madison Andrews, MANJUR OYASIM AKRAM, Ragene Thornton, Caleb Martin. Chemistry and Biochemistry, Baylor University, Waco, Texas, United States*

A ^{19}F NMR spectroscopic probe, *p*-fluorobenzonitrile is used to assess borane Lewis acidity, an alternative to the well-established ^{31}P NMR Gutmann–Beckett method. The Gutmann–Beckett method is ineffective for bulky boranes. This work was inspired from a study by Müller and co-workers to assess the Lewis acidity of intramolecularly stabilized silylium species. In this work, the ^{19}F NMR results from this method, the ^{31}P NMR data from the Gutmann–Beckett method, and computed fluoride ion affinities are evaluated. The key finding is that the ^{19}F probe correlates better with the fluoride affinities than the ^{31}P probe. The Müller approach is appealing due to the probe's commercial availability, minimal steric bulk from the linear geometry, and ease of ^{19}F NMR spectroscopy. The drawback to this method is that it is not effective with weak Lewis acids. This development provides chemists with an alternative tool to evaluate borane Lewis acidity that is crucial for understanding and predicting Lewis acid reactivity in organic synthesis and catalysis.

SWRM 2026 SW667

Towards fluorinated germanium cages

***Noah Holt**[1], noahasholt@icloud.com, Natie Karten[1,2], Mira Kessler[1]. (1) Chemistry, Oklahoma State University, Stillwater, Oklahoma, United States(2) Oklahoma Baptist University, Shawnee, Oklahoma, United States*

Computational studies show the properties of fluorinated Germanium cages make them viable candidates for thin film semiconductor applications. Exploration of excited state geometries using TDDFT and one photon spectroscopy give further insight into the properties and limits of this chemical motif. Small (4-8 Ge) fluorinated Ge cages show a low degree of stability, especially in excited states. Larger cages are much more stable, but may be harder to achieve synthetically. Synthetic access to a fluorinated germanium cage can be approached in two ways: fluorination of pre-assembled Ge cages or the use of fluorinated germanes to construct a cage. A Ge-Ge bond is typically weaker than a Si-Ge or C-Ge bond, which restricts leaving group choice. Careful kinetic control and gentle fluorine sources are likely required to avoid cleaving the Ge-Ge bonds in a pre-assembled cage and producing GeF4. Some progress has been made optimizing the synthesis of potential starting materials. Ge4(SiR3)4 cages have literature precedence: a tedious multi-step procedure with poor yields. Ge4(SitBu3)4 may accept fluorination however the published SitBu3Cl synthesis takes 4 steps and is very slow. To this end, a one pot synthesis using SiCl4 and tBuLi was investigated. Halogermane substrates, e.g. GeCl3F, may undergo reductive coupling to obtain the cage molecules. chelated GeF2 and GeCl3F were synthesized for this purpose. The outcome/limitations of computational studies along with potential synthetic routes to fluorinated cage molecules will be discussed.

SWRM 2026 SW668

Calcium phenoxyimine complexes for application towards C-H activation

***Carolyn Brown**, cb116@rice.edu, Kaitlyn Birkhoff, Samantha Yruegas. Chemistry, Rice University, Houston, Texas, United States*

C–H activation is a powerful strategy for the selective functionalization of organic substrates, which has been traditionally dominated by complexes of the late transition metals. Contrastingly, early main group complexes have garnered interest for their potential to promote C–H activation through alternative mechanisms and metal–ligand cooperativity. Access to well-defined alkaline earth metal complexes remains synthetically challenging as aggregate formation of ill-defined clusters and disproportionation by the Schlenk equilibrium is prominent. Sterically bulky ligands, such as the ubiquitous β-diketiminate (NacNac) scaffold, are often required to stabilize reactive s-block metal centers. The bidentate, LX type NacNac has been historically used in main group chemistry, but the phenoxyimine (FI) moiety binds in a similar LX fashion while offering higher denticity through modification of the substituents at the iminic nitrogen. This work outlines the synthesis and characterization of a library of phenoxyimine ligands with tunable steric and electronic properties. Contiguous metalation studies with the calcium metal precursor, $Ca[N(SiMe_3)_2]_2(solv)_2$ (solv = THF, dioxane) has enabled the isolation of well-defined, heteroleptic calcium phenoxyimine complexes. With the goal of synthesizing and isolating stable catalysts for substrate-based C-H activation, modification of the FI scaffold has furthered the exploration of the strength of metal-ligand interactions and the effects of basicity on complex reactivity. Complexes of the general form $[(FI)Ca(HMDS)_n(solv)_n]$ (HMDS = $N(SiMe_3)_2$) were characterized by observing shifts in ^{1}H, ^{13}C, and ^{29}Si NMR, as well as analysis of 2D NMR spectra. Time-course NMR monitoring and single-crystal X-ray diffraction (SC-XRD) studies allowed for further insight into coordination and solubility. These observations suggest that discrete ligand design can significantly impact the stability and reactivity of calcium centers. Ongoing efforts target the application of these stabilized complexes to the C–H activation of substituted pyridines and other heteroarenes, enabling new approaches to main group mediated functionalization.

SWRM 2026 SW669

Synthesis and preparation of germanium amides as precursors to germanium telluride dimers

***Patrick Kitzel**, patrick.kitzel@okstate.edu, Charles S. Weinert. Oklahoma State University, Stillwater, Oklahoma, United States*

Trimethylsilane ($-Si(CH_3)_3$) is a well explored bulky ligand used for a variety of reactions. This ligand can be utilized in helping to stabilize various otherwise reactive compounds. Germylenes are one example of this as they can be stabilized by trimethylsilyl ligands as a result of their steric and electron donating characteristics. The bis(amido) germylene ($Ge[N(Si(CH_3)_3)_2]_2$) is one of these established germylenes and has been shown to react with chalcogens like tellurium to generate $[Ge\{N(Si(CH_3)_3)_2\}_2(\mu\text{-}Te)_2]_2$ dimers. Research regarding germylene compounds with varying ligands and their tellurium dimer counterparts has not been widely investigated. As a result, an exploration into germylene compounds and their successful usage for synthesizing new chalcogen dimers, such as $[Ge\{N(SiPh(CH_3)_2)_2\}_2(\mu\text{-}Te)_2]_2$, is provided along with additional material characterization using ^{29}Si NMR, ^{125}Te NMR, and XRD analysis.

SWRM 2026 SW670

Divergent outcomes from the reactions of borole with Michler's ketone and thioketone

***Dinithi Alwis**, dinithi_alwis1@baylor.edu, Ayesha Begum, Caleb Martin. Chemistry and Biochemistry, Baylor University, Waco, Texas, United States*

The reactivity of borole systems with carbonyl compounds is well established, often leading to ring-expanded boracycles via C=O insertion. In contrast, the chemistry of thiocarbonyl analogues has not been investigated. In this study, the reactivity of pentaphenylborole with Michler's thioketone is examined and compared with Michler's ketone. In these reactions, ring expanded BOC_5 ring, an adduct, and an unexpected BSC_4 ring are obtained. These findings shed light on the roles of the heteroatom and electronic effects in insertion versus adduct reaction pathways.

SWRM 2026 SW671

Investigating sequential quantum yield steps of LMCT photocatalysts via cyclic voltammetry

***Nya E. Black**, nyaeblack@gmail.com, Weitong Gao, Dylan G. Boucher. Chemistry and Biochemistry, Baylor University, Waco, Texas, United States*

Ligand-to-metal charge transfer (LMCT) is common process among earth abundant metals where an electron is excited from the ligand to the electron deficient metal center upon illumination. This electronic transition induces bond homolysis that can produce high energy radical intermediates. The unique reactivity and relative abundance of LMCT photocatalysts makes them promising alternatives to expensive, precious metals used in many photocatalytic processes. Since LMCT photocatalysts experience relatively short, excited state lifetimes causing low yields and efficiency in reactions, researchers must investigate the fundamental properties of the photocatalyst and reaction conditions to optimize them. Recently, electrochemistry was used as a simple and quantitative approach for studying a $[FeCl_4]^-$ LMCT photocatalyst, demonstrating the first direct measurement of quantum yield via cyclic voltammetry. To further expand the utility of this method, we obtained quantum yield measurements for $[CeCl_6]^{2-}$ and $[CuCl_4]^{2-}$ LMCT photocatalysts, which demonstrated similar bond homolysis properties but different ligand environments and quantum yield efficiencies. As the quantum yield measured through cyclic voltammetry is a composite value of the LMCT quantum yield and hydrogen atom transfer quantum yield, we introduced substrates at different concentrations and performed a nonlinear least squares regression to determine the individual quantum yield values in the sequential, multi-step process. Finite element simulations were used to support the quantum yield measurements and LMCT quantum yield calculations. The simulations were also utilized to determine the limits of the cyclic voltammetry measurement for nonideal LMCT photocatalysts. This research presents an effective method for comparing LMCT photocatalyst efficiencies and quantifying the limiting quantum yield step to advance photocatalysis measurements.

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Directing selective photocatalytic C-H activation with electrochemistry

***Nalinda C. Senevirathna Mudiyanselage**, nalinda_senevirathn1@baylor.edu. Chemistry and Biochemistry, Baylor University, Waco, Texas, United States*

Selective C(sp^3)–H functionalization using chlorine radicals is a difficult task because chlorine radicals are highly reactive and diffuse freely. As a result, they often remove hydrogen atoms from many different C–H bonds during hydrogen atom transfer (HAT) reactions, leading to poor site selectivity. In this study, we show that combining electrochemical regulation with ligand to metal charge transfer (LMCT) photocatalysis offers a reliable method to control the concentration of chlorine radicals, recombination rates, and overall, HAT selectivity. In this study, 2,3-dimethylbutane was used as a model substrate to assess site selectivity. Electro photocatalytic activation utilizing $FeCl_3$ as the photocatalyst yielded a 7:1 primary to tertiary functionalization ratio, whereas the corresponding $CeCl_3$ system exhibited substantially lower selectivity under identical conditions. Further evaluation of the reaction kinetics of both Fe and Ce photocatalytic systems via cyclic voltammetry and quantum yield measurements suggested that chlorine radical recombination dynamics play a critical role in regulating productive chlorine radical flux and, consequently, C–H activation selectivity. Overall, these findings allowed us to develop an efficient method for the electrochemical regulation of LMCT photocatalysts as an effective method of directing selective C(sp^3)–H functionalization and controlling the reactivity of chlorine radicals.

SWRM 2026 SW673

[5+2] Cycloaddition reactions of oxidopyrylium, oxidopyridinium, oxidothiopyrylium ylides derived from hetero-substituted maltol derivatives

***Thanuja Thilakarathna**, thanuja_thilakarath1@baylor.edu, Patrick J. Farmer. Chemistry and Biochemistry, Baylor University, Waco, Texas, United States*

We investigated heteroatom-substituted maltol derivatives as precursors to air-stable, isolable pyrylium, pyridinium, and thiopyrylium salts, and evaluated how heteroatom substitution affects their reactivity in [5+2] cycloaddition reactions. Among the systems examined, the N-phenyl-substituted pyridinium salts showed reduced aromatic stabilization and, correspondingly, the greatest reactivity toward dipolarophiles. These ylides were readily intercepted by dipolarophiles before self-dimerization could occur, highlighting their utility as flexible reagents for constructing structurally complex seven-membered ring systems while minimizing competing dimer formation.

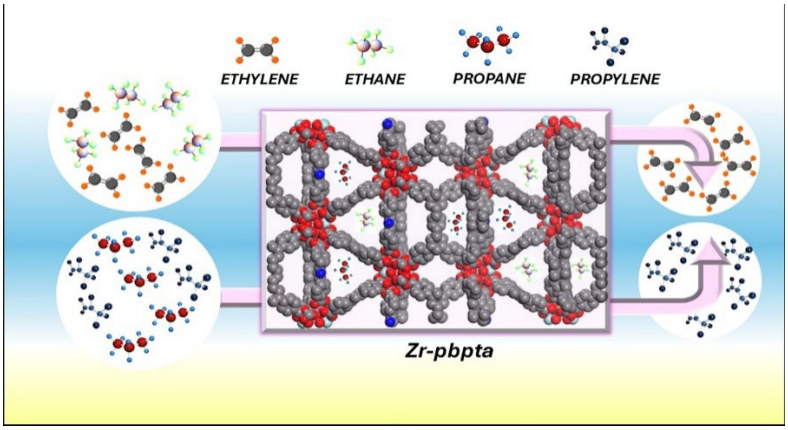
SWRM 2026 SW674

Highly robust Zr-MOF platform featuring aromatic rich cores for efficient paraffin/olefin separation

***Gaurav Verma**, gauravv003@gmail.com. University of North Texas System, Dallas, Texas, United States*

Paraffin–olefin separations are central to the production of polymer-grade feedstocks, yet they remain among the most energy-demanding processes in the chemical industry due to the nearly indistinguishable physical properties of these hydrocarbons. Metal–organic frameworks (MOFs) have emerged as transformative materials in this space, offering exceptional surface areas, precisely tunable pore architectures, and rich chemical functionality. Notably, reverse-selective MOFs that are capable of preferentially adsorbing paraffins via C–H--pi interactions, present a compelling pathway to achieve olefin-enriched streams under significantly milder and more energy-efficient conditions. In this work, we report a zirconium-based framework, Zr-pbpta, constructed from robust [$Zr_6(\mu_3\text{-}O)_4(\mu_3$-

$OH)_4(OH)_4]^{8+}$ clusters and a meticulously designed aromatic tetracarboxylate linker, H_4pbpta (pbpta = 4,4,4,4-(1,4-phenylenebis(pyridine-4,2,6-triyl))tetrabenzoic acid), featuring pyridyl functionalities. This architecture integrates extended aromatic systems with a high density of nitrogen donor sites, creating an optimal environment for strong and selective alkane–framework interactions. Consequently, Zr-pbpta delivers outstanding adsorption performance, achieving capacities of 4.55 mmol g^{-1} for ethane and 8.50 mmol g^{-1} for propane at 298 K and 1 bar, exceeding many benchmark MOFs. Moreover, the framework exhibits pronounced selectivity for C_2H_6/C_2H_4 and C_3H_8/C_3H_6 separations, driven by enhanced C–H---pi interactions, as confirmed by in situ infrared spectroscopy. These results position Zr-pbpta as a highly promising candidate for next-generation, energy-efficient paraffin–olefin separations, and underscore the power of deliberate MOF design in tackling critical challenges in industrial hydrocarbon purification.



SWRM 2026 SW675

Synthesis of MOF-based composites

***Marianna Espeleta**, mxe23c@acu.edu, Diego F. Zometa Paniagua. NEXT Lab, Abilene Christian University, Abilene, Texas, United States*

At NEXT Lab, our goal is to provide clean energy, water, and medical isotopes on a global scale through the use of molten salt reactor technology. Metal-organic frameworks (MOFs) have emerged as a potential material for the use of medical isotope extraction. MOFs are formed by the self-assembly of metal clusters and organic linkers, creating 3D frameworks. This property allows MOFs to be a highly tunable material. Scientists can control both physical and chemical properties through linker engineering and metal ion exchange. The first challenge for using a MOF in the reactor is temperature. Reactor operation temperature is higher than the majority of any known MOF thermal stability; another challenge is the corrosive behavior of the molten salt. MOF composites can be investigated with increased stability against corrosive environments and high temperatures. Research has begun with the use of solvothermal and electrochemical synthesis. The chosen MOFs: ZIF-8, MIL-53, and HKUST-1, along with their respective linkers, solvents, and metals, were mixed within a separate beaker before being transferred to an autoclave. Different metals such as zinc, copper, and Monel were used as substrates for MOF composite growth at different temperatures that ranged from 40°C-120°C in a furnace. Afterward, tests and imaging were taken with a scanning electron microscope, infrared spectroscopy, and a light microscope to see their physical and chemical properties. Synthesized MOF composites each had unique crystalline distributions and sizes that reflected the effects of different pretreatments. This presentation will cover the details of MOF composite synthesis and the effects of pretreating the metal substrate.

SWRM 2026 SW676

Synthesis and characterization of anion receptors featuring hydrogen and chalcogen bonding

***Andres Perez Gomez**, andrespgomez78@gmail.com. Department of Chemistry and Biochemistry, The University of Texas at Arlington, Arlington, Texas, United States*

Noncovalent interactions play an important role in molecular recognition and anion binding. Hydrogen bonding (HB) is widely employed in receptor design because of its accessibility and effectiveness; however, its strength and selectivity can be limited in competitive environments. Chalcogen bonding (ChB), by contrast, offers a highly directional and tunable interaction that can complement conventional HB motifs. Herein, we report the synthesis and characterization of two tellurium-containing anion receptors designed to incorporate both HB and ChB donor sites for anion recognition. The receptors were characterized by multinuclear and multidimensional NMR spectroscopy, and their anion-binding properties were further investigated through complementary spectroscopic titrations. Together, these receptors provide complementary platforms for probing the interplay between HB and ChB interactions and how receptor architecture influences anion recognition.

SWRM 2026 SW677

Beyond hydrogen bonding: Multidentate anion receptors integrating chalcogen bonding

***Francisca Gonzalez Ortiz**, gfrancisca50@gmail.com, Gyeongjin Park. Department of Chemistry and Biochemistry, The University of Texas at Arlington, Arlington, Texas, United States*

Synthetic receptors featuring multiple hydrogen-bonding (HB) interactions have been widely employed for strong anion recognition. In contrast, multidentate systems incorporating main-group noncovalent interactions remain underexplored, largely due to their inherent directionality. In this work, we report the design, synthesis, and characterization of multidentate anion receptors that integrate hydrogen-bonding and chalcogen-bonding (ChB) donor sites within a single molecular architecture. By combining these complementary interaction motifs, the receptors were designed to investigate the potential for cooperative HB and ChB interactions in anion recognition. The multidentate receptors were synthesized through a multistep synthetic route and characterized by multinuclear NMR spectroscopy, while single-crystal X-ray crystallography provided structural insight into the spatial arrangement of the HB and ChB donor sites. Their anion-binding properties were evaluated toward a series of anionic guests, while catalytic investigations across several mechanistically distinct transformations were used to assess the broader functional properties of these receptor systems. Together, these studies provide a platform for probing cooperative hydrogen- and chalcogen-bonding interactions and highlight the potential of integrating HB and ChB donor sites in the development of multifunctional supramolecular receptors for anion recognition and catalysis.

SWRM 2026 SW678

From oxygen-atom transfer to electronic frustration in antimony–borane Lewis pairs

***Thien Nguyen**, thien.nguyen7@mavs.uta.edu, Gyeongjin Park. Chemistry and Biochemistry, The University of Texas at Arlington, Arlington, Texas, United States*

Lewis acid stabilization provides access to reactive antimony species that are otherwise difficult to isolate, while offering a platform for probing the boundary between classical Lewis adducts (CLAs) and frustrated Lewis pairs (FLPs). We first found that the Lewis acid-stabilized stibine oxide $Ph_3SbOB(C_6F_5)_3$ undergoes oxygen-atom transfer (OAT) to PPh_3 through the discrete $Ph_3Sb{\bullet}B(C_6F_5)_3$ Lewis pair. This species also reacts with trace water to form the unusual monomeric hydroxoantimony(III) adduct $Ph_2SbOH{\bullet}B(C_6F_5)_3$ through Sb–C protonolysis, highlighting reactivity enabled by the labile nature of the Sb→B interaction. Building on these observations, we isolated and structurally characterized $Ph_3Sb{\bullet}B(C_6F_5)_3$ and related triarylstibine–borane adducts. Single-crystal X-ray diffraction reveals persistent yet elongated Sb–B bonds, supporting their classification as CLAs, yet their reactivity exhibits FLP-like characteristics. Notably, these complexes display reactivity distinct from that of the lighter phosphorus and arsenic analogs, which we attribute to the increased s-character of the antimony lone pair, as supported by computational studies. These findings position triarylstibine–borane complexes as electronically weakened CLAs whose labile Sb→B interactions enable unusual OAT and bond-activation chemistry.

SWRM 2026 SW679

Selective inhibition of HAT1 using AB oligomers: A tunable platform for targeting enzymes

***Ismail Lalami**[1], ixl170230@utdallas.edu, David Bork[1], Henry Neal[1], Shreenidhi Rajkumar[2], Jung-mo Ahn[1], Joshua Gruber[2], Jacob Soares[1], ishrat durdana[2], kiran kicinski[2,1]. (1) The University of Texas at Dallas, Richardson, Texas, United States(2) The University of Texas Southwestern Medical Center, Dallas, Texas, United States*

Histone acetyltransferase 1 (HAT1), an enzyme that catalyzes the acetylation of terminal lysines on histone H4, remains a challenging therapeutic target due to the poor cellular permeability of peptide-based inhibitors and the lack of specificity in small-molecule alternatives. Here, we present a novel class of compounds—AB oligomers—as selective and synthetically accessible inhibitors of HAT1. These oligomers are composed of alternating amino acid (A) and functionalized aminobenzoic acid (B) monomers, synthesized via solid-phase methods that enable rapid, modular assembly without the need for extensive purification. AB oligomers exhibit excellent flexibility and rigidity, enhanced membrane permeability, enzymatic stability, and chemical diversity, making them ideal candidates for structure-activity relationship (SAR) studies. One such compound, B21-2, demonstrates selective inhibition of HAT1 with a dissociation constant (Kd) of 1 μM, acting as a substrate-based inhibitor and effective biochemical probe. The ease of synthesis, coupled with the potential for AI-guided design and library screening, positions AB oligomers as a promising platform for targeting unknown enzymes and pathways in chemical biology and drug discovery.

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Edman sequencing evolved: Precise native peptide *C*-terminal ligation

***Aisosa Omere**, aisosaomere@gmail.com. Chemistry and Biochemistry, The University of Texas at Arlington, Arlington, Texas, United States*

Proteins, the workhorses of life, are complex macromolecules whose functions are precisely dictated by their amino acid sequences. These sequences, encoded by DNA, determine a protein's three-dimensional structure and specific biological activity. Proteins can also serve as biomarkers for various disease states, with alterations in their expression or structure signaling pathological conditions. Early detection and characterization of these disease-specific proteoforms, the diverse molecular forms arising from post-translational modifications, genetic variations, or alternative splicing, is paramount for accurate diagnosis and effective therapeutic intervention. The current state-of-the-art protein sequencing methodologies employing single-molecule detection predominantly utilize tandem mass spectrometry (LC-MS/MS), encompassing both top-down and bottom-up proteomic strategies. Bottom-up proteomics, characterized by the proteolytic fragmentation of proteins followed by separation via liquid chromatography prior to analysis, may result in the irreversible loss of post-translational modification data and compromises the contextual integrity of proteoform information. Conversely, while top-down approaches analyze intact proteins, both methodologies are constrained by elevated operational costs, limited throughput, and the necessity of substantial sample volumes to attain satisfactory resolution. These limitations impede widespread implementation and restrict the analysis of low-abundance proteoforms. To overcome these challenges, we propose a novel Edman-based multiplexing protein sequencing strategy. This technology suite utilizes chemoselective probes and advanced computational techniques to enable comprehensive and quantitative proteoform analyses. This presentation will focus on the foundational aspect of our technology: the development of a C-terminal specific ligation strategy, a critical step enabling subsequent Edman degradation and precise protein sequencing. Contemporary immobilization strategies utilize unnatural amino acids to facilitate the adherence of a peptide to a solid surface, or the results are very low yielding. Here, we report the ability to successfully immobilize a native peptide onto a solid surface.

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Reprogrammed autophagy for targeted organelle degradation using engineered protein therapeutics

***Ura Kang**, ura.kang@utdallas.edu, Ziwen Jiang. Chemistry and Biochemistry, The University of Texas at Dallas, Richardson, Texas, United States*

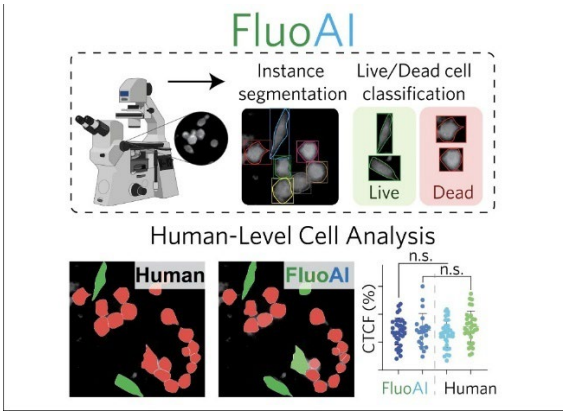
Autophagy acts as the waste disposal mechanism of cells, degrading intracellular content such as harmful protein aggregates and damaged organelles. It has been observed that when autophagy is impaired as a result of genetic defects or senescence, normal cellular processes are subsequently disturbed. Autophagy therefore plays an important role during aging and diseases that are associated with the accumulation of toxic protein aggregates or dysfunctional organelles. Overall, autophagy contributes a vital role in maintaining cellular homeostasis and can be harnessed for potential therapeutic development. Currently, there is no available broadly applicable system for the targeted degradation of selected organelles. Our lab has developed a novel methodology termed AceTAC to utilize engineered protein constructs with antibody-enabled specificity, transporting the selected target to undergo the autophagic degradation process. The fundamental mechanism for our design involves an engineered protein construct that can simultaneously bind to the autophagic membrane and the cellular target. We will highlight our recent progress using the AceTAC degradation technology for targeted degradation of several organelles, including mitochondria, peroxisome, and ER. We expect that our technology can be broadly tailored to selectively modulate the intracellular organelle dynamics.

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Assesment of *in vitro* nano-cytotoxicity with fluorescence microscopy through convolutional neural network-based live/dead cell classification

Ugur C. Topkiran[1], *ugur.topkiran@tcu.edu, Ali Gasimli*[2], *Anton V Naumov*[1]. *(1) Physics and Astronomy, Texas Christian University College of Science & Engineering, Fort Worth, Texas, United States(2) Computer Science, Texas Christian University College of Science & Engineering, Fort Worth, Texas, United States*

Nanomaterial use continues to rise in biomedical applications, and the demand for rapid, accurate, and non-invasive cytotoxicity measurements has become increasingly clear. Existing approaches for evaluating nanomaterial cytotoxicity tend to be indirect and typically rely on well-plate, salt-based fluorescence assays or complicated microscopy methods. To tackle these problems, we introduce FluoAI, a two-stage neural network workflow that directly determines live/dead cells from the nanomaterial's fluorescence, eliminating the need for additional labeling. The workflow employs two consecutive convolutional neural networks: Mask R-CNN first performs instance segmentation of individual cells from grayscale, single-channel fluorescence images, after which a DenseNet-121 classifier assigns alive or dead labels to each segmented cell, achieving performance values of up to 92.0%. Alongside viability classification, FluoAI also performs expert-level analyses of corrected total cell fluorescence (CTCF), mean fluorescence, and cell area, with results showing minimal to no significant differences compared with human measurements of Graphene Quantum Dot (GQD) and fluorescein dye-treated model cells. Since the entire pipeline is automated, these quantitative fluorescence metrics are generated faster than manual analysis while preserving comparable accuracy. Overall, this AI pipeline enables non-invasive cytotoxicity assessment and automated *in vitro* analysis using routine fluorescence microscopy. With its dataset continuing to expand, FluoAI provides a substantial foundation for reliable, high-throughput nano-cytotoxicity assays and automated data analysis, ultimately supporting the development of novel and safer nanomedicines.



SWRM 2026 SW683

Improving the stability of food-dye-based optical clearing agents with polymer additives

Rohit Kajla[1], *rohit.kajla@utdallas.edu, Kelsey I. Arze*[2], *Zihao Ou*[1]. *(1) Physics, The University of Texas at Dallas, Richardson, Texas, United States(2) Psychology, The University of Texas at Dallas, Richardson, Texas, United States*

Optical clearing improves tissue transparency by reducing refractive-index mismatch between tissue components and the surrounding medium. Achieving sufficiently high refractive indices with aqueous clearing agents can require dye concentrations approaching their stable solubility range. FDA-approved food dyes provide strong refractive-index tuning at high concentrations, but these solutions are only temporarily stable. Over time, molecular association through counterion-mediated interactions, hydrogen bonding, and π–π stacking leads to crystallization and precipitation. The resulting crystals introduce additional light scattering, shortening the time available for imaging. We approached this limitation as a problem of crystallization control. We hypothesized that water-soluble neutral and negatively charged polymers could stabilize concentrated dye solutions by disrupting dye–dye interactions and inhibiting crystal growth. Polymers with different charge and hydrogen-bonding characteristics were tested, and precipitation was monitored by time-lapse imaging. Kymograph analysis was used to quantify the onset and propagation of precipitation. Polymer addition substantially delayed precipitation, extending solution stability and usable imaging time. The most effective formulations delayed precipitation onset by 1.9- to 3.35-fold. We then applied the stabilized formulation to visualize different organs like small intestine from a fluorescent-reporter mouse and imaged labelled neuronal networks that are difficult to resolve in uncleared tissue without sectioning. Fluorescence intensity changed minimally after clearing, indicating preservation of the fluorescent signal. Neuronal structures were resolved against the background with a 3.37-fold improvement in signal-to-noise ratio. Together, these results demonstrate that water-soluble polymers can extend the working lifetime of food-dye-based optical clearing solutions while preserving optical performance and fluorescence signal. This provides a simple strategy for improving the stability of high-refractive-index aqueous clearing media for fluorescence imaging of intact tissues.

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Accelerating transient *in vivo* tissue optical clearing

***David Asante-Asare**, dpa240001@utdallas.edu, Zoya Chaudhry, Zihao Ou. The University of Texas at Dallas, Richardson, Texas, United States*

Transient tissue optical clearing can improve visualization of structures beneath the skin, but its *in vivo* use is often limited by the slow diffusion of clearing agents through biological tissue. This slow transport can increase clearing time and make uniform, large-area clearing difficult to achieve. Here, we investigated a strategy to enhance tissue permeability and improve the delivery of optical-clearing dyes such as tartrazine. Different enhancer concentrations were applied to skin samples before exposure to the clearing agent. Changes in optical transmission were monitored over time to quantify clearing kinetics and determine how these enhancers affected dye transport through tissue. Under optimized conditions, the enhancers produced an approximately 10-fold reduction in characteristic clearing time compared with clearing without enhancers. The response was concentration-dependent, highlighting the need to balance accelerated transport with the resulting optical transmission. The optimized approach was subsequently evaluated *in vivo*. Enhancers followed by topical application of the optical-clearing agent enabled rapid clearing over relatively large areas of mouse skin and improved visualization of underlying tissue. Animals were also monitored afterward to assess visible recovery over time. Together, these results show that modifying tissue permeability with chemical enhancers can substantially improve the speed and practicality of transient *in vivo* tissue clearing. This strategy addresses a major transport limitation of optical clearing and potentially supports broader applications of transient tissue transparency in biological imaging.

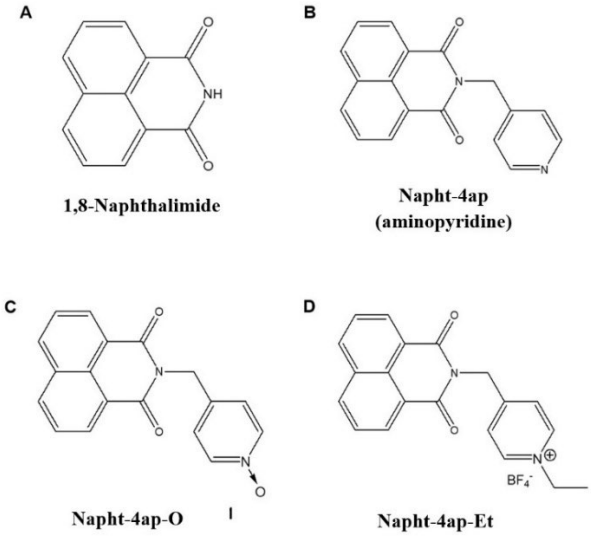
SWRM 2026 SW685

Spectroscopic investigation of bifunctional naphthalimide salt interactions with calf thymus DNA

Perla M. Tovar[1]*, tovarpm@jacks.sfasu.edu, Wolfgang Kramer*[2]*, Bidisha Sengupta*[1]*. (1) Department of Chemistry and Biochemistry, Stephen F Austin State University, Nacogdoches, Texas, United States(2) Department of Chemistry and Biochemistry, Millsaps College, Jackson, Mississippi, United States*

1,8-Naphthalimide derivatives (Scheme 1) have attracted considerable interest as DNA-binding molecules because their planar aromatic structures can facilitate intercalation between DNA base pairs, potentially disrupting DNA structure and replication. Structural modifications to the naphthalimide scaffold can alter its charge distribution, hydrophobicity, and interactions with DNA, providing opportunities to tune molecular recognition and biological activity. In this study, the interactions of three bifunctional 1,8-naphthalimide derivatives, napht-4ap (4-aminopyridine), napht-4ap-O, and napht-4ap-Et, with calf thymus DNA were investigated using UV–visible absorption spectroscopy, fluorescence spectroscopy, circular dichroism (CD), and agarose gel electrophoresis. Spectroscopic measurements revealed changes in the electronic and fluorescence properties of the naphthalimide derivatives upon DNA addition, consistent with their association with the DNA structure. CD spectroscopy indicated modest perturbation of the native right-handed DNA conformation, with the most pronounced changes observed for napht-4ap-Et. These results suggest that the ethyl-substituted derivative may exhibit enhanced DNA association, potentially involving both intercalative and electrostatic interactions with the DNA phosphate backbone. Gel electrophoresis further supported stronger DNA interaction for napht-4ap-Et compared with the other derivatives. Temperature-dependent spectroscopic studies will further characterize the thermodynamic stability and strength of these DNA–naphthalimide interactions. This work demonstrates how structural modification of naphthalimide salts can influence DNA recognition and provides a foundation for evaluating their potential in chemical biology and therapeutic research.

Scheme 1: Chemical structures of the 1,8-naphthalimide derivatives



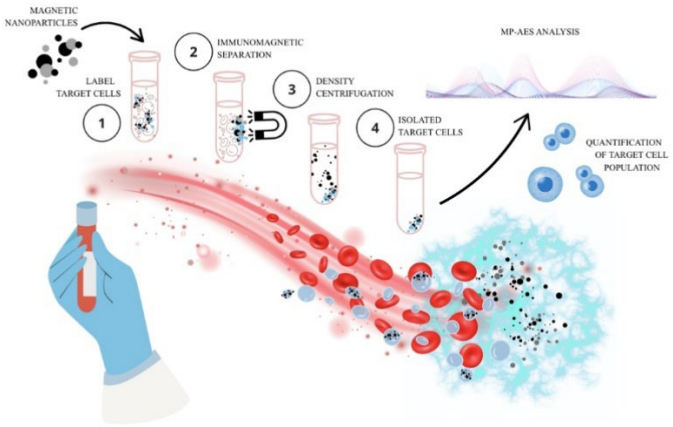
The following scheme shows the chemical structures of (A) 1,8-naphthalimide and the derivatives used in this study: (B) napht-4ap, (C) napht-4ap-O, (D) napht-4ap-Et.

SWRM 2026 SW686

Improving leukocyte-mediated cell-based disease diagnostics across diverse biomatrices via a novel MP-AES cytometry assay

***McKenna McKay**, mckenna.m.mckay@ttu.edu, Dimitri Pappas. Chemistry & Biochemistry, Texas Tech University, Lubbock, Texas, United States*

Blood-based disease diagnostics are a relatively common avenue of interest for liquid-biopsy informed assays. However, this limits detection to systemic disease, leaving potential for identification of localized inflammation and/or infection untapped. To address this, we have developed a nanomaterial-mediated microwave plasma atomic emission cytometry assay with flexible applications across various biological matrices. From cancerous leukocytes in acute leukemia and activated neutrophils in septicemia (peripheral blood) to leukocyte activation in urinary tract infections (UTI; urine), success in achieving sensitive and specific detection of target cell populations elucidates potential for further applications for detection of infectious, inflammatory, and carcinogenic disease. Current diagnostic methods, such as bacterial cultures, are limited in sensitivity, often yielding false negatives in blood samples and false positives in urine samples (e.g. distinguishing asymptomatic bacteriuria from UTIs), prompting misguided administration of prophylactic antibiotics. Improved sensitivity, selectivity, and shorter diagnostic time scales (<1 hour) offer early disease detection, elucidation of upstream contributors to disease development, and simplified monitoring of disease progression and severity, informing improved prognoses for patients. Currently, we have displayed efficacy in blood and urine samples, but anticipate future work aimed at informing cell-based diagnoses in a variety of biological matrices, informing the detection of both systemic and localized disease.



Overview of original assay workflow.

SWRM 2026 SW687

Targeting intracellular uropathogenic *Escherichia coli* with a small-molecule antibacterial agent

***Miguel Gaspar**[1], miguel.gaspar@utdallas.edu, Emily Osborn[1], Ujjaini Basu[2], Swami Sadanala[2], Rakhat Alakenova[1], Samuel Cornelius[2], Wilson Tyler[1], Michael Pustejovsky[1], Alexander J. Mathai[1], Shailendra Koirala[1], Hedieh Torabifard[1], Nicole De Nisco[2], Jeremiah J. Gassensmith[1]. (1) Chemistry,*

The University of Texas at Dallas, Richardson, Texas, United States(2) Biology, The University of Texas at Dallas, Richardson, Texas, United States

Intracellular bacterial infections present a persistent challenge for antimicrobial therapy. A variety of bacterial pathogens can invade or persist within host cells, where the intracellular environment can provide protection from host immune defenses and limit exposure to antibiotics that do not efficiently access these compartments. Consequently, antibacterial activity measured against extracellular bacteria may not translate to effective elimination of intracellular populations, which can survive treatment and contribute to persistent or recurrent infection. Uropathogenic *Escherichia coli* (UPEC), a major cause of urinary tract infection (UTI), exemplifies this challenge by invading bladder epithelial cells and establishing intracellular bacterial populations that can persist within the urothelium and contribute to recurrent infection. Here, we describe BV Jr, a bacterial-targeting small molecule with direct antibacterial activity against UPEC. BV Jr demonstrated antibacterial activity against UPEC and additional clinically relevant Gram-positive and Gram-negative bacterial pathogens and produced rapid reductions in viable bacterial burden. Mechanistic studies provided insight into the processes underlying the antibacterial activity of BV Jr. Given the challenges associated with treating intracellular bacterial populations, we next investigated whether this activity could be extended to UPEC residing within bladder epithelial cells. BV Jr accessed infected bladder epithelial cells and significantly reduced recoverable intracellular bacteria while maintaining short-term compatibility with host cells. In an acute murine model of UTI, a single intravesical treatment with BV Jr significantly reduced both luminal and intracellular UTI89 bacterial burden and outperformed dose-matched gentamicin treatment. Together, these findings demonstrate that BV Jr combines bacterial targeting with antibacterial activity against both extracellular and intracellular UPEC and supports its further development for targeting persistent bacterial infections.

SWRM 2026 SW688

Dual-function molecular probe for fluorescent detection and photothermal treatment of intracellular urinary tract infections

Emily Osborn[1]*, emily.osborn71240@gmail.com, Miguel Gaspar*[1]*, Michael Pustejovsky*[1]*, Alexander J. Mathai*[1]*, Ujjaini Basu*[2]*, Nicole De Nisco*[2]*, Jeremiah J. Gassensmith*[1]*. (1) Chemistry and Biochemistry, The University of Texas at Dallas School of Natural Sciences and Mathematics, Richardson, Texas, United States(2) Biological Sciences, The University of Texas at Dallas School of Natural Sciences and Mathematics, Richardson, Texas, United States*

Intracellular bacterial infections, including urinary tract infections (UTIs) caused by uropathogenic *E. coli*, remain difficult to eradicate because bacteria residing within host cells are protected from both immune surveillance and many conventional antibiotics. Most clinically available antibiotics exhibit poor intracellular activity, while those capable of entering host cells may still be limited by bacterial efflux, enzymatic degradation, or acquired resistance. These challenges motivate the development of targeted therapeutic strategies capable of selectively accessing intracellular bacterial reservoirs. Zn(II)-dipicolylamine (Zn-DPA) complexes selectively recognize anionic phosphates present on bacterial membranes. Conjugation of Zn-DPA to functional imaging or therapeutic platforms therefore provides a means to preferentially target bacteria over mammalian cells. BactVue is a Zn-Oxy-DPA-Cy7 probe that combines an oxygen-substituted DPA targeting ligand with a sterically shielded, zwiterionically modified heptamethine cyanine fluorophore (s775z). This molecular design enables reversible mammalian cell membrane permeation while preserving high bacterial affinity, allowing labeling of intracellular bacteria. This near-infrared (NIR) s775z fluorophore exhibits high fluorescence brightness for imaging and moderate photothermal activity, potentiating it as a dual-function

diagnostic and photothermal therapeutic (PTT) agent. Upon NIR irradiation, localized mild hypothermia (42-45 °C) is expected to induce immunogenic cell death (ICD), enhancing immune recognition of infected cells and intracellular bacterial clearance. Current studies are evaluating the photothermal performance of BactVue in both extracellular and intracellular infection models. Initial findings show reduction in bacterial burdens as a result of PTT. Ongoing work is focused on optimizing irradiation conditions to induce ICD and quantifying damage-associated molecular patterns (DAMPs).

SWRM 2026 SW689

Strain-dependent interactions between lactic acid bacteria and *Bacillus thuringiensis* in mixed-species cultures

***Cephus Bess-Grunewald**, bessgruner@jacks.sfasu.edu, Georgetta Zuo, Violet Bumah, Bidisha Sengupta. Stephen F Austin State University, Nacogdoches, Texas, United States*

Biofilms formed by pathogenic bacteria are difficult to control because interactions among microorganisms can alter bacterial growth, biofilm development, and community structure. Lactic acid bacteria (LAB) can influence microbial communities through competition, biofilm formation, and production of antimicrobial metabolites. This study investigated strain-dependent interactions between selected LAB and Bacillus thuringiensis (Bt) using mono- and co-culture systems. Three LAB strains, Pediococcus acidilactici K19D, Pediococcus pentosaceus K18F, and Lactiplantibacillus plantarum F201, were evaluated individually and in combination with Bt. Growth kinetics were monitored to compare mono- and co-culture responses and determine whether LAB strain identity influenced Bt-associated growth. Scanning electron microscopy (SEM) was used to characterize changes in bacterial attachment, cellular morphology, and biofilm architecture, providing structural evidence of interactions within the mixed-species communities. Ion chromatography (IC) was used to characterize changes in ionic composition associated with the different culture conditions and to complement the morphological observations. The co-culture systems demonstrated distinct, strain-dependent growth patterns. In particular, K18F + Bt exhibited greater growth than the corresponding single cultures, whereas K19D + Bt and F201 + Bt showed different growth responses. SEM and IC analyses provided complementary structural and chemical perspectives on these interactions. Together, the results demonstrate that LAB-Bt interactions are complex and dependent on the interacting LAB strain. Understanding these strain-specific responses may provide a foundation for developing biological approaches to modulate pathogenic biofilms while preserving beneficial microorganisms.

SWRM 2026 SW690

β-carotene production from CO_2-fed microbial electrosynthesis using adaptively evolved and metabolically engineered *Rhodobacter sphaeroides*

***Yuri Kim**[1,3], yuri@kier.re.kr, Hwi Jong Jung[1,3], Minsu Noh[1,3], Jiye Lee[1], Sangmin Lee[2], Changman Kim[3], Soo Youn Lee[1]. (1) Korea Institute of Energy Research, Daejeon, Daejeon, Korea (the Republic of)(2) Chungnam National University, Yuseong-gu, Daejeon, Korea (the Republic of)(3) Chonnam National University, Buk-gu, Gwangju, Korea (the Republic of)*

The utilization of microbial electrosynthesis (MES) has emerged as a promising platform for converting carbon dioxide (CO_2) into value-added biochemicals. *Rhodobacter sphaeroides*, a photoautotrophic and electroactive, has been found to produce spheroidenone-type carotenoids form CO_2. In this study, a strain of *R. sphaeroides* that had been adaptively evolved and metabolically engineered *R. sphaeroides* was developed for the production of β-carotene, which is a high-value carotenoid, through MES. The heterologous *Crtl*4 and *Crt*Y genes were introduced into the wild type (WT) and 30% CO_2-adapted ALE strains with the objective of establishing a β-carotene biosynthetic pathway. The MES experiments were conducted in an H-type reactor under photoautotrophic conditions with a 5% CO_2 supply at −0.6 V (vs. Ag/AgCl) under continuous illumination. It was confirmed that the final product was β-carotene, while lycopene was detected as an intermediate. This confirmed the functional expression of the heterologus carotenoid biosynthetic pathway under MES conditions. The 30% CO_2-adapted ALE strain demonstrated higher β-carotene productivity in comparison to WT under CO_2-fed MES conditions, indicating enhanced metabolic robustness during the process of CO_2 conversion. The results demonstrated that the potential of combining adaptive evolution and metabolic engineering to enable β-carotene production from CO_2 using R. sphaeroides baed MES.

SWRM 2026 SW691

Confidence as an oracle for orthogonal protein design: Boltz-2 and ESMFold2 lead the way for designed proteins

Colter I. Buffford[1,2]*, colterbufford@gmail.com, Zyaja Huggan*[2]*, Jeffrey J. Gray*[2]*. (1) Chemistry, Southern Nazarene University, Bethany, Oklahoma, United States(2) Chemical and Bimolecular Engineering, Johns Hopkins University Department of Chemical and Biomolecular Engineering, Baltimore, Maryland, United States*

Orthogonal protein pairs consist of two proteins that selectively bind to each other and not to their native counterpart that they either evolved or were engineered away from. These systems have therapeutic potential, with applications in cell-based therapies and synthetic signaling networks. Engineering such orthogonal pairs can be difficult because traditional physics-based modeling software like Rosetta has largely approximative energy functions and struggles to capture entropic effects and long-range allosteric changes. This led us to ask if we could supplement and/or complement traditional physics-based analysis with contemporary ML approaches to accelerate the identification of key residues in these orthogonal protein interactions.
To test this, we benchmarked four models, AlphaFold3, ESMFold2, Boltz-2, and Chai-1,on a computationally designed heterodimer and a crystallized dataset. We gathered all of their native metrics and analyzed them to see which metrics correlated best with experimentally determined protein binding. We computed ROC-AUC, ranking-based accuracy, and score margin for each model's native confidence metrics. We then took the structures produced by all models and ran them through Rosetta Fast Relax and its Interface Analyzer Mover to see if the physics-based adjustments and analysis better mediated between correct protein interactions.
Across models, ESMFold-2 and Boltz-2 outperformed the rest of the ML-based models at identifying protein-protein interactions in computationally designed heterodimers. The Fast Relax protocol improved ML-based model predictions mainly when the ML models were already unconfident, but when they were confident, their own native metrics were often better at discriminating protein binders. Moving forward, we are looking to expand our dataset so that we can find a cutoff to aid our endeavors at predicting correct protein interactions and accelerating orthogonal protein design.

SWRM 2026 SW692

Unravelling the impact of linker architecture on PROTAC conformations via atomistic simulation

***Shikshya Bhusal**, shikshyabhusal@my.unt.edu, Austin Thompson, Omar Valsson. Chemistry, University of North Texas, Denton, Texas, United States*

One promising strategy in targeting undruggable proteins is Targeted Protein Degradation (TPD) that employs PROteolysis TArgeting Chimeras (PROTACs). PROTACs are large molecules that include two protein-binding moieties connected by a flexible linker, which can induce proximity and formation of ternary complexes by binding to the target protein and the E3 ligase and forming stable protein-protein interactions. It is known that the linker architecture plays a significant role in the potency and cell membrane permeability. Therefore, understanding the conformational behavior of PROTACs in solution is crucial for optimizing their design and efficacy. While some PROTACs share the same target protein and E3 ligase moieties, they differ in the linker orientation. An example is dBET6 and dBET23 PROTACs, which target bromodomain-containing protein-4 (BRD4) for degradation via Cereblon (CRBN) E3 ligase, and have the same BRD4 and CRBN binding moieties, but differ in the binding orientation to the alkyl group linker. Despite having nearly identical molecular descriptors, these subtle structural differences may lead to distinct conformational behavior and affect their therapeutic potential. In this study, we utilize atomistic simulations to investigate the conformational behavior of dBET6 and dBET23 in different solvents, including chloroform, which has been proposed to mimic the apolar environment of the cell membrane. We apply an enhanced sampling methodology based on Parallel Bias Metadynamics to accurately characterize the conformational ensembles in terms of global CVs. For further analysis, we apply Sketch-map for dimensionality reduction and clustering to identify representative structures and assess conformational diversity. Our findings reveal that, despite being composed of the same moieties, different binding orientations result in significantly distinct conformations for each PROTACs. This shows that subtle differences in the linker can significantly affect conformational behavior, which has implication for the cell membrane permeability. Additionally, our methodology proves an efficient way to characterize PROTAC's conformational ensembles.

SWRM 2026 SW693

Closing the experiment–model–decision loop in chemical science: Chemistry and physics-informed scientific machine learning tools

***M M Faruque Hasan**, hasan@tamu.edu, M G Toufik Ahmed, Rahul Golder, Bimol Nath Roy. Texas A&M University, College Station, Texas, United States*

The emergence of autonomous laboratories offers an opportunity to accelerate catalyst discovery by tightly integrating experiments, mechanistic models, artificial intelligence, and decision-making. However, purely data-driven machine learning can struggle with limited experimental data, extrapolation, physical feasibility, and mechanistic consistency. We present a suite of physics- and chemistry-informed scientific machine learning (SciML) approaches that embed governing equations, thermodynamic relationships, kinetic mechanisms, conservation laws, and operational constraints directly into learning and decision-making. These methods combine first-principles knowledge with experimental data to develop reliable hybrid models for catalytic systems. We present several constraint-embedded SciML tools and open-source codes that can support several interconnected functions required for autonomous laboratories, including hybrid modeling, simulation, parameter

estimation, mechanism selection, optimization, and closed-loop control. Projection- and optimization-based architectures enforce physical constraints during learning and inference, while differential-algebraic equation-informed models capture dynamic behavior and reaction kinetics. These models can be coupled with optimization and control algorithms to identify promising experiments, estimate uncertain kinetic parameters, discriminate among competing reaction mechanisms, and determine operating conditions that balance activity, selectivity, stability, and safety. The resulting framework establishes a pathway toward autonomous laboratories in which experiments and computation continuously inform one another. By integrating chemical knowledge with machine learning and mathematical optimization, physics- and chemistry-informed SciML can enable autonomous catalyst discovery and process development that are not only faster, but also physically consistent, interpretable, and reliable.

SWRM 2026 SW694

Learning slow collective variables via spectral autoencoder maps and iterative metadynamics

sara alinejad[1]*, sara.alinejad@unt.edu, Jakub Rydzewski*[2]*, Omar Valsson*[1]*. (1) Chemistry, University of North Texas, Denton, Texas, United States(2) Faculty of Physics, Astronomy and Informatics, Institute of Physics, Nicolaus Copernicus University, Toru, Poland*

Abstract: Collective variables mediate nearly every modern strategy for accessing slow molecular processes. Metadynamics, transition path sampling, Markov state models, and the emerging generative diffusion models for molecular conformations all depend on low-dimensional representations that faithfully encode the slow degrees of freedom. How well these approaches perform is largely determined by CV quality, and yet constructing good CVs for systems with nontrivial conformational landscapes remains a problem that resists general solutions. We present the Spectral Autoencoder Map, which learns slow CVs by training a (deep) autoencoder whose latent space is shaped by a spectral objective. Specifically, the network maximizes the spectral gap of a Markov transition matrix built from anisotropic diffusion kernels evaluated in the CV space. This forces the learned coordinates to align with the eigenmodes that govern the longest-lived dynamical processes. A reconstruction loss regularizes the latent space against degenerate mappings, while a decorrelation penalty based on pairwise Pearson coefficients ensures that each CV resolves a distinct slow mode. Because the framework incorporates reweighting for biased data, it naturally supports iterative refinement. CVs trained on existing trajectories are deployed in well-tempered metadynamics, and the resulting data are fed back to retrain improved CVs. We apply this scheme to alanine dipeptide in vacuum and to Aib9 in explicit solvent where interconversion between left- and right-handed helical folds occurs on the microsecond timescale. In both systems, the iteratively refined CVs drive sustained barrier crossing and yield free energy surfaces that converge reproducibly across independent simulations. These results show that embedding spectral objectives within an autoencoder architecture offers a practical route to CVs that are suitable for enhanced sampling and more broadly, for any framework that requires a compact, kinetically informed description of molecular dynamics.

SWRM 2026 SW695

AI-accelerated *ab-initio* bottom-up polymer structure prediction of amorphous polyethylene glycol

***Kriti Alam**, kritialam@my.unt.edu, Bharatha K. Gunawardana, Yizhi Song, Hsin-Yu Ko. Chemistry, University of North Texas, Denton, Texas, United States*

Polymers are ubiquitous materials with many applications, ranging from consumer plastics to functional materials in the medical and energy sciences. For example, polyethylene glycol (PEG) is widely used in drug delivery, nerve repair, and surface protection. Disproportional to the wide range of applications, reliable assignment of amorphous polymer structures for PEG (and most other polymers) at atomistic resolution remains an open challenge, impeding theory-guided design of targeted properties. Here, we present an ab initio bottom-up polymer structure prediction (AI2-BPSP) for PEG structures that employs a reactive machine-learning force field trained on first-principles electronic-structure data generated with van der Waals-inclusive hybrid density functional theory (DFT). To achieve sufficient statistical-mechanical sampling of amorphous macromolecules, we further develop a Kubernetes-based cloud computing workflow to enable the scalable deployment of AI2-BPSP. Using this approach, we simulate the living polymerization of PEG under experimentally relevant conditions to generate atomistically resolved structural ensembles as a function of the chain length.

SWRM 2026 SW696

Computational study of Zr/Hf-MOF-808 catalyzed sulfoxide oxidation

***Lauryn Guzman**[1], laguzman@smu.edu, Hafsa Ghuffar[2], Haoyuan Chen[1], Hyunho Noh[2]. (1) Chemistry, Southern Methodist University, Dallas, Texas, United States(2) The University of Oklahoma, Norman, Oklahoma, United States*

Oxygen atom transfer (OAT) reactions are important to a variety of chemical processes, namely within heterogeneous catalysis. Previous research has shown that Zr-MOF-808 acts as an effective catalyst in inducing OAT reactions with a specific substrate, thioanisole, and oxidant, *t*-butyl hydroperoxide. This computational study analyzes two proposed reaction pathways for the Zr/Hf-MOF-808-catalyzed oxidation of methyl phenyl sulfoxide with two oxidants, hydrogen peroxide (H_2O_2) and methyl hydrogen peroxide (CH_3OOH). Experimental research provides the basis for this computational study, presenting opposing trends in the rate of reaction for each oxidant with methyl phenyl sulfoxide depending on the metal identity of the metal-organic framework (MOF), Zr or Hf. The contradictory trends necessitate a detailed focus on the relationship between oxidant strength and reactivity. Within this work, density functional theory is employed to model the catalytic cycle of this reaction via quantum chemical calculations. Free energy diagrams were constructed, and the free energy barrier was calculated for each MOF with each oxidant. In modeling the two reaction schemes for each oxidant with methyl phenyl sulfoxide on both MOF nodes, comparisons of the free energy barrier are drawn to provide insight into the experimentally observed rates of reaction. This study serves to help elucidate the conflicting rate mechanisms and how these mechanisms vary depending on the nature of the oxidant utilized in reaction.

SWRM 2026 SW697

Structural plasticity and functional dynamics of pigeon cryptochrome 4 as avian magnetoreceptor

***CHUANYE XIONG**, chuanyexiong@gmail.com, Palanisamy Kandhan, Brian D. Zoltowski, Peng Tao. Department of Chemistry, Southern Methodist University, Dallas, Texas, United States*

Cryptochromes (CRYs) are flavoproteins involved in circadian regulation and magnetoreception, with Type IV CRYs proposed as candidates for avian magnetic sensing. However, the dynamics of flexible regions such as the cryptochrome C-terminal extension (CCE) and phosphate-binding loop (PBL) remain poorly understood experimentally. Here, we combined temperature replica-exchange molecular dynamics (T-REMD), conventional molecular dynamics, and dimensionality-reduction analyses to characterize the conformational landscape of *Columba livia* cryptochrome 4 (*Cl*CRY4). Full-length *Drosophila* cryptochrome (*d*CRY) was used to benchmark T-REMD sampling and guide the selection of representative *Cl*CRY4 conformations. Autoencoder and time-lagged independent component analysis (t-ICA) projections showed that the selected and conventional *Cl*CRY4 ensembles were contained within the broader T-REMD conformational space, supporting the sampling strategy. *Cl*CRY4 populated multiple distinct CCE conformations and exhibited stronger CCE–PBL dynamic coupling than *d*CRY. Several states also showed differences in PBL gating and CCE orientation. Together, these results reveal distinct conformational dynamics in *Cl*CRY4 and establish a reference-guided computational framework for studying cryptochromes with structurally unresolved flexible regions.

SWRM 2026 SW698

Understanding hydrogen evolution reaction on CoCrFeNi(111) high-entropy alloy surface

*Ahmad Arshadi, **Ye Xu**, yexu@lsu.edu. Department of Chemical Engineering, Louisiana State University, Baton Rouge, Louisiana, United States*

High-entropy alloys (HEAs) offer exciting opportunities for engineering new catalytic materials among many other potential applications, but the complex, heterogeneous nature of HEAs has prevented a clear understanding of their surface reactivity. We take the equimolar CoCrFeNi as an example, which has been shown to catalyze the electrochemical hydrogen evolution reaction (HER) in a 0.5 M sulfuric acid solution with significantly higher activity and stability than all its constituent metals, but why it is so is not understood. We computationally investigate the HER on the CoCrFeNi(111) surface using both density functional theory (DFT) and machine-learning interatomic potentials (MLIPs)-based total energy calculations. Monte Carlo-based sampling of the surface configurations is combined with transition state calculations and microkinetic modeling to enable the simulation of the polarization curves, which successfully reproduce the small activity gap measured between CoCrFeNi and Pt. We conclude that the HER activity originates from protons deposited on weakly binding sites populated at high coverage and proceeds on a subset of the surface sites at ambient temperature.

SWRM 2026 SW699

Task-specific design of metal-organic frameworks for selective gas adsorption

***Shengqian Ma**, shengqian.ma@unt.edu. University of North Texas, Denton, Texas, United States*

Metal–organic frameworks (MOFs) represent a new class of materials, and one of their striking features lies in the tunable, designable, and functionalizable nanospace. The nanospace within MOFs provides virtually plenty of room for imagination, allowing designed incorporation of different

functionalities for targeted applications, such as gas storage/separation, sensing, drug delivery, catalysis. This seminar will illustrate different approaches to engineer the nanospace of MOFs thereby affording MOFs as a versatile platform for applications in selective gas adsorption.

SWRM 2026 SW700

Taming molecular boron nitride

Todd W. Hudnall[1]*, todd_hudnall@baylor.edu, Junyi Wang*[1,2]*. (1) Chemistry and Biochemistry, Baylor University, Waco, Texas, United States(2) Chemistry and Biochemistry, Rice University, Houston, Texas, United States*

Boron nitride (BN) is a highly reactive 8 valence electron diatomic molecule, unstable under ambient conditions; however, at temperatures >900 °C, ceramic $(BN)_n$ polymorphs can be prepared. Isoelectronic to carbon isosteres such as diamond, graphite, and carbon nanotubes (CNTs), $(BN)_n$ polymorphs exhibit remarkably different properties owing to the highly polar B–N bonds. The high temperature synthesis of $(BN)_n$ materials preclude the isolation and study of molecular BN. This presentation will describe our recent report on the synthesis of ^{Et}CAAC-B≡N-B$(C_6F_5)_3$, a donor-acceptor stabilized molecular boron nitride. Single-crystal X-ray diffraction as well as nuclear magnetic resonance, infrared, and Raman spectroscopic studies coupled with density functional theory calculations support the notion that the central B≡N unit exhibits triple bond character.

SWRM 2026 SW701

Intramolecular cooperativity of polytopic Lewis acids in frustrated Lewis pair catalyzed hydrogenations

Clemens Krempner*, clemens.krempner@ttu.edu. Department of Chemistry & Biochemistry, Texas Tech University College of Arts and Sciences, Lubbock, Texas, United States*

Polytopic Lewis acids offer unique opportunities to enhance substrate activation through cooperative interactions between multiple Lewis acidic sites. In this work, various polytopic boranes were evaluated as Lewis acid components in frustrated Lewis pair-catalyzed hydrogenation reactions. In combination with suitable organic bases, the di-, tri- and tetratopic boranes selectively hydrogenate a range of aromatic aldehydes to the corresponding alcohols under mild conditions, whereas structurally related monotopic Lewis acids show little or no catalytic activity. Spectroscopic, crystallographic, and computational studies suggest that the enhanced reactivity of these polytopic acids arises from cooperative substrate binding and hydrogen activation involving multiple boron centers. These findings highlight the importance of spatially organized Lewis acidic sites in promoting bond activation and provide design principles for the development of advanced main-group catalysts for hydrogenation and small-molecule activation.

SWRM 2026 SW702

Harnessing tetrel bonding in donor–acceptor molecular design

***Gyeongjin Park**, gyeongjin.park@uta.edu. Chemistry and Biochemistry, University of Texas at Arlington Research Institute, Arlington, Texas, United States*

As part of our interest in main-group noncovalent interactions, we have developed tetrel-bonding-mediated donor–acceptor systems. Here, we report our efforts to utilize tetrel-bonding motifs as acceptor components in donor–acceptor systems and explore their influence on photophysical properties. Unlike more established noncovalent interactions, such as hydrogen and halogen bonding, tetrel bonding remains relatively underexplored in the design of donor–acceptor systems. We first synthesized and characterized systems incorporating a carbazole donor and an electron-deficient silane as a tetrel-bonding acceptor. While the silicon center exhibited effective fluoride binding, its electronic properties were not ideally matched for the desired donor–acceptor photophysics. This observation led us to extend our design to a stronger carbenium-based acceptor paired with a carbazole donor, providing access to distinct cationic and radical electronic states. These studies highlight the potential of tetrel-bonding-inspired strategies for developing new donor–acceptor architectures and functional optical materials.

SWRM 2026 SW703

Bimetallic catalysis for polymer synthesis and degradation

***Robert Comito**[1], rjcomito@central.uh.edu, Simran Simran[1], Oshani Wijesinghe[1], Pratyush Naik[1], Maxym Tansky[2], Zipeng Gu[3], Qingqing Dong[1]. (1) Chemistry, University of Houston, Houston, Texas, United States(2) Tokyo Kagaku Daigaku, Meguro, Tokyo, Japan(3) Proteogenomics Research Institute for Systems Medicine, La Jolla, California, United States*

This talk will describe our development of bimetallic main group and early transition metal catalysts based around binucleating ligands. Firstly, we introduced binucleating bis(pyrazolyl)alkanes as supports for di(main group) catalysts, including zinc, magnesium, and lithium. We have used them to prepare biodegradable polyesters, including with new selectivity such as highly alternating polyesters. We have also clarified the mechanism of anionic polymerization using dilithium catalysts, providing well-defined poly(aldehydes). Second, we developed heterocycle-bridged binucleating ligands that form well-defined divanadate complexes. Among these complexes, we have found unexpected ferromagnetic complexes and mixed-valent oxidation states. Some of our catalysts are exceptionally active in the aerobic oxidation of diols and of lignin model complexes. We have also depolymerized organozolv lignin into chemical commodities. Overall, our work also provides insight into the mechanism of cooperativity in main group and early transition metal catalysis.

SWRM 2026 SW704

Intraligand secondary interactions as a design principle for organometallic catalysts

***LeGrande M. Slaughter**[1], legrande.slaughter@unt.edu, Fanji Kong[2], Aaron Ruch[1], Matthew C. Ellison[1], Vladimir Nesterov[1]. (1) Department of Chemistry, University of North Texas, Denton, Texas, United States(2) Department of Chemistry, University of Virginia, Charlottesville, Virginia, United States*

The deliberate use of noncovalent secondary interactions to control ligand conformations and ligand-metal or ligand-substrate interactions is a forefront area of ligand design in organometallic catalysis,

with potential to greatly enhance the traditional synthetic toolkit focused on steric and electronic tuning. This synthetic principle is demonstrated in two projects focused on enantioselective gold(I) catalysis. First, in a series of chiral acyclic diaminocarbene ligands derived from isocyanobinaphthyl derivatives, computational and experimental studies implicated weak metal-aryl interactions as a critical factor for creating chiral induction in gold-catalyzed enantioselective transformations of allenes and alkynylbenzaldehydes. In the second study, sterically encumbered, C3-symmetric chiral tris(binaphthyl)phosphite ligands exhibited noncovalent CF3-aryl contacts between binaphthyl substituents that appear to play a key role in creating a rigid chiral pocket around the metal despite these contacts being remotely located. This was exploited to improve enantioselectivities in gold-catalyzed intramolecular hydroaminations of allenes. The chiral phosphite ligands also afforded moderate enantioselectivities in asymmetric Suzuki-Miyaura coupling reactions, including challenging substrate pairs involving minimally substituted aryl and naphthyl partners. X-ray crystallographic and diffusion-ordered NMR studies provided a model to help interpret the substituent-dependent selectivities in these systems.

SWRM 2026 SW705

Exploring the synthesis, characterization, and reactivity of various home- and heteroleptic mono-N-heterocyclic carbene Cu(I) complexes

***Laleh Tahsini**, tahsini@okstate.edu. Chemistry, Oklahoma State University, Stillwater, Oklahoma, United States*

Over the last decade, our group has developed various homo- and heteroleptic Cu(I)-complexes containing imidazole-based NHC, bis(imino)acenaphthene (BIAN)-based NHC, diamino carbene NHC (DAC-NHC), and N-picolyl substituted NHC ligands. Some of these complexes, such as the cationic, three-coordinate [Cu(I(R))(Me_2dpa)]PF_6 and [Cu(SI(R))(Me_2dpa)]PF_6 complexes (R = Dipp, Mes), performed as blue emitters in the solid state.[1] In contrast, changing the NHC backbone to BIAN suppressed the luminescent properties. The complexes [Cu(BIAN-IPr)(Hdpa)]PF_6, [Cu(BIAN-IPr)(3,3′-Me_2Hdpa)]PF_6, [Cu(BIAN-IPr)(3,4′-Me_2Hdpa)]PF_6, [Cu(BIAN-IPr)(3,5′-Me_2Hdpa)]PF_6, [Cu(BIAN-IPr)(3,6′-Me_2Hdpa)]PF_6, [Cu(BIAN-IMes)(Hdpa)]PF_6, and [Cu(BIAN-IMes)(3,3′-Me_2Hdpa)]PF_6, wherein IPr = 1,3-bis(2,6-diisopropylphenyl)imidazole-2-ylidene and IMes = 1,3-bis(2,4,6-trimethylphenyl)imidazol-2-ylidene, have been characterized by ^{1}H and ^{13}C NMR spectroscopies, elemental analysis, CV, and X-ray crystallography. The complexes were moderately effective catalysts for the Buchwald-Hartwig amination of halo- and aminopyridines alongside their imidazole-based NHC counterparts, a reaction previously catalyzed by $Pd_2(dba)_3$.[2] Furthermore, the diamino carbene-based NHC complexes, [Cu(DAC-Dipp)Cl] and [Cu(DAC-Mes)Cl] performed as effective catalysts for the direct carboxylation and esterification of terminal alkynes. The Cu-acetylide complexes bound to the NHC were isolated and characterized crystallographically and spectroscopically as active intermediates in the reaction. Recently, we have also developed the first examples of mononuclear Cu(I)-NHC complexes using 2-picolyl-functionalized NHC ligands and demonstrated an impressive effect of the wingtip substituents on tuning the copper coordination geometry.

SWRM 2026 SW706

Construction and reactions of bidentate bis-chalcogenium Lewis acids

***Brendan Murphy**, blm238_1996@tamu.edu, Francois P. Gabbai. Texas A&M University, College Station, Texas, United States*

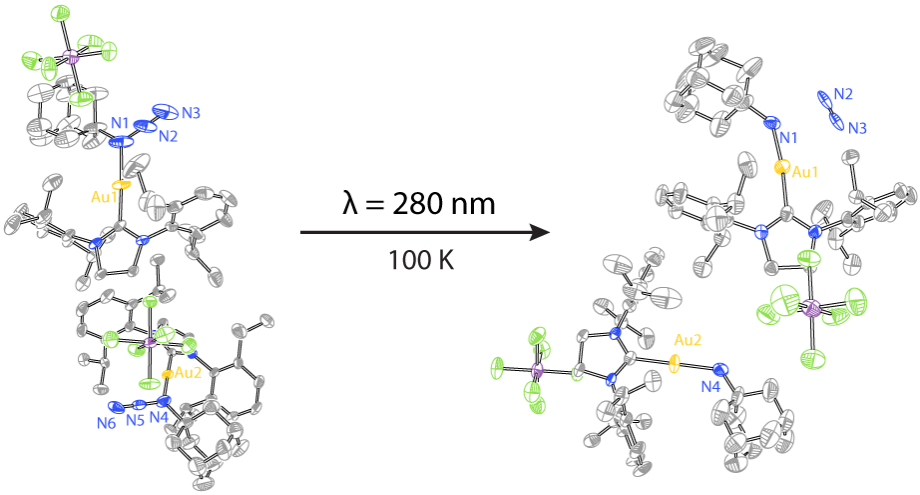
Bidentate main group Lewis acids are often coveted for their capacities to bind anions and to facilitate chemical transformations, especially when these centers are cationic. Well-known examples of such constructs juxtapose telluronium, stibonium, and iodonium moieties to afford a two-point binding pocket. Notably, examples of lighter chalcogenium bidentate Lewis acids are lacking. We report the synthesis and characterization of bidentate Lewis acids featuring sulfonium and selenonium centers. We explore their fundamental Lewis acidic properties, including their affinities towards anions and other Lewis bases, experimentally and computationally. We also apply these towards several Lewis acid-catalyzed transformations. These compounds represent new entries into a growing class of bifunctional Lewis acids.

SWRM 2026 SW707

Trapping gold(I) nitrenes with crystalline matrix isolation

***Debasmita Dutta**, debasmitadutta@tamu.edu, Nattamai Bhuvanesh, David C. Powers. Chemistry, Texas A&M University System, College Station, Texas, United States*

Coinage metal nitrenes have emerged as sought-after reactive intermediates for important transformations like C–H amination and C=C aziridination. Several terminal Cu and Ag nitrenes have been proposed as reactive intermediates in these nitrene-transfer reactions. While nitrenes of Cu and Ag have been characterized, through either synthetic efforts to deliver kinetically stable versions or via photocrystallography, the heavier Au congener (*i.e.*, L_nAu–NR) has thus far eluded experimental scrutiny. Here, we describe the *in crystallo* synthesis of a Au(I) nitrene generated by N_2 photoelimination in the solid state. Both nitrenes, and the anti-Bredt imines that results from formal C-to-N migration within a nitrene complex have been observed and the reaction outcome depends on the extended crystal lattice (dictated by the supporting counterion). The *in crystallo* results are further supported by solid-state IR spectroscopy. The results of related computational studies will be discussed to provide preliminary mechanistic details.



In crystallo photolysis of [(SIPr)AuN(1-Ad)NN][SbF_6] to generate the Au nitrene at 100 K

SWRM 2026 SW708

Stabilizing boravinylidenes through interrupted 1,1-hydroboration and 1,1-carboboration reactions

***MANJUR OYASIM AKRAM**, manjur_akram@baylor.edu, Ayesha Begum, Kirk A. French, Kevin L. Shuford, Caleb Martin. Department of Chemistry and Biochemistry, Baylor University, Waco, Texas, United States*

Vinylidenes (I) represent an important class of fleeting intermediates encountered in a wide range of organic transformations, including the Corey-Fuchs, Seyferth-Gilbert, and Fritsch-Buttenberg-Wiechell reactions. These carbene species feature a six-electron vinyl carbon center, rendering them highly reactive and often poorly selective. In contrast, transition metal-stabilized vinylidene complexes, metal-vinylidenes (II), are well-established organometallic intermediates that enable controlled tuning of vinylidene stability and reactivity, thereby unlocking a broad range of synthetic transformations. The bonding in such systems is well understood, involving σ-donation from the vinylidene to the metal and π-backdonation from the metal to the vacant p-orbital of the vinylidene fragment. Bora-vinylidenes (III), adducts of vinylidene carbenes with boranes, have been proposed as key intermediates in the 1,1-hydroboration and 1,1-carboboration reactions of alkynes and the boranes. Despite extensive studies of these transformations, studies on bora-vinylidenes are inherently elusive. Unlike transition metals, boron lacks d-electrons and therefore cannot engage in π-backbonding to stabilize the electron-deficient vinylidene center. We found that appropriate substituents on the alkynes and borane could enable the stabilization and isolation of bora-vinylidene species in the 1,1-hydroboration or 1,1-carboboration reactions. Furthermore, the insertion reactivity of the isolated bora-vinylidene was investigated, revealing new pathways for bond construction. This work opens new avenues for the development of main-group-stabilized vinylidene chemistry, an underexplored area with significant potential in catalysis and synthetic chemistry.

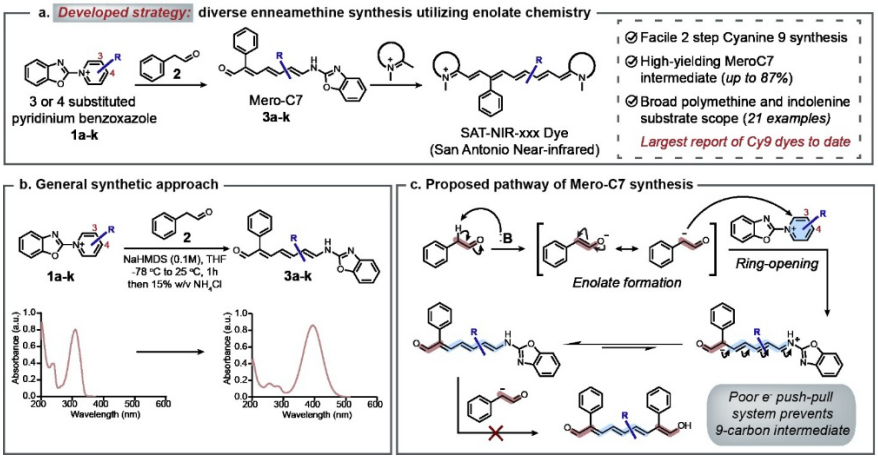
SWRM 2026 SW709

Carbon nucleophile-mediated pyridine ring-opening enables polymethine-functionalized cyanine 9

***Syed Usama**[1], syedmuhammad.usama@utsa.edu, Jared Head[1], Hailee McCulloch[1], Alyssa Kornegay[1], Ulrich Bickel[2]. (1) Chemistry, The University of Texas at San Antonio, San Antonio, Texas, United States(2) Pharmaceutical Sciences, Texas Tech University Health Sciences Center, Lubbock, Texas, United States*

Near-infrared (NIR) fluorophores are widely utilized in biomedical imaging due to reduced light scattering, minimal autofluorescence, and improved tissue penetration, enabling real-time visualization of biological processes. Among these, polymethine cyanines have become indispensable tools owing to their high molar absorptivity, tunable electronic structure, and compatibility with biological environments. Heptamethine cyanines (Cy7), in particular, are ubiquitous NIR fluorophores in biomedical imaging. Significant efforts have therefore focused on diversifying this scaffold through versatile synthetic strategies that enable functionalization of the polymethine backbone. However, most Cy7 derivatives remain limited to absorption below 850 nm, and do not take advantage of the further NIR spectra (850-1000 nm). To address these limitations, we report a general two-step strategy for the synthesis of functionalized Cy9 from commercially available precursors. Inspired by synthetic approaches for Cy7 diversification, the developed method herein exploits the reactivity of electron-deficient pyridinium benzoxazole salts, which undergo pyridyl ring-

opening with enolate nucleophiles derived from phenylacetaldehyde to form a merocyanine-like intermediate (Mero-C7). Knoevenagel condensation with diverse indolenine partners afforded a library of polymethine- and heterocycle-substituted Cy9 derivatives (21 examples; SAT-NIR Fluorophore), representing the most extensive Cy9 series reported to date. Collectively, this method offers a concise, and modular route to Cy9 dyes with absorption beyond 850 nm, bridging the gap between traditional NIR fluorophores and next-generation long-wavelength imaging agents.



SWRM 2026 SW710 - Withdrawn

SWRM 2026 SW711

Biocatalytic, asymmetric oxa-Pictet-Spengler reaction for the synthesis of oxazinoindole derivatives

***Pratap Rijal**, prataprijal052@gmail.com, Beau Thompson, David C. Miller. Chemistry, Oklahoma State University, Stillwater, Oklahoma, United States*

The oxazinoindole core is present in various synthetic compounds with biological activities, such as antidepressant, anticancer, and anti-inflammatory activities. The oxa-Pictet-Spengler (OPS) reaction can be used to synthesize oxazinoindoles. Asymmetric OPS reactions are known for the synthesis of isochroman and dihydropyrans using chiral organocatalysts. Organocatalytic asymmetric OPS reactions of indoles require that the chiral catalyst hydrogen bonds to the indole nitrogen, directly or during post-functionalization, which is not possible with 1-(hydroxyethyl)indole precursors in OPS reactions. Only one example of an asymmetric OPS reaction for the synthesis of oxazinoindoles has been reported using a chiral-BINOL phosphoric acid organocatalyst, achieving 80:20 er and 75% isolated yield. To date, this is an outstanding challenge for modern organocatalysis. Our group recently reported that Squalene-Hopene Cyclase (SHC) enzyme demonstrates promiscuous activity for asymmetric OPS reactions for the synthesis of tetrahydropyranoindoles. We hypothesized that this new-to-nature activity could address existing limitations for the preparation of chiral oxazinoindoles. In this study, we report an engineered SHC enzyme with initial activity for the synthesis of oxazinoindoles, originating from *Zymomonas Mobilis, Zmo*SHC1. With three rounds of additional directed evolution, we identified a highly active mutant that can achieve up to 72% yield and >99:1 er on a 0.5-mmol scale. Also, upon exploring the substrate scope, enantioselectivity is uniformly excellent among all substrates. Our work represents the best reported enantioselective OPS reaction

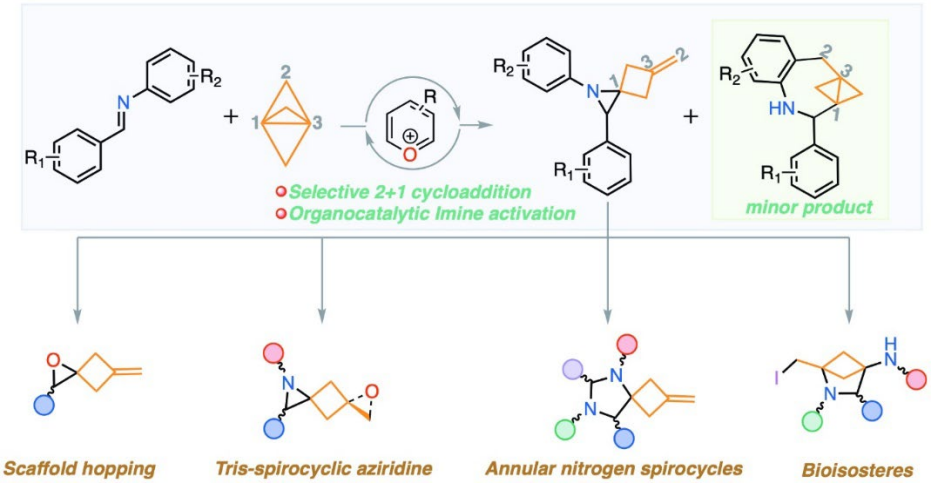
for oxazinoindoles. This finding adds to the versatility of the SHC enzyme and its potential for the synthesis of different fused heterocyclic compounds, which are prohibitively challenging for modern organocatalyst platforms.

SWRM 2026 SW712

5-Methylene 1-azaspiro[2.3]hexanes: Gateway to high Fsp^3 amine chemical space

***Uddalak Sengupta**, udda@tamu.edu, Mason Moreau, David C. Powers. Chemistry, Texas A&M University System, College Station, Texas, United States*

Aziridines, the smallest nitrogen containing saturated heterocycle, have long served as an entry point to biologically relevant amine-containing scaffolds *via* predictable strain-release chemistry. Since the introduction of the concepts of escape from flatland and conformational restriction, high F_{sp}^3 compounds — defined as the number of sp^3 carbon atoms/total carbon count — have garnered significant attention in medicinal chemistry. These three-dimensional architectures maintain rigidity, resulting in improved entropically driven bio-selectivity, reduced lipophilicity, enhanced pharmacokinetics, and metabolic stability. Here, we describe an efficient and modular [2+1] cycloaddition between aldimines and [1.1.1] propellane, promoted by a pyrylium Lewis acid to furnish methylene azaspiro[2,3]hexanes. This simple organocatalytic activation allows rapid generation of an array of spirocyclic aziridines with an exocyclic methylene handle. Systematic manipulation of this product class allows us cover the high Fsp^3 biologically important amine chemical space.



SWRM 2026 SW713

Carbenium-enhanced halogen bonding and applications to catalysis

***Dylan Zhong**[1], dylanz9000@proton.me, Sean Rooney[2], Mohammadjavad Karimi[2], Francois P. Gabbai[2]. (1) Westlake High School, Austin, Texas, United States(2) Texas A&M University, College Station, Texas, United States*

Halogen bonding has recently emerged as an appealing concept in organocatalysis. The design and synthesis of platforms featuring halogen bond donors has been heavily investigated for application in catalysis. In this presentation, we demonstrate that halogen bonding may be augmented by the

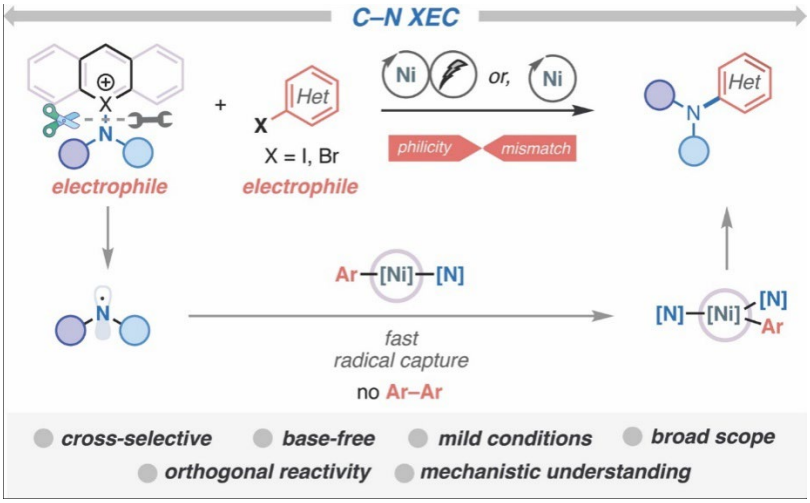
interaction of the halogen bond donor with a Lewis acidic carbenium center. The motif that we will describe consists of an aryl bromide or aryl iodide moiety functionalized by a nearby carbenium ion. The position of the carbenium center in the molecular constructs dictates the possible formation of the X→C$^+$ interaction, as confirmed by Natural Bond Orbital calculations. The catalytic properties of these carbenium-decorated systems were evaluated in the bromination of anisole with *N*-bromosuccinimide, providing evidence for the favorable influence of the X→C$^+$ interaction present in these systems. Our results suggest that the activity of the aryl iodide derivative is markedly higher than that of its bromide counterpart. To enhance the extent of X→C$^+$ charge transfer, we tested the bromination reaction under irradiation with green light and observed faster rates of catalysis in the case of the iodide-containing system.

SWRM 2026 SW714

Base-free C−N cross-electrophile coupling

***Lauv Patel**, lauv@tamu.edu, Samya Samanta, David C. Powers. Chemistry, Texas A&M University System, College Station, Texas, United States*

Metal-catalyzed carbon–nitrogen (C–N) cross-coupling, a philicity-matched reaction of carbon electrophiles with nitrogen nucleophiles under basic conditions, is a foundational tool in modern medicinal chemistry. Here, we report a philicity-mismatched nickel-catalyzed C–N cross-electrophile coupling (XEC) that combines electrophilic carbon and nitrogen precursors. Because the method relies on electrophilic nitrogen precursors, basic additives are not required to activate the nitrogen coupling partner. This mild protocol exhibits broad functional group tolerance, including base-sensitive substrates, and is compatible with late-stage applications. The electrophilic nitrogen precursors can be accessed from diverse starting materials, including C–H bonds and olefins. We demonstrate a two-step, one-pot *N*-phenothiazination, C–N XEC sequence that provides the platform for application of C–N XEC to the functionalization of amine-containing bioactive small molecules. Strategic implementation of C–N XEC enables synthesis of designer secondary and tertiary amines as well as unsymmetrical diamines. Mechanistic investigations indicate the C–N XEC proceeds via a Ni(II)–aryl-amido intermediate and enforces cross-selectivity by avoiding Ni(II)–aryl-halide intermediates associated with homocoupling. These findings establish a paradigm for base-free C–N bond construction and introduce a mechanistic rationale for controlling C–X XEC selectivity.

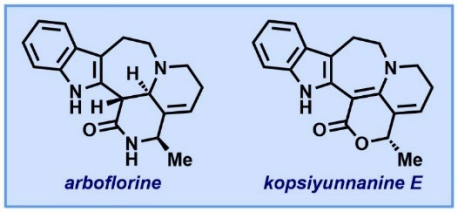


SWRM 2026 SW715

Concise synthesis of kopsiyunnanine E and synthetic efforts toward arboflorine

***Tarak Nayak**, nayaktarak1998@gmail.com, Swapnamoy Ganguly, Myles Smith. Biochemistry, The University of Texas Southwestern Medical Center, Dallas, Texas, United States*

Arboflorine and kopsiyunnanine E are complex pentacyclic monoterpenoid indole alkaloids (MIA) isolated from *Kopsia arborea*. We showcase a concise total synthesis of kopsiyunnanine E proceeding via a known Pictet–Spengler reaction/rearrangement sequence to access indoloazepine core, followed by construction of the remaining six-membered rings via a key radical cyclization/lactonization cascade. A late-stage oxidation protocol completes the total synthesis of kopsiyunnanine E in 10 total steps. Currently, we are focused on the total synthesis of the more complex target, arboflorine, which incorporates an uncommon third nitrogen atom into its MIA framework along with two additional stereocenters. We highlight several early, unproductive approaches toward this natural product, as well as the adaptation of our successful kopsiyunnanine E strategy to ultimately enable the construction of the complete pentacyclic scaffold of arboflorine.



The structures of two MIAs: Kopsiyunnanine E and Arboflorine

SWRM 2026 SW716

Anti-amyloidogenic behaviour of 1,3,6-trisubstituted 4-cinnolinols

***SIDDHARTHA MAJI**, smaji@okstate.edu, Richard A Bunce. Chemistry, Oklahoma State Regents for Higher Education, Stillwater, Oklahoma, United States*

A new approach to 1,3,6-trisubstituted 4-Cinnolinols has been developed and optimized. The method begins with the preparation of the imine from a 2-(2-fluoro-5-nitrophenyl)-1-phenylethan-1-one and a phenyl hydrazine hydrochloride derivative with five drops of triethylamine to neutralize the acid attached to the phenyl hydrazine. Treatment of this imine with the K_2CO_3 in DMF and followed by workup to give the 4-Cinnolinols. Non-aromatic hydrazines were also evaluated as reacting partners but didn't work. Twenty-three derivatives were synthesized and biologically evaluated against hen egg-white lysozyme (HEWL) model to study amyloid fibrillization and its inhibition and the results will be presented with a discussion of factors important to the process.

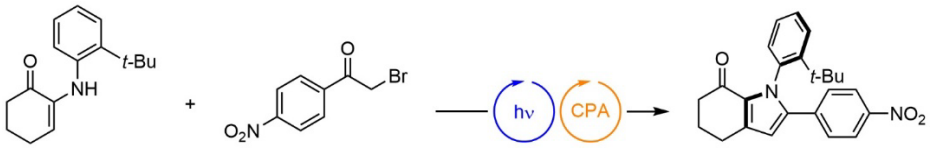


SWRM 2026 SW717

Atroposelective synthesis of axially chiral N-aryl pyrroles from α-enaminones by merging photo redox and chiral phosphoric acid catalysis

***Ashwani Chauhan**, ashwanichauhan@my.unt.edu, Saad Shaikh, Hong Wang. Chemistry, University of North Texas, Denton, Texas, United States*

α-Enaminones have been widely utilized for the synthesis of diverse nitrogen-containing heterocycles, including pyrroles, quinolones, and tetrahydro-1H-carbazol-1-ones, by leveraging their amphiphilic nature. Recent studies from our group have revealed that these substrates can also participate in single-electron transfer (SET) processes under oxidative conditions, affording highly substituted tetrahydroquinolinones and functionalized carbazoles. Building on this insight, we have decided to exploit the intrinsic redox activity of enaminones under photochemical conditions. Initial investigation utilized a well-known radical precursor, 2-bromo-4'-nitroacetophenone, with α-enaminones, leading to the formation of N-aryl tetrahydroindol-7-ones in moderate yield and promising enantioselectivity. N-aryl tetrahydroindol-7-ones is an axially chiral N-aryl pyrrole class molecule, which has great importance in asymmetric catalysis and medicinal chemistry, however their synthetic methodology is limited to ionic condensation of 1,4 diketone and aniline and required very long reaction time and high catalytic loading. Here we are developing an atroposelective route to axially chiral N-aryl pyrroles that merges visible-light photo redox with chiral phosphoric acid (CPA) catalysis. in which $Ir(ppy)_3$ photocatalyzed radical addition of α-bromoketones to α-enaminones is followed by CPA-catalyzed cyclodehydration. The atropisomers are configurationally stable, showing no erosion of enantiopurity over three days in solution at ambient temperature. Ongoing efforts toward catalyst and solvent optimization, suppression of the competing racemic background pathways will be presented.



Synthesis of axially chiral N-aryl pyrroles from α-enaminones by merging photo redox and chiral phosphoric acid catalysis

SWRM 2026 SW718

Nickel-catalyzed deaminative C–C cross-coupling via photosensitized 1,2-dialkyldiazene intermediates

***Mark Jeffrey Diaz**, markjeffreydiaz04@tamu.edu, Quentin Michaudel. Chemistry, Texas A&M University, College Station, Texas, United States*

The intrinsic thermodynamic stability of the C–N bond in aliphatic amines constitutes a fundamental limitation to their utility as electrophilic coupling partners in complex molecule synthesis. Conventional strategies typically necessitate preactivation via bulky activating groups, which raises both practical and environmental concerns. In this presentation, we discuss an atom-economical strategy for C–N bond activation and subsequent cleavage in primary amines, achieved through sequential application of sulfur(VI) fluoride exchange (SuFEx) click chemistry followed by an *aza*-Ramberg–Bäcklund (*aza*-RB) rearrangement. This reaction sequence furnishes 1,2-dialkyldiazenes, which serve as radical pair precursors via extrusion of N_2 upon photoexcitation with blue light under iridium catalysis. Following diffusion from the solvent cage, the resultant carbon radicals are intercepted by a nickel catalyst,

enabling formation of C(sp^3)–C(sp^2) bonds. This presentation details our efforts toward expanding the scope of accessible 1,2-dialkyldiazene substrates, optimizing reaction parameters, elucidating mechanistic pathways, and applying this methodology to the coupling of diverse natural products and pharmaceutically relevant scaffolds.

SWRM 2026 SW719

Rapid mechanochemical synthesis of biologically important enamino carbonyl compounds via ball milling

***Maqhawe Ndlovu**, man8259@utulsa.edu. Chemistry and Biochemistry, University of Tulsa, Tulsa, Oklahoma, United States*

Enamino carbonyl compounds are valuable intermediates in organic synthesis and play an important role in the preparation of pharmaceuticals, bioactive molecules, peptidomimetics, and catalytic ligands. Their conjugated amine–alkene–carbonyl framework provides both nucleophilic and electrophilic character, making these structures versatile building blocks and pharmacophores in medicinal chemistry. As a result, the development of efficient and sustainable synthetic routes to enamino carbonyl scaffolds continues to attract significant attention. The Eschenmoser coupling reaction is a well-established method for the synthesis of enamino carbonyl compounds. This transformation typically involves the reaction of a thioamide with an α-halo carbonyl compound in the presence of a base and has been widely used due to its broad substrate scope and synthetic utility. However, conventional approaches are generally carried out in solution and often require extended reaction times, motivating the search for faster and more sustainable alternatives. In this work, we investigate a mechanochemical approach to the Eschenmoser coupling using ball milling. This method enables the reaction to proceed under solvent-free conditions, eliminating the need for bulk solvents while providing efficient mixing of the solid reactants. Mechanical energy generated during milling promotes effective contact between reagents and facilitates rapid bond formation. Notably, the ball-milling approach allows the formation of enamino carbonyl products within minutes, representing a substantial reduction in reaction time compared with conventional methods. Overall, this study demonstrates that mechanochemical activation provides a rapid, solvent-free, and practical route to biologically important enamino carbonyl compounds, highlighting the potential of ball milling as an efficient tool for sustainable organic synthesis.

SWRM 2026 SW720

Proton relaying in carbenium-based oxygen reduction

***Sean Rooney**, sean1033tr@gmail.com, Mohammadjavad Karimi, Francois P. Gabbai. Chemistry, Texas A&M University System, College Station, Texas, United States*

This presentation will detail our recently published work into proton relaying in the Oxygen Reduction Reaction (ORR) using a carbenium based catalyst.[1] The ORR is an important catalytic process that is relevant to fuel cells, metal-air batteries, organic oxidations, and biological respiration. Traditional ORR catalysts employ transition metals; however, metal-free systems have emerged as powerful alternatives. This study details the preparation of quinoline-carbenium species as a catalyst for the ORR. The investigation shows the quinoline nitrogen can act as proton relay depending on its

position, thereby increasing the rate of H_2O_2 production. The presentation will also disclose kinetic studies, electrochemical studies, kinetic isotope effect studies, and overpotential analysis.

SWRM 2026 SW721

Carbenium ions enabled by proximal phosphine oxides: Redox chemistry, radical formation and hydrogen evolution catalysis

***Xinyue Tan**, x.tan@tamu.edu, Wei-Chun Liu, Francois P. Gabbai. Texas A&M University System, College Station, Texas, United States*

Intramolecular donor-acceptor interactions between Lewis-basic donors and electrophilic carbon centers provide a strategy for tuning the electronic structure and reactivity of carbenium ions. Herein, we report a series of phosphine oxide-supported carbenium ions and their redox and catalytic chemistry. These compounds exhibit reversible one-electron reduction, enabling the synthesis and characterization of the corresponding neutral radicals, while different phosphine oxide groups were found to influence the redox properties of the molecular framework. Notably, these systems also promote the hydrogen evolution reaction under acidic conditions, whereas an analogous carbenium compound lacking the P=O group shows no catalytic activity. Mechanistic studies further support a homolytic pathway for H2 formation. These results showcase the potential of intramolecular donor-acceptor interactions as a versatile platform for tuning the redox properties and reactivity of carbenium-based systems.

SWRM 2026 SW722

Leaving group controlled skeletal editing of pyrroles

***UPASANA CHATTERJEE**, upasana.chatterjee-1@ou.edu, Indrajeet Sharma, Prakash Kafle, Shuhei Yasuda. Department of Chemistry and Biochemistry, The University of Oklahoma, Norman, Oklahoma, United States*

Skeletal Editing plays a very crucial role in diversifying the N-containing heterocycles. In this work, we present a programmable approach for converting pyrroles to pyridines using sulfenylcarbenes. Systematic modulation of leaving groups in the carbenic carbon atom in sulfenyl carbenes enables precise control over the site and nature of functional-group installation during ring expansion. By using this strategy, we will transform pyrroles into privileged meta-functionalized pyridines under mild conditions, while accommodating diverse substitution patterns, including thioalkyl, thioaryl, sulfonyl, and so on. The programmable nature of this approach provides a versatile platform for the synthesis and late-stage diversification of pyridine derivatives, demonstrating the potential of sulfenylcarbene-mediated skeletal editing for controlled heterocycle synthesis.

SWRM 2026 SW723 - Withdrawn

SWRM 2026 SW724

Stereochemically defined cyclohexylamide scaffolds as chiral peptidomimetics for mimicking α-helical surfaces

***Henry Neal**, hxn220012@utdallas.edu, Julia Floyd. Chemistry, The University of Texas at Dallas, Richardson, Texas, United States*

α-Helix-mediated protein–protein interactions (PPIs) are challenging to inhibit because it is difficult to reproduce the exact side chain orientation and spacing necessary for effective molecular recognition. To date, α-helix mimetics, such as aromatic scaffolds, stapled peptides, and foldamers, have shown notable conformational rigidity but often lack systematic stereochemical control and tunable side chain positioning. In contrast, the chiral cyclohexylamide scaffolds we designed uniquely combine enhanced structural rigidity with precise stereochemical control in side chain positioning. This dual advantage allows accurate replication of side chain arrangements found in α-helices and overcomes limitations of previously reported helix mimetics. This is a new class of peptidomimetics engineered to present side chains found at the *i, i+4, i+7,* and *i+11* positions of three helical turns. They comprise stereochemically defined, tri-substituted cyclohexanecarboxylic acids, serving as modular building blocks. Through regio- and stereoselective bromo-lactonization, eight distinct cyclohexane stereoisomers were synthesized and efficiently assembled into cyclohexylamide oligomers. These combinations of rigid three-dimensional structure and stereochemical diversity expand the design space of α-helix mimetics, enabling more selective disruption of PPIs. These scaffolds were employed to emulate the BH3 domains of pro-apoptotic Bcl-2 proteins and induce apoptosis. They were tailored to engage the 3-4 helical turn hydrophobic pocket in anti-apoptotic Bcl-2 proteins like Bcl-xL, where extended scaffolds can maximize molecular contacts, enhancing both binding affinity and biological activity.

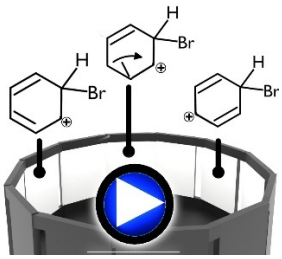
SWRM 2026 SW725

Atom Animator: An open-source plugin for generating animated mechanisms from Chemical Markup Language files

***Timothy Bonzon**, hokeysmoke1123@gmail.com, Jonathan Clinger. Chemistry and Biochemistry, Baylor University, Waco, Texas, United States*

Chemical reactions are intrinsically dynamic processes. The motion of electrons is fundamental to chemistry. However, conventional depictions of chemistry rely on static arrow pushing that can fail to convey the rich dynamics of the transformation and become inefficient for long mechanisms. For this reason, dynamical depictions, such as animations, have been used by researchers and educators to depict mechanisms and chemical transformations. Animations have seen a wide range of use cases from simple callouts to full 3D depictions of cellular processes. Research suggests animation positively contributes to student understanding and concept retention. However, roadblocks exist for the widespread use of animations for depicting chemical reactions and mechanisms. These roadblocks, such as the steep learning curve of software designed for animation, and the difficulties in sensibly incorporating chemistry into animation pipelines, prevent educators from using animation to convey chemistry to students in many cases. We describe Atom Animator, an open-source plugin for Blender that generates ready-to-animate 2D structures from Chemical Markup Language (CML) files. It is designed to facilitate a pipeline from static structure to animated mechanisms for use in the classroom and beyond. CML files can be generated by drawing a mechanism in ChemDraw and imported into Blender using Atom Animator. Current features of Atom Animator include 1) generating

ready-to-animate structures from CML files, 2) creating dynamic bonds between atoms, 3) generating animated arrows for depicting “arrow pushing” mechanisms, and 4) handling lone pairs. Atom Animator handles this all inside the Blender interface, allowing advanced control over mechanism depiction and easy export for use in presentations. We describe the motivation for a 2D animation tool, how to use Atom Animator to animate chemical mechanisms, and selected use cases of Atom Animator for the classroom.



SWRM 2026 SW726

Practical strategies for integrating programming into existing chemistry courses: Lessons from the ACT-CMS community

***Prajay Patel**, pmpatel@udallas.edu. Chemistry, University of Dallas, Irving, Texas, United States*

The growing importance of data analysis, automation, and computational modeling across the chemical sciences has increased the need to develop students' computational literacy throughout the undergraduate curriculum. Yet many chemistry instructors face significant barriers to incorporating programming into their courses, including limited instructional time, a lack of computational expertise, and uncertainty about where programming naturally fits within existing laboratory and lecture experiences. Rather than requiring the development of entirely new computational courses, the Accelerating Curricular Transformation in the Computational Molecular Sciences (ACT-CMS) community affiliated with the Molecular Software Sciences Institute (MolSSI) promotes the integration of modular, openly available computational activities into traditional chemistry curricula.
This presentation will introduce the ACT-CMS community and web portal as a collection of adaptable instructional resources designed to support instructors and their students at a range of computational experience levels. Drawing from experiences as an ACT-CMS Fellow and educator, the talk will discuss practical strategies for adopting Jupyter Notebook–based activities that reinforce core chemical concepts while simultaneously developing foundational programming and data analysis skills. Examples spanning multiple chemistry disciplines will illustrate how computational activities can complement existing laboratory and classroom instruction without requiring substantial curricular redesign. Beyond showcasing available resources, the presentation will highlight lessons learned from implementation, including approaches for scaffolding programming for novice learners, selecting meaningful computational tasks that enhance disciplinary understanding, and fostering student confidence through authentic scientific workflows.

SWRM 2026 SW727

From generative AI to VASR: Integrating AI into advanced chemistry education

***Peng Tao**, ptao@smu.edu. Chemistry, Southern Methodist University, Dallas, Texas, United States*

Generative AI (GenAI) is rapidly changing scientific research and education. In my advanced chemistry courses, I integrate GenAI as a tool for inquiry, critical evaluation, and scientific creativity rather than as a shortcut. Students are expected to document AI use, verify outputs against chemical principles and evidence, and demonstrate independent reasoning. In CHEM 6382, Physical Chemistry of Proteins, students used advanced AI research tools in a class-wide project to explore quantitative measures of protein flexibility and dynamics. They surveyed current literature, connected experimental and computational approaches, evaluated existing methods, and proposed new metrics and validation strategies. Building on this experience, I am developing VASR—Virtual Assistant for Scientific Research, a framework that guides students in using AI throughout the research process while keeping scientific judgment at the center. This presentation will share practical strategies for AI-assisted research, responsible-use expectations, assessment, and lessons learned from the classroom.

SWRM 2026 SW728

From classroom to research: Engaging undergraduate chemists in wine metabolomics through the Freshman Research Initiative and the UT Wine Initiative

Diana Zamora-Olivares[1,2]*, dianapauzo@gmail.com. (1) Undergraduate Education, The University of Texas at Austin, Austin, Texas, United States(2) Chemistry, The University of Texas at Austin, Austin, Texas, United States*

The Freshman Research Initiative (FRI) at The University of Texas at Austin engages undergraduate students in authentic research through a multi-semester curriculum that combines classroom instruction with faculty-mentored projects. As part of FRI, the UT Wine Initiative (UTWI) provides students with opportunities to participate in industry-focused research in partnership with the Texas wine industry. During the spring semester, students develop foundational skills in general and analytical chemistry, experimental design, and data analysis. These skills are subsequently applied to interdisciplinary research projects that address real-world challenges in wine chemistry and enology.

SWRM 2026 SW729

Building-in student success in general chemistry

David L. Catlett*, dlcatlett@udallas.edu,* ***Ellen Steinmiller****, esteinmiller@udallas.edu. Chemistry, University of Dallas, Irving, Texas, United States*

General Chemistry presents significant challenges for many students, including adapting to the pace and rigor of the course, developing effective problem-solving strategies, and connecting lecture concepts with independent practice. This presentation will describe our approach to supporting students through a combination of recitation instruction, pre-exam review sessions with the professor, online homework and the intentional reintroduction of paper-based, hand-written homework notebooks. While online homework provides immediate feedback and opportunities for repeated practice, paper-based work offers a complementary environment in which students can show their reasoning, organize their work, identify errors, and develop problem-solving habits without relying exclusively on digital platforms. Recitation sessions provide additional opportunities for guided problem solving, discussion, and feedback. Together, these practices illustrate how relatively simple

changes to course design can create a more supportive and active learning environment for students beginning their study of chemistry.

SWRM 2026 SW730

Making laboratory skill assessment make sense

***Eszter Trufan**, trufane@uhd.edu. Natural Sciences, University of Houston-Downtown, Houston, Texas, United States*

Practical laboratory competency has long been recognized as a defining outcome of chemistry laboratory instruction. Yet chemistry laboratory instruction and assessment continue to rely largely on assumptions of competency, self-reported capability, and written proxies rather than direct evidence that students can independently perform essential laboratory techniques. In virtually every other domain where procedural competency matters—nursing, engineering, aviation, or the skilled trades—such evidence would be considered insufficient to justify a claim of competency. If practical laboratory competency is truly an intended learning outcome, does it make sense to claim students are competent without ever asking them to demonstrate it? Practical final examinations represent an important step toward answering that question because they replace assumptions with direct evidence of performance. Ironically, they often reveal that many students are unable to independently perform skills they were assumed to have mastered. Yet endpoint assessment introduces a second inconsistency. It documents deficiencies only after instruction has ended, leaving little opportunity to correct them or to understand why they developed in the first place. If the purpose of assessment is not only to verify learning but also to support it, does it make sense to discover students' deficiencies only after the opportunity to address them has passed? The learning sciences have spent decades investigating how procedural expertise develops. Across disciplines, evidence consistently demonstrates that competency emerges through intentionally designed sequences of explicit instruction, observation, guided practice, retrieval, feedback, error correction, and progressively independent performance. These developmental principles are well established, yet chemistry laboratories frequently continue to rely on assumptions that competency will emerge through participation alone or that endpoint assessment will somehow compensate for missing developmental experiences. If we already know how procedural competency develops, does it make sense to design laboratory instruction around assumptions that contradict that evidence? In this presentation, we present a scaffolded skill portfolio that intentionally integrates these evidence-based developmental principles into laboratory instruction and assessment.

SWRM 2026 SW731

From following procedures to scientific reasoning: Redesigning the general chemistry I laboratory

***Jordan Rector**, jordan.r94@proton.me, **Pamela Auburn**, pamela.r.auburn@lonestar.edu. Chemistry, Lone Star College, The Woodlands, Texas, United States*

Our General Chemistry I laboratory curriculum at a large community college had evolved into a collection of loosely connected experiments with inconsistent formats, unclear learning objectives, unnecessarily complex calculations, and limited attention to common misconceptions. Students could successfully follow procedures without fully understanding the chemical reasoning behind them or

how experimental evidence supports scientific conclusions. This presentation describes a comprehensive redesign of the laboratory sequence conducted collaboratively by a course instructor and a student who had recently completed the course. Their partnership combined instructional expertise with firsthand insight into sources of student confusion, unnecessary cognitive load, and disconnection among experiments. Using backward design, the experiments were developed as a progressive sequence that revisits established skills while introducing increasingly complex concepts and techniques. Each laboratory was organized around a central question and designed so that students use experimental data to evaluate a chemical model, confront common misconceptions, and construct evidence-based conclusions. Streamlined procedures allow students to focus on scientific reasoning while developing confidence and transferable skills in measurement, data analysis, graphing, and scientific argumentation. Authentic problem contexts further connect laboratory decisions to applications in environmental monitoring, public health, and industry.Green chemistry principles informed the selection of lower-hazard reagents, smaller quantities, and reduced-waste procedures. These changes improve safety and sustainability while simplifying preparation, storage, and waste management for laboratory staff. Attendees will gain practical strategies for redesigning introductory laboratory curricula to strengthen conceptual understanding, scientific reasoning, student engagement, and confidence while also addressing the operational demands of laboratory instruction.

SWRM 2026 SW732

Start data collection, organization, and analysis in general chemistry lab week one: Why wait?

Scott J. Donnelly*, scott.donnelly@azwestern.edu. Arizona Western College, Yuma, Arizona, United States*

There is no disagreement in the chemistry education community about the importance - from a learning perspective - in students collecting, organizing, analyzing, interpreting empirical data, and comparing/contrasting conclusions drawn from the same data set. This should begin as soon as possible so students have as many opportunities as possible over the course of a semester to hone their interpretive and analysis skills and become more confident in sifting through increasing data complexity. This presentation discusses several 'quick and easy' data collection activities that can be employed week one of the semester either in lab or in the classroom. The activities are easy to set up, use equipment that can be bought at a local Walgreens or DIY big box store, are simple for students to carry out, class data can be collected in less than 15 minutes, and students can instead spend valuable lab time the first week of class (or lab) actually engaged in looking at data for patterns. The activities to be discussed include but are not limited to thermography, the use of handheld IR thermometers, pulse oximeters, and good ol' 5 gallon plastic buckets.

SWRM 2026 SW733

GC-MS, ^{13}C NMR, polarimetery, and thermography: Advancing the teaching of general chemistry with modern instrumentation

Scott J. Donnelly*, scott.donnelly@azwestern.edu. Arizona Western College, Yuma, Arizona, United States*

For students enrolled in first-semester general chemistry, it may be their first encounter with a college-level science course. Unfortunately, too many times both the classroom and lab experiences

do not convey the realities of modern scientific inquiry, nor how science measures what seemingly is immeasurable, nor how scientists see what to the human eye is invisible. This presentation describes a motley mix of classroom and lab activities created so general chemistry students can probe the invisible world of molecules and energy. The activities involve students comparing the gas chromatographic and mass spectral data from the GC-MS analysis of a variety of essential oils, deciphering the structure of a mystery antioxidant from ^{1}H decoupled and DEPT-135 ^{13}C NMR data, comparing the optical properties (and chemistry) of soda beverages produced for US and Mexican consumers, and exploring invisible thermal phenonmena through the use of thermal cameras interfaced to a cell phone.

SWRM 2026 SW734

Simultaneous electro-oxidation and electrocoagulation of contaminated water using modified carbon electrodes under pulse and steady current

riju s robin*, rijusrobinr@gmail.com, Meggan A. Collicelli, Teresa Golden, Saeed Hemmati. Chemistry, University of North Texas, Denton, Texas, United States*

Electrochemical oxidation of contaminants in water can be strongly influenced by mass transport, surface charge distribution, electrode geometry, double layer charging, and electric field screening. In this study we designed a dynamic modulated electrochemical reactor, implementing two rotating and revolving plate electrodes integrated with custom built circuits to control frequency of electrooxidation and double layer chemistry. This mechanic electrode-pulse system is studied under galvanostatic, potentiostatic, and pulse conditions to evaluate how dynamic geometry affects the electric field distribution and double layer, thus influencing the degradation efficiency. Continuous changes in electrode orientation and inter-electrode distance will generate a time-dependent electric field redistribution resulting in periodic disruption and reformation of the electrical double layer. The electro-oxidation of selected PFAS and hormones (including β-estradiol (E2), progesterone, PFOA, PFNA, and PFBA) in water was investigated under extreme current and voltage conditions. COMSOL studies were done to model how electric fields extend behind the electrode in a parallel electrode and how that affects electrode degradation. Our study showed that dynamic changes in geometry and distance affect the electric field distribution and thus changes the double layer. As a result, charged molecules experience enhanced long-range electrostatic attraction toward the electrode surface and can undergo effective degradation.

SWRM 2026 SW735

Runways to waterways: Fate of PFAS and tire-derived organic pollutants in Louisiana’s airports

Md Firoz Al Mamun*, MdFirozAl.Mamun@lsu.edu, Zachary H. Gregg, Khaga R. Sharma, Bikram Subedi. Enviornmental Sciences, Louisiana State University, Baton Rouge, Louisiana, United States*

While aqueous film-forming foam usage makes airports a significant source of PFAS contamination, the extreme friction of heavy aircraft landings simultaneously generates tire-derived organic pollutants (TDOPs) and associated transformation products such as 6-PPDQ. Approximately 2 million annual takeoffs and landings occur across Louisiana's 68 public-use airports. Heavy annual precipitation (>60 inches) and frequent severe storms in Louisiana accelerate the transport of airport-derived

pollutants into regional waterways, threatening both local drinking water sources and the state's vital commercial fishing industry. In this study, we measured PFAS and tire-derived contaminants in surface water collected around five major airports in Louisiana: Louis Armstrong New Orleans International, Alexandria international, Baton Rouge Metropolitan, Shreveport regional, and Lake Charles regional airports. Forty-five PFAS and their precursors and 6 TDOPs were analyzed using LC-MS/MS. Several PFAS including PFBA, PFPrS, PFPeA, PFBS, PFHxA, PFPeS, PFHpA, PFHxS, PFOA, 6:2 FTS, PFNA, PFOS as well as 6-PPD, 6-PPDQ, BTH, 2-OH BTH, MBTH, HMMM were detected at concentrations ranging from ng/L to µg/L. These findings provide critical baseline data for airport runoff management, environmental risk assessment, and regulatory monitoring around aviation facilities in vulnerable coastal regions.

SWRM 2026 SW736

Statewide wastewater monitoring of psychostimulants and synthetic opioids in Louisiana

***Ramesh Sapkota**, rsapko3@lsu.edu, Bikram Subedi. Environmental Sciences, Louisiana State University, Baton Rouge, Louisiana, United States*

Emerging highly potent synthetic opioids, polysubstance abuse, and associated overdose mortality warrant a near-real time surveillance of these substances. Wastewater analysis for residual drugs has been considered an important complementary approach to existing drug surveillance. In this ongoing study, raw wastewater samples are collected from 10 wastewater treatment facilities monthly over a year across five major urban communities in Louisiana and analyzed over 30 psychostimulants, opioids, synthetic opioids, and medications for opioid use disorder utilizing a validated solid-phase extraction and UPLC-MS/MS method. The spatial and temporal drug-use patterns across the state were examined based on the flow and population normalized mass load (mg/day/1,000 people) of drug residues. Integrating wastewater surveillance with forensic toxicology, statewide prescription metrics, and overdose mortality rates provides a comprehensive, multi-dimensional view of drug use trends across Louisiana. By delivering these actionable insights to key stakeholders, this framework can directly inform targeted public health interventions and ultimately save lives.

SWRM 2026 SW737

MgFe layered double hydroxide for excess NO_3^- and PO_4^{3-} nutrient remediation

***aaron caesar**, aacaesa@okstate.edu. chemistry, Oklahoma State University The College of Arts and Sciences, Stillwater, Oklahoma, United States*

Eutrophication, caused by excess nutrients such as nitrates and phosphates, is a major environmental issue that degrades water quality. These excess nutrients can lead to harmful algal blooms and lower dissolved oxygen levels. This study investigates the optimization of magnesium-iron layered double hydroxide (MgFe LDH) with varying Mg: Fe molar ratios for the simultaneous removal of phosphate and nitrate, which can subsequently be employed as a time-release fertilizer. The preparation involved mixing a low-cost, earth-abundant salt solution with a sodium hydroxide solution, followed by overnight aging of the precipitated mixture at room temperature. The precipitates were isolated by centrifugation and washed extensively with water. The final sorbent was obtained by calcining the materials at 500°C. Nitrate and phosphate uptake capacities were determined for

different Mg: Fe ratios, where a 5:1 Mg: Fe LDH ratio showed the maximum capacity for both NO_3^- and PO_4^{3-}. The equilibrium isotherms of NO_3^- and PO_4^{3-} were performed on the optimal material.

SWRM 2026 SW738

Bypassing the spatial limits of acoustic remediation: From interfacial partitioning to anaerobic solid-state nanozymes

***Yunxiang Gao**, yugao@pvamu.edu. Department of Chemistry, Prairie View A&M University, Prairie View, Texas, United States*

Conventional advanced oxidation processes (AOPs) for water remediation rely heavily on outer-sphere reactive oxygen species (ROS). However, ROS-mediated degradation is severely handicapped by short radical diffusion radii and a mandatory reliance on aerobic environments, causing catastrophic catalytic failure in impacted, oxygen-depleted sub-surface systems. Herein, we present a unified physicochemical framework that bypasses the spatial limits of acoustic remediation. First, by evaluating mechanochemically activated cerium oxide against a diverse dye structural library, we delineate the thermodynamic boundaries of classical sonolysis. We demonstrate that non-coordinating emerging contaminants degrade solely via amphiphilic partitioning to the gas-liquid bubble interface. Conversely, entirely hydrophilic contaminants remain geometrically isolated in the safe bulk aqueous phase, evading oxidative attack near the surface of the solid-state catalyst. To overcome this spatial diffusion bottleneck, we also engineered a biomimetic CeO_2 solid-state nanozyme capable of strictly anaerobic, ROS-independent reductive cleavage. Mechanochemical activation unmasks hyper-dense Ce^{3+} oxygen vacancy craters acting as Hard Lewis-acid traps. Deploying a 16-molecule logic matrix, we establish a strict inner-sphere electronic mandate: degradation requires target chelation coupled with an unbroken π-conjugated inner quantum loop. This architecture enables the direct, zero-distance injection of localized 4f polarons into the target's lowest unoccupied molecular orbital (LUMO). Surprisingly, Argon-purged conditions accelerate degradation, confirming a fundamentally ROS-independent pathway driven by flexoelectric shockwaves. Equivalently ball-milled ZrO_2 ($4d^0$) and Al_2O_3 controls exhibit absolute catalytic failure, explicitly isolating the sterically shielded 4f orbital as the mandatory quantum engine. This unified mechanism provides a predictive materials chemistry blueprint for the highly selective, energy-agnostic remediation of emerging contaminants in impacted anaerobic environments.

SWRM 2026 SW739

Removal of per- and polyfluoroalkyl substances from contaminated water using scalable metal-organic frameworks

***Arefeh Mirsharifian**, axm230157@utdallas.edu, Mario Wriedt. Chemistry and Biochemistry, The University of Texas at Dallas School of Natural Sciences and Mathematics, Richardson, Texas, United States*

Per- and polyfluoroalkyl substances (PFAS) are persistent pollutants widely detected in water sources, posing significant environmental and human health concerns due to their toxicity, mobility, and resistance to degradation. Conventional treatment technologies, including activated carbon adsorption and ion exchange resins, often face limitations in removal efficiency, selectivity, and cost-effectiveness. Metal-organic frameworks (MOFs) have emerged as promising adsorbent materials for

PFAS remediation because of their high surface area, tunable porosity, and adaptable chemical functionality. However, translating MOF-based PFAS capture from laboratory studies to real-world applications requires the development of materials that can be produced economically and at scale while maintaining high adsorption performance. In this study, we evaluated Al-fum, a scalable and commercially relevant MOF, for the removal of PFAS mixtures from aqueous systems through both batch adsorption experiments and Rapid Small-Scale Column Testing (RSSCT). The results demonstrated efficient uptake of PFAS across a range of compounds and strong performance under conditions relevant to continuous-flow water treatment. These findings highlight the potential of scalable MOFs as practical adsorbents for PFAS remediation and support their further development for large-scale water treatment applications.

SWRM 2026 SW740

Semiconducting copper(II) oxide sulfate: Synthesis, solid-state chemistry, and electronic structure

Katheryn R. Cruz[1]*, katheryncruz@yahoo.com, Eric J. Cyganowski*[1]*, Abhishek Rawat*[1]*, Alberto Carta*[2]*, Abhishek Adak*[3]*, Chuzhong Zhang*[4]*, Stanley A. Chavez Portillo*[1]*, Efstathios I. Meletis*[4]*, Rajeshwar Krishnan*[1]*. (1) Department of Chemistry & Biochemistry, The University of Texas at Arlington, Arlington, Texas, United States(2) Center for Scientific Computing, Theory, and Data (CSD), Paul Scherrer Institut PSI, Villigen, AG, Switzerland(3) The Abdus Salam International Centre for Theoretical Physics (ICTP), Trieste, Italy(4) Department of Materials Science and Engineering, The University of Texas at Arlington, Arlington, Texas, United States*

An integrated experimental and theoretical approach was used in this study on an intriguing compound variously described in the literature as copper(II) oxide sulfate, $CuO{\bullet}CuSO_4$, or by its mineral name, dolerophanite. Specifically, contrasting with the magnetic and structural aspects previously studied by other authors, the synthesis, solid-state chemistry, and electronic structure are described below with particular emphasis on the thermal, surface, and optoelectronic (semiconductor) properties of this compound. We performed density functional theory (DFT) calculations to simulate the electronic structure of this material. Because standard semilocal DFT is insufficient to capture the strong electron correlations in $CuO{\bullet}CuSO_4$, we refined our approach using two advanced methods: hybrid functionals and dynamical mean-field theory (DMFT) (see below). The results of these calculations are in good agreement with our experimental findings on bandgap energy values from diffuse reflectance spectroscopy. The thermal aspects of the synthesis and decomposition pathways were probed by thermogravimetric analysis; these data were complemented by powder X-ray diffraction, selected area electron diffraction, and Raman spectroscopy. The $CuO{\bullet}CuSO_4$ surface showed very high proclivity to bind an organic dye molecule such as rhodamine B. The adsorptive removal of the dye was studied via cyclic voltammetry and UV–visible spectrophotometry and the applicability of models to describe the adsorption process is finally presented.



SWRM 2026 SW741

Advances toward the Ewing sarcoma cytotoxin altertoxin II

***Max Balderas**, max.balderas@utsouthwestern.edu, Joseph Ready. Biochemistry, The University of Texas Southwestern Medical Center Department of Biochemistry, Dallas, Texas, United States*

Ewing sarcoma (ES) is an aggressive pediatric bone and soft tissue cancer with only 20–30% survival in patients with metastatic or recurrent disease. Current options for treatment-refractory ES are limited, underscoring the need for novel therapies. In 2021, Mooberry and co-workers identified the fungal metabolite altertoxin II (ATXII, Fig 1a.) as a potent cytotoxin (GI_{50} = 8 ± 3 nM) with 25-fold selectivity for ES *in vitro* and in xenograft models. Motivated by its therapeutic profile, we initiated a synthetic campaign toward the first total synthesis of ATXII and subsequent target identification studies. ATXII is a perylenequinone-derived mycotoxin, first isolated from the fungus *Alternaria mali* in 1973. Its highly oxidized, fused hexacyclic framework and four contiguous stereocenters present a significant synthetic challenge. We explored two complementary retrosynthetic strategies: (1) a biomimetic approach enabling a late stage desymmetrization (Fig 1b), and (2) a sequential fragment coupling approach (Fig 1a.). Initial studies have established efficient routes to advanced intermediates relevant to both approaches. In the biomimetic route, stepwise assembly rapidly furnished the perylenequinone core, while optimization of a late-stage desymmetrization remain ongoing. Our fragment coupling approach joins naphthol-derived fragments of comparable complexity. We evaluated complementary sequences in which the biaryl and C(sp3)–C(sp3) bonds were formed in either order. Formation of the right-hand C(sp3)–C(sp3) bond was feasible, although redox manipulations were required to prevent rearomatization and avoid a challenging late stage dearomatization. Alternatively, biaryl bond formation followed by functional group interconversion provided advanced intermediates for evaluating diverse methods to forge the remaining key C–C bond. Both sequences provided access to advanced intermediates en route to ATXII, enabling completion of the total synthesis and future biological evaluation.

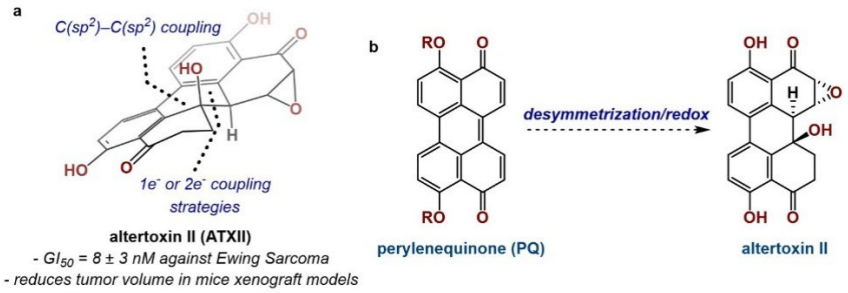


Figure 1. Chemical structure of altertoxin II, fragment-based coupling and biomimetic strategies

SWRM 2026 SW742

Synthesis and evaluation of 6-chloro-N-hydroxy-1H-indole-4-carboxamide as a potential HDAC1 inhibitor

***Inioluwa Adetiloye**, adetiloye.inioluwa@mcm.edu. Biology & Biochemistry, McMurry University, Abilene, Texas, United States*

Histone deacetylases (HDACs) are epigenetic enzymes that regulate gene expression, cell proliferation, and apoptosis. Dysregulation of HDAC activity has been associated with cancer

progression, making HDACs attractive targets for anticancer drug development. Hydroxamic acid-containing compounds are promising HDAC inhibitors because their hydroxamic acid moiety can coordinate the catalytic zinc ion within the HDAC active site. This study investigated the synthesis and anticancer potential of 6-chloro-N-hydroxy-1H-indole-4-carboxamide, an indole-based hydroxamic acid proposed as a potential HDAC1 inhibitor. The target compound was synthesized by converting the indole ester to the hydroxamic acid using hydroxylamine hydrochloride under basic conditions. The product was characterized by using infrared (IR) and proton nuclear magnetic resonance (^{1}H-NMR) spectroscopy. IR analysis showed characteristic O–H, N–H stretching and a carbonyl absorption consistent with the hydroxamic acid functionality, supporting formation of the desired product. ^{1}H-NMR analysis further supported conversion of the starting ester to the hydroxamic acid. The cytotoxic activity of the synthesized compound was evaluated against four cancer cell lines: G361, A375, MCF7, and MB231. Cells were treated with concentrations ranging from 0.01 to 1000 μM, and CC50 values were determined. G361 exhibited CC50 values of 330 and 300 μM, A375 exhibited 410 and 470 μM, MCF7 exhibited 380 and 260 μM, and MB231 exhibited 98 and 130 μM across two experimental determinations. MB231 demonstrated the greatest sensitivity to the compound, exhibiting the lowest CC50 values among the cell lines tested. These results demonstrate differential cytotoxicity across cancer cell lines and support further investigation of 6-chloro-N-hydroxy-1H-indole-4-carboxamide as a potential HDAC-targeting anticancer compound. Future studies will investigate HDAC1 binding, isoform selectivity, and the molecular mechanisms underlying the observed cytotoxicity.

SWRM 2026 SW743

Design and synthesis of self-assembling peptides for the formation of coacervates

***Raniyah Ali**, aliraniyah1126@gmail.com, He Dong. Department of Chemistry and Biochemistry, The University of Texas at Arlington, Arlington, Texas, United States*

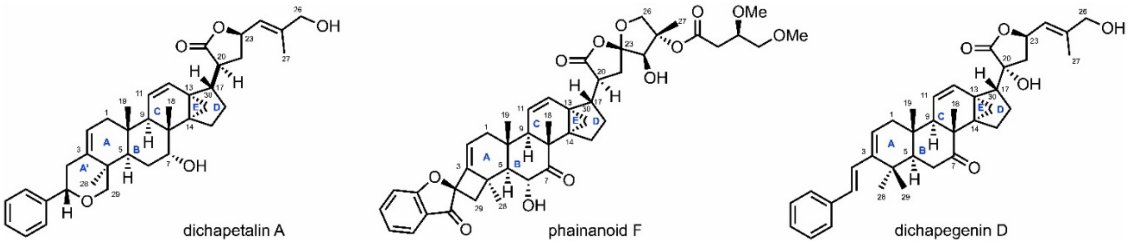
Peptides are versatile molecules that can be engineered to form a variety of nanostructures, which can subsequently be used to construct hydrogels and nanoparticles. In addition, the recent discovery of biomolecular condensates has attracted significant interest for applications in cellular engineering and biological systems. While most current studies on biomolecular condensates primarily focus on intrinsically disordered structures, the role of molecular ordering has received comparatively little attention. However, understanding this aspect is crucial for improving mechanistic insight and expanding the design space of synthetic peptides for constructing functional condensates. Multidomain peptides (MDPs) have emerged as promising candidates in this field because their amino acid composition, sequence length, assembly and disassembly domains, and secondary structural propensity can be tuned to generate partially ordered structures that promote condensate formation. These peptides typically contain amphiphilic regions that facilitate self-assembly into secondary structures, along with arginine residues that play a key role in promoting interactions during coacervate formation. The peptides were synthesized using a solid-phase peptide synthesizer and purified by high-performance liquid chromatography (HPLC). Circular dichroism (CD) spectroscopy was used to analyze the partial secondary structures of the peptides, while matrix-assisted laser desorption/ionization (MALDI) mass spectrometry confirmed successful peptide synthesis. These peptides were further utilized to generate enzyme-triggered condensation, enabling the formation of complex materials suitable for a wide range of biological applications.

SWRM 2026 SW744

Application of pharmacophore-directed retrosynthesis to the dichapetalin family: Synthetic studies toward the C8 side chain and cyclopropane

***Alyssa N. Garcia**, alyssangarc@gmail.com, Nobuyuki Matsumoto, Daniel Romo. Department of Chemistry and Biochemistry, Baylor University, Waco, Texas, United States*

The dichapetalin family, that includes the dichapetalins, the phainanoids, and dichapegenins (representative examples shown below) possess a rare type of triterpenoid carbon framework that includes a unique tetra-substituted cyclopropane and a gamma lactone. Various family members possess potent biological activities which led us to apply pharmacophore-directed synthesis to the dichapetalin family. We developed a synthetic strategy that will allow access to simplified intermediates that possess key structural features that we propose are required for bioactivity. This synthetic strategy will provide structure-activity relationship data toward discovering the minimum structural requirements for bioactivity. Model studies employing a CD-bicycle will be described that have uncovered methods for introduction of the C8 side chain and the cyclopropane which will inform our overall synthetic strategy to the dichapetalin family.



SWRM 2026 SW745

Expanding the fluorinated natural product space: Synthesis of novel phytocannabinoid derivatives

***Jessica C. Thompson**, jessica.c.thompson-1@ou.edu, Prashant Mandal, Shanteri Singh. Chemistry and Biochemistry, The University of Oklahoma, Norman, Oklahoma, United States*

The benefits of incorporating fluorine into pharmaceuticals have been known for decades. This application stems from the chemical properties fluorine possesses resulting from its small size, electronegativity, and ability to form strong polar covalent bonds with carbon. Upon fluorination, pharmaceuticals see a significant difference in metabolic stability, bioavailability, and adjacent hydrogen acidity as compared to nonfluorinated counterparts. Despite the prevalence of fluorine in medicine, especially in the realm of natural products, the structural introduction of fluorine to cannabinoids is virtually unexplored. Cannabinoids, more specifically phytocannabinoids, are compounds which originate in the Cannabis sativa plant and interact within the body's endocannabinoid (EC) system. This involves the binding of cannabinoids to receptors like the CB_1 and CB_2 which can be found throughout the central nervous system and peripheral tissues, respectively. Cannabigerol (CBG) in particular has been shown to bind mainly to the CB_2 receptor and holds antimicrobial and anti-inflammatory properties. The acidified form of CBG, cannabigerolic acid (CBGA), is a precursor for a number of other cannabinoids, the structures of which come about through the enzymatic cyclization of CBGA and subsequent decarboxylation. These "secondary" cannabinoids (i.e. cannabichromene (CBC), cannabidiol (CBD), and tetrahydrocannabinol (THC)) are ones with great pharmacological application. Synthetic routes to fluorinated CBG and CBGA present some practical difficulties given the novelty of the system with methods of fluorination ranging from heavy metal catalysis to electrophilic addition. Additionally, exploration into the structural relationship

of CBG, and its cyclized products, as it relates to its bioactivity has been limited to nonfluorinated analogues. The aim of this study is to develop a variety of novel fluorinated cannabigerol and cannabigerolic acid analogs, perform enzymatic cyclizations, and analyze the biological activity of the derivatives thus expanding the currently limited area of fluorinated natural products.

SWRM 2026 SW746

Asymmetric Ir-catalyzed migratory alkene hydrosilylation: Chirality transfer from chiral *N,O*-silyl acetals

***Linda Lallawmsangi**, lxl9194@mavs.uta.edu. Chemistry & Biochemistry, The University of Texas Arlington College of Science, Arlington, Texas, United States*

An iridium-catalyzed approach to the stereoselective reduction and cyclization of chiral auxiliaries is reported. This method enables chemoselective hydrosilylation to generate stereodefined cyclic *N,O*-silyl acetals under mild conditions with low catalyst loading. Subsequent ring opening provides access to aldehydes with high stereochemical integrity, which can be further transformed into β-hydroxy aldehydes, introducing an additional stereogenic center. The protocol exhibits broad substrate scope, functional group tolerance, and scalability, highlighting its practicality for synthetic applications. Extension to structurally diverse systems demonstrate the versatility of this strategy in constructing stereochemically defined frameworks. Stereochemical assignments of the cyclic *N,O*-silyl acetals were established by ^{1}H NMR coupling constant analysis, while the newly formed stereogenic center was further confirmed by Mosher ester derivatization. Overall, this work outlines a general and efficient platform for stereocontrolled synthesis, providing access to valuable aldehyde intermediates and β-hydroxy motifs relevant to complex molecule synthesis.

SWRM 2026 SW747

Synthesis of highly substituted electron-rich [*n*]-dendralenes via one-pot electrocyclic ring-opening and enolate protection

***Dinorah Ponce**[1], lilianadinorah.perezlimaponce@utsa.edu, Shawn Blumberg[2], Stanton F. McHardy[1]. (1) Chemistry, The University of Texas at San Antonio College of Sciences, San Antonio, Texas, United States(2) Southwest Research Institute, San Antonio, Texas, United States*

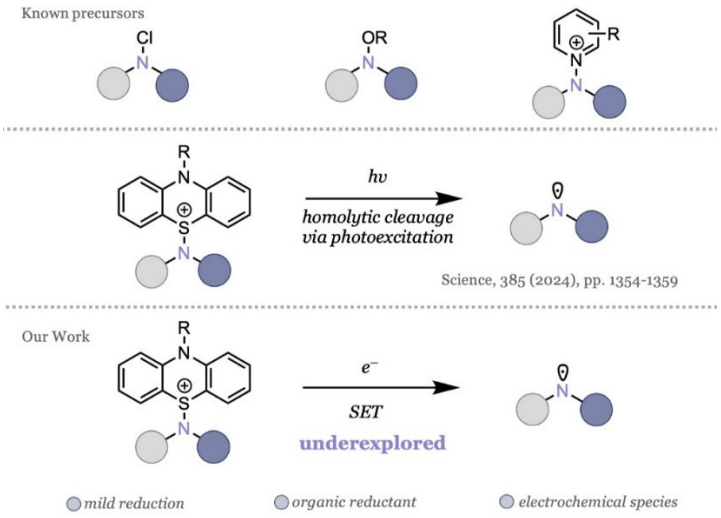
[*n*]-dendralenes have served as reactive entities that enables the formation of complex molecules bearing multicyclic frameworks, which are characteristic of many natural products. This work proposes a novel approach for the preparation of highly substituted electron-rich [3]- and [4]-dendralenes through a one-pot electrocyclic ring-opening and enolate protection reactions. Such [*n*]-dendralenes could later be utilized to assess the synthesis of new classes of antibiotics and novel natural product-inspired molecules using Diene-Transmissive Diels-Alder (DTDA) reactions.

SWRM 2026 SW748

***N*–phenothiaziniums as *N*–centered radical precursors**

***Melissa Ojeda**, melissaojedawwsec@gmail.com, Samya Samanta, Phong Nguyen, David C. Powers. Texas A&M University System, College Station, Texas, United States*

N-Phenothiazinium amine salts are bench-stable precursors to nitrogen-centered radicals. Here, we demonstrate reductive activation of N-phenothiazinium amine salts with tetrakis(dimethylamino)ethylene (TDAE), a soluble organic reductant, generates aminyl radicals and phenothiazine. We utilize the modularity of N-phenothiazinium synthesis to examine the electrochemical properties of a library of salts featuring variation of both the amine and phenothiazine moieties. We have evaluated both N-phenothiazinium amine salts, as well as other available N-centered radical precursors, by cyclic voltammetry to enable quantitative comparison of the facility of radical generation. Our results demonstrate a platform for reductive generation of N-centered radicals that enables the potential needed for radical generation to be systematically controlled by reagent design, which positions N-phenothiazinium salts as attractive precursors to combine with downstream chemistry. Aminyl radicals generated from N-phenothiazinium amine salts are synthetically useful for the formation of base-free C–N coupling and Giese-type additions to Michael acceptors.

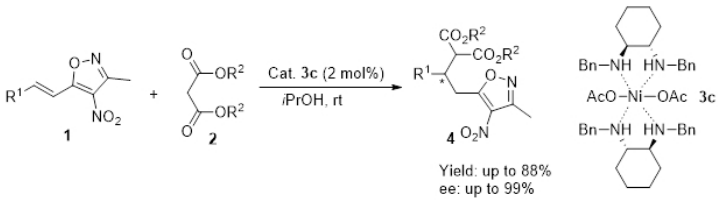


SWRM 2026 SW749

Enantioselective Michael addition of malonate to 3-methyl-4-nitro-5-alkenyl-isoxazoles using chiral Ni(II)-diamine catalysts

*Grace Bediako, Usoshi Moshin, Rion Dell, **Bukuo Ni**, bukuo.ni@etamu.edu. Department of Chemistry and Biochemistry, East Texas A&M University, Commerce, Texas, United States*

A readily prepared Ni(II) complex, Ni(II)-bis(R,R)-N,N′-dibenzylcyclohexane-1,2-diamine, has been developed as an efficient chiral catalyst for the asymmetric Michael addition of 1,3-dicarbonyl compounds to 3-methyl-4-nitro-5-alkenyl isoxazoles. The reaction proceeds smoothly at room temperature to furnish the corresponding Michael adducts in good yields and with high enantioselectivities. Mechanistic studies indicate that the two diamine ligands in the Ni(II) catalyst play distinct and complementary roles: one diamine ligand coordinates to the nickel center and provides the chiral environment responsible for stereochemical induction, while the second functions as a Brønsted base to facilitate enolization of the 1,3-dicarbonyl substrate. This cooperative ligand–base activation mode provides an effective strategy for asymmetric conjugate addition and highlights the potential of readily accessible Ni(II) complexes for the catalytic construction of highly enantioenriched functionalized molecules.

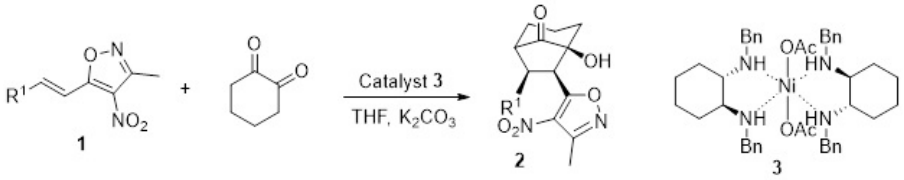


SWRM 2026 SW750

Asymmetric Michael-aldol cascade reactions of 1,2-diones with 3-methyl-4-nitro-5-alkenyl-isoxazoles catalyzed by Ni(II)-diamine complex

*Brandy Grinstead, Rebecca Villalobos, **Bukuo Ni**, bukuo.ni@etamu.edu. Department of Chemistry and Biochemistry, East Texas A&M University, Commerce, Texas, United States*

The development of efficient catalytic methods for the stereoselective synthesis of chiral molecules remains an important objective in organic synthesis because the biological and pharmaceutical activities of many compounds are highly dependent on their stereochemistry. In this study, we investigated the Ni(II)-diamine complex-catalyzed asymmetric Michael–Aldol cascade reaction of 1,2-diones with 3-methyl-4-nitro-5-alkenyl isoxazoles to access structurally complex chiral isoxazole derivatives in a single synthetic operation.



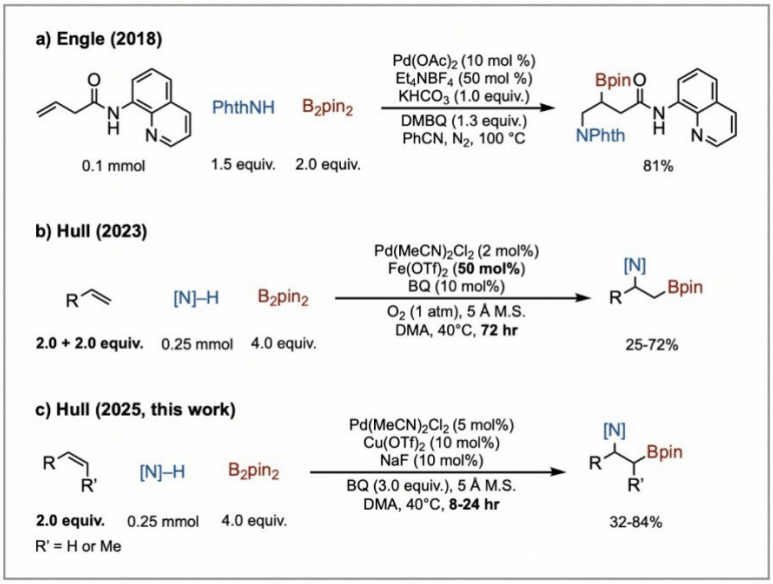
SWRM 2026 SW751

Pd- and Cu-cocatalyzed anaerobic olefin aminoboration

*Saurabh S. Satpute, **Clay West**, ctw2334@utexas.edu, Hannah Wendlandt, Ryan Storteboom, Amol Vibhute, Serhii Vasylevskyi, Cassandra E. Callmann, Kami Hull. The University of Texas at Austin Department of Chemistry, Austin, Texas, United States*

The ability to efficiently and selectively install boron- and nitrogen-containing moieties across an olefin, a cheap and abundant synthetic feedstock, in one step represents a highly practical method for the synthesis of value-added products. *N*-containing moieties are present in a vast majority of FDA-approved drugs, and boronic acids/esters can be utilized as both a synthetic handle and carboxylic acid bioisostere. Utilizing oxidative Pd catalysis with a Lewis acidic metal triflate co-catalyst, the selective formation of β-aminoboronic esters from an olefin has been achieved; however, current methods suffer from rapid Pd-nanoparticle formation that require inefficient leaching to remain catalytically active. In this work, improved conditions for the aminoboration of unactivated olefins have been developed which allow for a broader substrate scope, improved yields, and drastically shorter reaction times using $Cu(OTf)_2$ as cocatalyst, 1,4-benzoquinone (BQ) as terminal oxidant, and substoichiometric NaF as a transmetalation promoter. ICP-OES data show that, unlike previous work using $Fe(OTf)_2$ and O_2, BQ stabilizes Pd(0) and circumvents the need for oxidative leaching of Pd-nanoparticles, leading to a significant rate enhancement for aminoboration. Mechanistic studies on a

model Pd-alkyl complex show that $Cu(OTf)_2$ and NaF work in tandem to promote the borylation step. Finally, the synthetic utility of this process is demonstrated through further derivatization of the Bpin moiety and gram-scale reactions.



Overview of Pd-catalyzed aminoboration

SWRM 2026 SW752

Dearomative C2-borylation of indoles

Ayesha Begum, *ayesha_begum1@baylor.edu, MANJUR OYASIM AKRAM, Caleb Martin. Chemistry and Biochemistry, Baylor University, Waco, Texas, United States*

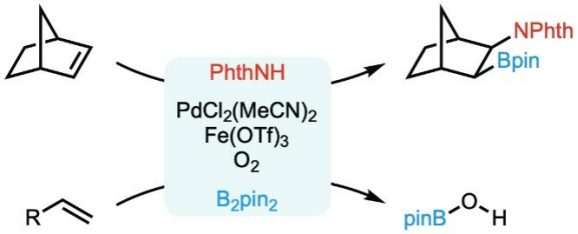
Indoles and indolenines are important structural motifs found in many biologically active molecules and natural products. Compounds bearing these systems have shown anticancer and antiinflammation activities. Considerable advances in metal and metal-free functionalization have been made in recent years. Among these functionalization methods, borylation is of particular interest due to the synthetic versatility of organoboron compounds. In this work, we demonstrate the use of a super-electrophilic borane to induce the dearomative C2- borylation of indoles in excellent yields and under mild reaction conditions to access a stable indolinium core. This method achieves better results in comparison to fluoroaryl boranes.

SWRM 2026 SW753

Olefin borylation with electrophilic palladium

Elizabeth G. Milem[1], *milemeg@utexas.edu, Lillian M. Skinner*[1], *Ya-Nong Wang*[2,1], *Brittany L. Gay*[3,1], *Shreeja Bhatt*[4,1], *Kami Hull*[1]. *(1) Chemistry, The University of Texas at Austin, Austin, Texas, United States(2) Merck, Philadelphia, Pennsylvania, United States(3) Merck & Co Inc, Rahway, New Jersey, United States(4) Mallinckrodt LLC, St. Louis, Missouri, United States*

Initial work for Pd and Fe co-catalyzed aminoboration established an aerobic system in which norbornene and terminal, unactivated olefins produce aminoboration products with a wide range of nitrogen nucleophiles and diboron B_2pin_2. Investigations into this system indicate that the active Fe co-catalyst is an Fe(III) species slowly produced from the aerobic oxidation of an $Fe(OTf)_2$ pre-catalyst, which then forms an electrophilic Pd species highly active within the borylation step. In the case of norbornene as the olefin coupling partner, direct use of the analogous $Fe(OTf)_3$ pre-catalyst species is robust, and results in high yields of selective aminoboration products across the nitrogen nucleophile scope with lower loadings of this Fe(III) source. However, terminal olefins produce low yields of the aminoboration product under these direct Fe(III) conditions. Reaction progress in the case of the terminal olefins reveals rapid and irreversible consumption of the diboron coupling partner occurring preferentially to that of expected olefin by-products. Further studies indicate that the absence of norbornene as olefin instead results in sequential diborylation of the active electrophilic Pd catalyst, which leads to diboron consumption and, ultimately, catalyst degradation. The role of norbornene is elucidated to act as a better ligand to stabilize the electrophilic Pd and, thus, intercepts the deleterious diboron consumption via strain release via product formation in the overall reaction. This furthermore has implications on the necessity of higher diboron loadings in the presence of poorer olefinic substrates under these conditions.

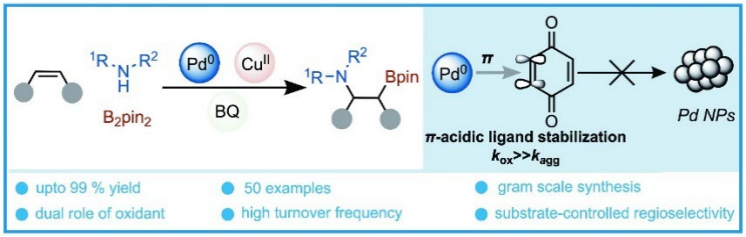


SWRM 2026 SW754

Pd- and Cu-cocatalyzed anaerobic aminoboration of unactivated alkenes

***Saurabh S. Satpute**, saurabh07@utexas.edu, Clayton West, Hannah Wendlandt, Ryan Storteboom, Amol Vibhute, Serhii Vasylevskyi, Cassandra E. Callmann, Kami Hull. Chemistry, The University of Texas at Austin College of Natural Sciences, Austin, Texas, United States*

We have developed an anaerobic Pd/Cu-cocatalyzed aminoboration of unactivated terminal and internal olefins using benzoquinone as the terminal oxidant. These conditions allow for enhanced turnover frequencies and an improved substrate scope relative to those of other Pd-catalyzed aminoboration reactions. These highly practical, selective, and high-yielding aminoboration conditions overcome many of the challenges associated with ligand-free oxidative Pd catalysis. The representative scope of the reaction includes 50 examples. This reaction has an improved scope, turnover frequency, and turnover numbers relative to those of our Pd/Fe-cocatalyzed aerobic aminoboration reaction. The reaction demonstrates substrate-dependent regiochemistry; with terminal alkenes, the Markovnikov regioisomer is favored, while internal vinyl arenes afford the anti-Markovnikov product. Mechanistic investigations support the idea that the rapid rate of oxidation by benzoquinone and Cu-(II) prevents the aggregation of heterogeneous Pd(0) species, allowing the Pd to remain homogeneous throughout the aminoboration reaction. The scalability and downstream synthetic utility of the aminoboration products are also demonstrated.



SWRM 2026 SW755

Green synthesis: Selective cleavage of isatin in peroxide free conditions

***Erika Rochelle**, erochelle@smu.edu, Sudershan R. Gondi, David Y. Son. Chemistry, Southern Methodist University Dedman College of Humanities and Sciences, Dallas, Texas, United States*

Isatin, a bicyclic heterocycle, can be selectively cleaved to create anthranilic acid derivatives. These aminobenzoic acids serve as intermediates in pharmaceutical synthesis and have broad applications in medicinal and organic chemistry. Traditional cleavage methods rely on peroxide oxidants or transition-metal catalysts, which raise safety concerns, add cost, and require difficult purification. In our work, we developed a peroxide- and catalyst-free method that generates sodium isopropoxide in situ to cleave the isatins at room temperature to 60 °C, giving anthranilic acid derivatives in 91-98% yield. Our reaction is selective for isatins containing electron-withdrawing groups at the 5- and 7-positions. This selectivity offers a practical advantage: it allows isomeric mixtures of isatins to be resolved by selectively hydrolyzing the reactive isomer, without the need to separate the isatins directly. Overall, these results produce a safer, more practical, and versatile route to pharmaceutically relevant anthranilic acid derivatives.

SWRM 2026 SW756

Synthesis and separation of hexose-6-phosphate utilizing ion exchange techniques

***Ashton Drake**, aed6477@mavs.uta.edu. The University of Texas at Arlington, Arlington, Texas, United States*

This study highlights the laboratory synthesis of ^{13}C-labeled hexose-6-phosphate for measuring bacterial enzyme activity by NMR. This work also presents a comparative evaluation of ion-exchange chromatography methods for downstream purification. Because crude mixtures often retain unreacted substrates, non-phosphorylated sugar, and alternative structural isomers, optimization of the isolation protocol is vital to eliminate chemical artifacts that distort kinetic data. This work establishes a workflow bridging chemical synthesis and functional biochemistry, providing a scalable template for producing assay-ready metabolic intermediates.

SWRM 2026 SW757

Reductive transformations of carbonyl compounds mediated by 1,4-dihydropyridine anions and visible light irradiation

***Viraj M. Miyuranga**, virajmiyu@gmail.com, Prasadi Gallage, Kayman Ross, Spencer Pitre. Chemistry, Oklahoma State University, Stillwater, Oklahoma, United States*

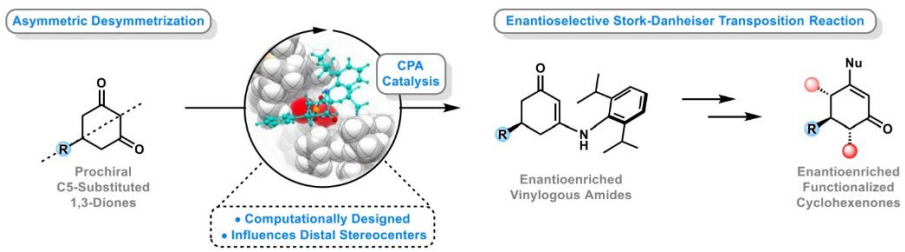
Ketyl radicals are useful reactive intermediates in organic synthesis, providing an umpolung of the reactivity of carbonyls that allows for C−C and C−heteroatom bond forming reactions. These radicals are usually produced by single-electron reduction of aldehyde or ketone, but this approach requires highly reducing conditions to satisfy the thermodynamic requirements of unactivated carbonyls, especially aliphatic substrates ($E_{1/2}$ < −2.2 V vs. SCE). Traditionally, this reduction has been achieved using air- and moisture-sensitive, toxic, and expensive-to-handle ground-state metal reductants like SmI_2 and Cp_2TiCl_2. Photoredox catalyzed methods are milder but can be restricted to aromatic substrates. In this work, we demonstrate that visible-light excitation (456 nm) of anionic 1,4-dihydropyridines can produce an excited state with an oxidation potential of −2.65 V vs. SCE, which is high enough to access ketyl radicals from both aromatic and aliphatic carbonyl groups. Our progress in applying this method to the reductive ring-opening of α-epoxyketones, pinacol coupling, imine homocoupling, and lactone formation will be presented.

SWRM 2026 SW758

Enantioselective Stork-Danheiser transposition enabled by a computationally designed chiral phosphoric acid catalyst

***Jordan M. Martinez**, jordanm1598@outlook.com. Biochemistry, The University of Texas Southwestern Medical Center, Dallas, Texas, United States*

The development of new Brønsted acid catalyzed methods to furnish asymmetric transformations persists at the forefront of synthetic chemistry. Since their introduction, chiral phosphoric acids (CPAs) have been established as versatile and reliable chiral Brønsted acid catalysts. However, the reports using these privileged chiral catalysts typically focus on their ability to control enantioselectivity near the reaction site – leaving distal enantioselectivity lagging. Herein, we disclose our recent work on the enantioselective synthesis of vinylogous amides with distal stereocenters via chiral Brønsted acid catalysis, which enables access to an enantioselective Stork–Danheiser Transposition (SDT) reaction. The SDT reaction is a landmark method for generating substituted cyclohexane architectures in complex molecular settings, however enantioselective versions often rely on the use of stoichiometric chiral auxiliaries. We rationalized that the historic SDT reaction could be made enantioselective through the asymmetric desymmetrization of cyclic 1,3-diketones using a computationally designed CPA. DFT calculations from the Tantillo Lab (UC Davis) identified key CPA-substrate interactions, which were experimentally confirmed to be crucial for achieving high distal enantioselectivity.



SWRM 2026 SW759

Copper-containing N/O-donor macrocycles for benzylic and allylic oxidation catalysis

***Amreet Kaur**, amrekaur@ttu.edu. Chemistry, Texas Tech University, Lubbock, Texas, United States*

Copper is an earth-abundant and less resource-intensive alternative to many late-transition-metal catalysts, motivating the development of copper-based systems for more sustainable oxidation chemistry. Copper complexes supported by N/O-donor polydentate macrocycles were examined as catalysts for benzylic and allylic C-H oxidation. The copper(II) species were generated by direct metalation of the macrocyclic scaffold and evaluated under varied conditions to establish general reactivity trends. These complexes promoted efficient oxygenation with tert-butyl hydroperoxide under modest heating and accommodated a range of substitution patterns across representative substrates. Preliminary scale-up trials indicated that the system can operate beyond small-batch screening. Overall, the study outlines a versatile copper-macrocycle oxidation platform and provides a foundation for further mechanistic and scope-driven exploration.

SWRM 2026 SW760

Synthesis of achiral squaramide catalysts for use in organocatalyzed reactions

***Francis K. Kekessie**, francis.kekessie@usm.edu, Elizabeth M. Shirley, Julie A. Pigza. Chemistry And Biochemistry, University of Southern Mississippi, Hattiesburg, Mississippi, United States*

Squaramide (SQ) organocatalysts are bifunctional catalysts composed most often of an acidifying group and a basic tertiary amine component. They can catalyze a wide range of reactions by taking advantage of noncovalent interactions (NCIs) between substrates. Noncovalent interactions (NCIs) are the collection of both favorable and unfavorable interactions between molecules that ultimately determine the fate of reactions. Chiral SQ organocatalysts employed in organic synthesis convert achiral or prochiral substrates to chiral products yet are difficult to make and are expensive to purchase. On the other hand, achiral squaramides yield racemic products or can be used to probe diastereoselectivity, but they are readily accessible in the lab. Our group has found them key for screening new organocatalyzed reactions towards the synthesis of small molecules of relevance in the pharmaceutical and chemical space to find ‘hits’. This work describes a two-step synthesis of achiral squaramide organocatalysts from commercially available materials with varying acidifying and basic groups. We successfully synthesized 40 achiral squaramide catalysts using this procedure. We also demonstrated their utility by screening them in various known reactions to show proof of concept.

SWRM 2026 SW761

Synthesis of β-diketone scaffolds for the selective formation of α-acyloxy ketone motifs

***Claire Martinez**, c.martinez022603@gmail.com, Reagan P. Carter, Sarah Walbridge, Sandra M. Simmons, Meagan E. Hinze. Chemistry, Sam Houston State University, Huntsville, Texas, United States*

The Baeyer-Villiger reaction oxidizes ketone functional groups into esters. Traditional chemical syntheses often utilize harsh reagents such as peroxyacids, may require excess reagents, increase safety risks at high concentrations, and create environmentally hazardous by-products. To address these obstacles and offer a greener alternative, we aim to investigate a biocatalytic strategy utilizing

flavin-dependent Baeyer-Villiger monooxygenases (BVMOs). These versatile enzymes have the potential to perform oxidations with regio-, chemo-, and stereoselectivity. Furthermore, BVMOs offer an eco-friendly solution due to their utilization of molecular oxygen, mild reaction conditions, and creation of non-hazardous by-products. To expand the synthetic utility of this class of biocatalysts, we aim to construct a diverse substrate library composed of scaffolds. Compounds incorporating symmetrical diketones would provide access to α-acyloxy ketone motifs. Preliminary results will compare chemical and enzymatic oxidation outcomes across our substrate library. Orthogonal synthetic routes for the α-acyloxy ketone standards will also be described.

SWRM 2026 SW762

Substituent effects on hydration equilibria of biomass-burning-relevant aromatic aldehydes by variable-temperature H NMR spectroscopy

***madiha mazhar**, madiha.mazhar@okstate.edu, Ahmadraza Chaudhary, Justus rogers, Elijah Schnitzler. chemistry, Oklahoma State University, Stillwater, Oklahoma, United States*

Biomass burning emits many further oxygenated phenolic compounds, including benzaldehydes like vanillin, into the atmosphere through the thermal decomposition of lignin. Atmospheric processing, including aqueous chemistry, can lead to further functionalization, e.g., nitro addition to vanillin has been observed in water. Consequently, benzaldehydes with hydroxy, methoxy, and nitro substituents can all result from biomass burning, and these species may undergo hydration to geminal diols in cloud droplets and aqueous aerosol particles, influencing their partitioning and fate. Here, we use variable-temperature H NMR spectroscopy to investigate the hydration equilibria for a series of these species, from benzaldehyde to nitro-substituted vanillin, in D_2O. For each compound, the methine-proton integrals were normalized to the non-exchangeable aromatic-proton integrals to account for fluctuations in overall intensity and allow determination of the hydration equilibrium constant, K_{hyd}, at each temperature. Spectra collected from 5 to 70 °C revealed strongly compound-dependent hydration. For 3- and 4-hydroxybenzaldehyde, the methine signal was strong enough to determine the hydration equilibrium and its temperature dependence, allowing van't Hoff analysis. For vanillin, the methine signal was too weak for reliable quantification of hydration, consistent with suppression of carbonyl electrophilicity by electron-donating substitution. In contrast, the nitro-substituted hydroxybenzaldehydes exhibited additional temperature-dependent resonances and more complex aqueous speciation, consistent with enhanced hydration associated with electron-withdrawing substitution. Our results demonstrate that even for large benzaldehydes hydration can be appreciable, and that atmospheric aging, e.g., aqueous addition of a nitro group to vanillin, can significantly shift the extent of hydration for biomass-burning emissions.

SWRM 2026 SW763

Developing prototype Raman-active drugs for real-time *in situ* drug delivery

***Christian Morkeh**, cxm5079@mavs.uta.edu. Chemistry, The University of Texas at Arlington, Arlington, Texas, United States*

Biofilm associated infections have become one of the most long lasting clinical challenges due to their extracellular polymeric matrix, reduced metabolic activity, and extensive resistance to conventional antibiotics. Current drug delivery platforms, such as nanoparticles, hydrogels, and label free Raman

methods, enable controlled release and material tracking but lack real time, drug specific monitoring inside bacterial biofilms, a crucial gap that limits mechanistic understanding and rational therapeutic design of antibiotics. This work presents a Raman active antibacterial drug system engineered by incorporating strong vibrational reporter groups such as nitro, alkyne, and nitrile groups into existing antibiotic scaffolds, enabling each drug to produce a unique, measurable Raman fingerprint. The modified drugs are loaded into a biocompatible, Raman silent pEtN PVA hydrogel, allowing non invasive, time resolved tracking of drug release and penetration. Using Raman spectroscopy, drug specific peak intensities can be monitored in situ to generate real time release kinetics, spatial distribution maps, and depth resolved penetration profiles within biofilm structures. This integrated system would provide the prototype platform for real time, in situ monitoring of antibacterial drug transport, offering new mechanistic insight into drug biofilm interactions and enabling data driven optimization of future antimicrobial delivery strategies.

SWRM 2026 SW764 - Withdrawn

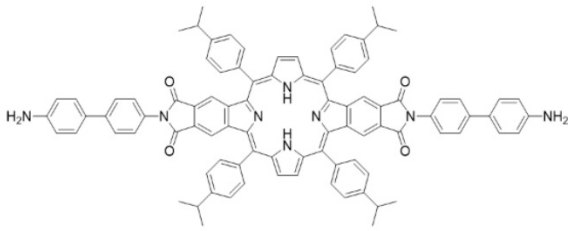
SWRM 2026 SW765 - Withdrawn

SWRM 2026 SW766

Synthesis and characterization of *β*-functionalized porphyrins as building blocks for covalent organic frameworks

***Rajendra Adhikari**, rajendraadhikari@my.unt.edu, Hong Wang. Chemistry, University of North Texas, Denton, Texas, United States*

Covalent Organic Frameworks (COFs) are crystalline, porous materials formed by connecting organic building blocks through strong covalent bonds to create highly ordered and tunable frameworks. They have high surface area, well-defined pore structure, and adjustable pore size. Porphyrins are used as building blocks for COFs due to their large π- conjugated system, strong visible light absorption at UV- visible region, metal binding ability and tunable functional groups. In this work, we are using *β*-functionalized porphyrins as one of the monomers to construct the COFs. Generally, porphyrins are used as electron donating units in donor-acceptor architectures. In this work, porphyrins are converted to electron-acceptors by attaching electron-withdrawing groups at the porphyrin *β,β*'-positions. This porphyrin monomer will be linked with another complimentary organic monomer to form extended COF frameworks. These porphyrin-based COFs will be characterized by Powder X-ray Diffraction (PXRD), Fourier Transform Infrared Spectroscopy (FTIR), solid state ^{13}C NMR spectroscopy and Brunauer–Emmett–Teller (BET) analysis. SEM (Scanning Electron Microscope) and TEM (Transmission Electron Microscope) will be used to study their morphologies. The ability of the COFs to transport electrical charge will be evaluated by measuring electrical conductivity. Finally, this study will be beneficial to understand the potential use of *β*-functionalized porphyrin-based COF for optoelectronic applications.



SWRM 2026 SW767

Thermodynamic characterization and optimization of imidazolium based ionic liquid modified reversed phase HPLC system

***Ayan Paul**, ayanpaul2@my.unt.edu, William E. Acree, Teresa D. Golden. Chemistry, University of North Texas College of Science, Denton, Texas, United States*

Fentanyl, fentanyl analogues and basic drugs face a critical analytical challenge in forensic and analytical science as their protonation on C18 reversed phased column triggers ion-exchange interaction with residual silanol groups in the column. This results in peak tailing, retention irreproducibility and co-elution of positional isomers. This research applies imidazolium Ionic Liquids (ILs) as dynamic surface modifiers and the Abraham solvation parameters (LSER) to convert empirical method development into a predictive mechanically sound framework.
Three specific aims are proposed: 1) Thermodynamic characterization such as derive Abraham system constants for C18 column modified by EMIM Cl (C_2), HMIM Cl (C_6) and OMIM Cl (C_8) across multiple concentrations using a diverse 60 compounds training set. 2) Model driven optimization: using derived constant to predict and validate optimal IL concentration for separating basic drugs, fentanyl analogues, and positional isomers. 3) Transfer and further optimize this method toward mass spectrometry compatible volatile additives and covalently bonded IL stationary phase.
Preliminary TLC and HPLC data show that IL modified silanol suppression depends on the compound hydrogen bond basicity (B-Value). Caffeine (B=1.28) and p-nitroso phenol (B=0.79) show maximum retention factor retention after addition of HMIM both in RP-HPLC and RP-TLC. The expected outcome is a validated, quantitative and broadly transferable approach to separating challenging basic pharmaceuticals and fentanyl analogues, converting analytical method development from trial and error into a predictive design with thermodynamic principles. This work extends the gas phase IL Abraham paradigm into the liquid phase, addressing a critical gap in forensic and toxicology chromatography.

SWRM 2026 SW768

Speciation of silver complexes and their effect on palladium-catalyzed C–H functionalization

***Sophia de Aquino Veras**, sxd200050@utdallas.edu, Faith Tung, Marianne Dizon, Dax Hildebrand, Lilith Voss, Connor Delaney. The University of Texas at Dallas School of Natural Sciences and Mathematics, Richardson, Texas, United States*

Palladium-catalyzed C–H functionalization is widely versatile and frequently used in late-stage functionalization of complex molecules. Commonly, these reactions employ a cocktail of directing groups, ligands and silver salt additives that are crucial for high yield. Although the interactions between these groups and the palladium catalyst have been studied, potential interactions between

the ligands and silver salts have not been investigated. However, the same motifs that facilitate metalation by palladium can also allow metalation by silver. This suggests that metalation by common silver salts could be possible, forming *in-situ* silver complexes that can influence the reactivity of silver towards the palladium catalyst. Our studies show that a variety of common ligands and directing groups, as well as other common additives, are metalated by silver acetateHH. The degree of metalation depends on the structure of the additive and the solvent, and in several cases the resulting silver complex is significantly more soluble than silver acetate. Further investigations show that soluble silver salts afford higher rates and yields for oxidation of a model Pd(0) complex than insoluble salts. Our studies suggest that, in addition to previously considered roles, ligands and directing groups can act as phase transfer catalysts that tune the reactivity of Ag(I) and facilitate catalyst regeneration by oxidation of Pd(0).

SWRM 2026 SW769

Light-activated natural products as deployable antimicrobials

Brayden Stackhouse*, brayden.stackhouse@mavs.uta.edu, Gurleen Kaur, Alisher Talgatov, Dalton Lucas, Broderick Nelson, Ge Shi, Sherri A. McFarland. University of Texas at Arlington Research Institute, Fort Worth, Texas, United States*

Antibiotic resistance poses a major global health and agricultural challenge, threatening both human and animal health. We propose that light-activated natural product extracts derived from widely cultivable plants could serve as inexpensive, deployable anti-infective agents for use in resource-limited settings, including field applications and veterinary medicine. Light-triggered natural products can be highly potent and are particularly suited for topical or surface treatments where illumination is feasible, reducing the need for systemic antibiotics. We hypothesize that these extracts act through the light-induced production of reactive molecular species (RMS), leading to broad oxidative damage that may be less prone to conventional resistance mechanisms. Our preliminary results show that plant extracts containing light-responsive secondary metabolites display strong light-dependent antimicrobial activity. Ongoing studies aim to quantify activity and evaluate formulation strategies suitable for portable, phototherapeutic anti-infectives to prevent or control infection in field and veterinary environments.

SWRM 2026 SW770

Nature meets light: Investigating natural product for antimicrobial photodynamic therapy

Kim Luu*, kimluu141203@gmail.com, Brayden Stackhouse, Gurleen Kaur, Alisher Talgatov, Chelsea Kimberlin, Colin Cameron, Sherri A. McFarland. Chemistry and Biochemistry, The University of Texas at Arlington, Arlington, Texas, United States*

Antimicrobial resistance (AMR) is a growing global health challenge that reduces the effectiveness of conventional antibiotics and increases the need for alternative antimicrobial strategies. This project investigates readily available North Texas plants as sources of natural photosensitizers for antimicrobial photodynamic therapy (aPDT), a light-activated treatment that generates reactive oxygen species to kill microorganisms through multiple mechanisms, reducing the likelihood of resistance. Plant extracts containing light-responsive compounds, including emodin-like anthraquinones, will be prepared and evaluated for their antibacterial activity against drug-resistant

Staphylococcus aureus under both dark and illuminated conditions. We hypothesize that selected extracts will demonstrate significant photoactivated antibacterial activity while exhibiting minimal toxicity in the absence of light. By identifying effective plant-derived photosensitizers from locally sourced species, this work aims to advance the development of sustainable, low-cost antimicrobial therapies and contribute to new approaches for combating antibiotic resistant infections.

SWRM 2026 SW771

Development of a synthetic route to highly substituted quinazolines via isatoic anhydride and phthalimide intermediates

***Mediha N. Siddiqui**, msiddiqui2024@gmail.com, Sudershan R. Gondi, David Y. Son. Chemistry, Southern Methodist University, Dallas, Texas, United States*

Quinazolines are nitrogen-containing fused heterocycles that represent an important scaffold in medicinal chemistry due to their broad range of biological activities and capacity for structural modification. In particular, substituted quinazolines have been extensively investigated as anticancer agents and protein kinase inhibitors, including inhibitors of the epidermal growth factor receptor (EGFR). The nitrogen atoms within the quinazoline core facilitate interactions with biological targets, while substitution around the fused ring system provides opportunities to modify the physicochemical and pharmacological properties of resulting compounds.
Building on previous approaches for the synthesis of quinazolines and trisubstituted anilines from isatin derivatives, this study investigates a synthetic strategy beginning with isatin-7-carboxylic acid. We sought to incorporate structural features associated with both isatoic anhydride and phthalimide intermediates into a common substituted aromatic precursor. This approach was designed to provide additional sites for chemical modification and enable access to a broader range of highly substituted quinazoline and aniline derivatives. Through sequential functional-group transformations of isatin-7-carboxylic acid and related intermediates, the feasibility of this synthetic pathway was evaluated. The development of such intermediates may provide a versatile platform for the preparation of structurally diverse quinazoline derivatives and facilitate future investigation of their potential medicinal chemistry applications.

SWRM 2026 SW772

Synthetic approach toward sulfonamide-substituted quinazolines from isatin sulfonic acid derivatives

***Mediha N. Siddiqui**, msiddiqui2024@gmail.com, Sudershan R. Gondi, David Y. Son. Chemistry, Southern Methodist University, Dallas, Texas, United States*

Sulfonamide-substituted quinazolines represent an important class of heterocyclic compounds that combine the structurally versatile quinazoline nucleus with sulfur-containing functional groups capable of modifying polarity, solubility, hydrogen-bonding interactions, and molecular recognition. These features have contributed to the investigation of sulfonamide-containing quinazolines in medicinal chemistry, particularly as anticancer and protein kinase inhibitors, as well as antimicrobial, anti-inflammatory, and enzyme-inhibitory agents. The ability to independently modify both the quinazoline ring and sulfur-containing substituents provides substantial opportunities for generating structurally diverse derivatives. Building on previous work involving the synthesis of quinazolines and

trisubstituted anilines through isatin-derived cyclic intermediates, this study explores analogous transformations using isatin sulfonic acid derivatives. We proposed that isatin-7-sulfonic acid could undergo sulfur-based cyclization to generate a six-membered cyclic intermediate analogous to previously investigated isatoic anhydride derivatives. In parallel, five-membered cyclic sulfonamide structures related to saccharin derivatives were investigated as alternative synthetic intermediates. These complementary cyclization pathways were considered as potential routes for introducing sulfur-containing functionality into subsequent quinazoline and substituted aniline products. Additionally, we envisioned incorporating functionalities capable of forming both six-membered sulfonic and five-membered saccharin-type cyclic structures within a single substituted aromatic system. Subsequent modification of these intermediates could provide access to a broader range of highly substituted sulfur-containing quinazolines and anilines. This approach establishes a synthetic framework for expanding structural diversity within quinazoline-based compounds and provides new intermediates for future investigation and functionalization.

SWRM 2026 SW773

Programmable C-H functionalization of N-heterocycles

***Buddhadeb Pal**, buddhadeb.pal@niser.ac.in. The University of Texas at Arlington, Arlington, Texas, United States*

Precise control over site-selective C-H functionalization of N-heterocycles remains a longstanding challenge in synthetic chemistry. Here, we introduce a programmable, thermocontrolled and photocatalytic platform that enables regiodivergent functionalization through deliberate modulation of external reaction parameters. CsPbBr3 perovskite shows promise as a visible light photocatalyst, though its instability in polar solvents limits practical applications. This work highlights its potential in organic transformations, such as the chemodivergent functionalization of N-methylalkanamides using CBr4. Additionally, we disclose a visible-light-induced, 9-mesityl-10-methylacridinium perchlorate catalyzed cascade chalcogenation and three-component reaction of aryl alkynoates or N-arylpropynamides and quinoxalin-2(1H)-one respectively. The thermocontrolled regiodivergent functionalization of quinoxalin-2(1H)-one further emphasizes the sustainability of our methodology.

SWRM 2026 SW774

Harnessing hypervalent silicon: In sustainable organic synthesis

***Neetesh Yadav**, nxy9115@mavs.uta.edu. Department of Chemistry and Biochemistry, The University of Texas at Arlington, Arlington, Texas, United States*

The stepwise heterodifunctionalization of dihydrosilanes has traditionally been hindered by multi-step sequences, selectivity issues, operational difficulties, and limited substrate scope. To overcome these challenges, this study presents a novel, telescoped Iridium-catalyzed alkynylative ortho-anilmation process for the heterodifunctionalization of dihydrosilanes. A central innovation of this methodology is the design and implementation of *N,O*-silyl acetal stabilizing (SAS) groups to effectively control reactivity. Optimization studies revealed highly efficient catalyst performance, enabling the rapid generation of silyl acetals with yields reaching up to 99%. Furthermore, this protocol demonstrates a broad substrate scope and successfully facilitates the late-stage modification of complex bioactive molecules. Ultimately, this streamlined synthetic strategy provides a direct and efficient pathway for

the synthesis of silicon-containing acetaminophen analogues (Si-APAPs), offering a valuable new tool for organosilicon chemistry and drug discovery.

SWRM 2026 SW775

Oxidant-efficient benzylic and allylic C–H oxidation using a water-soluble Cu(II) Schiff base/TEMPO system

***Xander Duke**, xaduke@ttu.edu, Ansh Chugh, Anne E. Gorden. Chemistry and Biochemistry, Texas Tech University, Lubbock, Texas, United States*

Benzylic and allylic C–H oxidation provides a direct route to valuable carbonyl-containing products used in pharmaceuticals and the materials industry, but conventional oxidation methods often require high oxidant loadings and organic solvents. Previous work in our group demonstrated that an imidazolium-functionalized, water-soluble Cu(II) Schiff base complex catalyzes the oxidation of benzylic and allylic substrates using tert-butyl hydroperoxide (TBHP) in aqueous media. Building on this work, we investigate the incorporation of 2,2,6,6-tetramethylpiperidine 1-oxyl (TEMPO) as a co-catalyst to improve the efficiency of Cu(II)-catalyzed C–H oxidation. To accommodate the solubility of TEMPO while maintaining a water-rich reaction environment, a 2:1 water/acetonitrile solvent system was employed. Under optimized conditions, the Cu(II) Schiff base catalyst is used at 2 mol% with 5 mol% TEMPO and 0.5–1.0 equivalents of TBHP. Reactions conducted at temperatures up to 70 °C over 8–24 hours afford moderate to high yields of the corresponding carbonyl products, with predominantly selective formation of a single oxidation product. Incorporation of TEMPO enables the use of approximately 3–5-fold less TBHP than the previously investigated Cu(II)/TBHP system. These results demonstrate that a water-soluble Cu(II) Schiff base/TEMPO catalytic system can promote selective benzylic and allylic C–H oxidation while substantially reducing the typical oxidant requirements.

SWRM 2026 SW776

Synthesis of benzoborole-based macrocycles utilizing dialkoxy phenylene linkers

***Kylie V. Bartusek**, kvb016@shsu.edu, Dustin E. Gross. Chemistry, Sam Houston State University, Huntsville, Texas, United States*

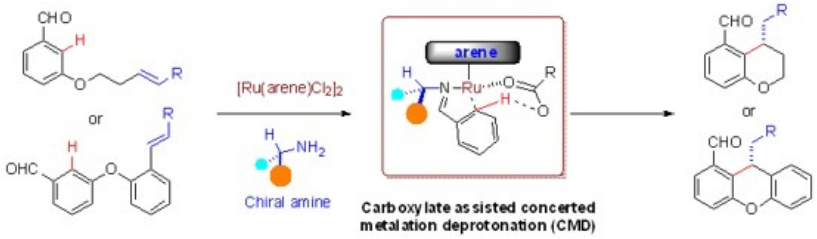
Diazaboroles and oxazaboroles are heterocyclic compounds known for their unique electronic properties and reversible dynamic covalent behavior, which allows them to be explored as stimuli-responsive or self-healing materials. In oligomeric systems, benzodiazaborole and benzoxazaborole motifs can serve as dynamic linkers that connect monomers into complex macrocyclic architectures. In this work we aim to synthesize benzodiazaborole- and benzoxazaborole-based macrocycles through the dynamic covalent assembly of dialkoxy phenylene linking units and diboronic acids. This will allow us to evaluate the potential of these dynamic covalent systems for the formation of well-defined, reversibly assembled architectures.

SWRM 2026 SW777

Stereoselective functionalization of carbon-hydrogen bond with collaborative enantiomeric control

***Weinan Tan**, wt411@msstate.edu, brian tran, Xin Cui. chemistry, University of North Texas, Denton, Texas, United States*

Asymmetric C–H functionalization provides a powerful approach to constructing stereogenic centers directly from readily available substrates. We developed a Ru-catalyzed platform using α-branched amines as chiral transient directing groups (cTDGs) to control enantioselectivity without preinstalled directing groups. The combination of tunable Ru(II)–arene complexes and chiral amines enables multiple reaction modes, including intramolecular hydroarylation to access chiral chromane and xanthene frameworks, intermolecular hydroarylation, and vinylic C–H functionalization. Mechanistic studies involving H/D scrambling, kinetic isotope effects, and DFT calculations reveal condition-dependent catalytic pathways and distinct rate-determining steps for the two enantiomeric pathways, providing insight into asymmetric induction in Ru-mediated d6-metal C–H functionalization. The retained aldehyde functionality further enables diverse downstream transformations to generate complex polycyclic structures. Overall, this work establishes cTDGs as a versatile strategy for asymmetric Ru-catalyzed C–H functionalization and expands access to structurally diverse chiral molecules.



SWRM 2026 SW778

Cell organelle-targeted Schaap's dioxetane for sub-cellular imaging

***Gen Chen**, genc@smu.edu. Chemistry, Southern Methodist University Dedman College of Humanities and Sciences, Dallas, Texas, United States*

Chemiluminescence is the emission of light from chemical reaction. Without excitation source like fluorescence, it can reduce autofluorescence, light scattering, and photobleaching, which has been widely used for biological study. Subcellular imaging of cells provides spatial and temporal information about biological processes, enabling to understand what happens inside a cell. While lots of fluorescent probes for cell organelle imaging have been developed, chemiluminescent probes remain relatively underexplored due to synthetic difficulty. We successfully synthesized a group of 1,2 dioxetanes for mitochondria, lysosome and nucleus imaging using chemiluminescence microscopy in our group characterize the for A549 human lung epithelial cells. This study provides a chemiluminescent 1,2-dioxetane platform for developing small molecules probe for sub cellular imaging.

SWRM 2026 SW779

Concentration-dependent photochemical evolution of primary brown carbon under irradiation

Sithumi M. Liyanage*, smadhus@okstate.edu, Colton T. Calvert, Holly B. Anthony, Elijah Schnitzler. Chemistry, Oklahoma State University The College of Arts and Sciences, Stillwater, Oklahoma, United States*

Brown carbon (BrC) components of biomass burning organic aerosol (BBOA) influence climate directly by absorbing and scattering solar radiation and indirectly by enhancing cloud formation. Absorption contributes to warming, but the magnitude of this effect depends on the aerosol's optical properties, which can vary over its atmospheric lifetime. Primary BrC undergoes atmospheric aging through irradiation and oxidation, which can alter its chemical and optical properties. Overall, this aging generally whitens organic aerosols; however, irradiation can also initially increase the visible light absorption of BrC species. Here, we address this variability in light-driven processing by examining the evolution of primary BrC optical properties under irradiation while varying the initial BrC concentration to modulate between these two scenarios. BrC aerosol was generated from eastern red cedar sapwood and prepared across a range of concentrations, from thin films to diluted solutions. Samples were irradiated from above in a solar simulator. Importantly, all samples appeared the same color from above, with sample thicknesses inversely proportional to mass concentration, so the number of photons absorbed at time zero was the same for all samples. The lowest BrC concentration exhibited the most rapid initial absorption enhancement and the highest quantum yield, whereas higher concentrations showed significantly lower values, indicating lower photochemical efficiency under concentrated aerosol conditions than under dilute cloud conditions. These results emphasize the importance of concentration in the atmospheric lifetime and optical evolution of BrC, with consequences for modeling its impact on climate change and visibility.

SWRM 2026 SW780

Synthesis and characterization of water-soluble prodrugs of a Toll-like receptor 4 (TLR-4) inhibitor, TAK-242

Jacquelin LaBerteaux*[1], Jacquelin_Laberteau2@baylor.edu, Kiah Sleiman[2], Santhalakshmi Ranganathan[2], Dwayne D. Simmons[2], Robert R. Kane[3]. (1) Baylor University, Waco, Texas, United States(2) Biology, Baylor University, Waco, Texas, United States(3) Chemistry & Biochemistry, Baylor University, Waco, Texas, United States*

The small molecule drug TAK-242 is a potent inhibitor of Toll-Like Receptor 4 (TLR-4) and has shown great promise in its ability to reduce inflammation in a variety of disease models. However, the poor aqueous solubility of TAK-242 presents a challenge. Many studies have shown that polyethylene glycol (PEG), dimethylammonium (DMA), and sulfonate moieties can be utilized to improve the water solubility of drugs and prodrugs. In this study, we synthesized four TAK-242 prodrugs that contains a β-eliminative sulfone trigger for drug release, a para-aminobenzyl spacer, and either a medium length PEG moiety (average 550 Da), a longer PEG structure (average 2k Da), a propyl DMA functionality, or a propyl sulfonate group. Preliminary studies with the PEG2k prodrug of TAK-242 demonstrated improvement of solubility enabling an effective TAK-242 concentration of 0.5mg/mL to be delivered. This prodrug slowly released TAK-242 which allowed for inhibition of TLR-4 in an in vitro cell assay and reduced LPS-stimulated cytokine production in an in vivo model. The synthesis and biological characterization of these water-soluble TAK-242 prodrugs will be described.

SWRM 2026 SW781

Speed of sound in a circular acoustic resonator

***Adam Mansell**, adam.mansell@chem.ufl.edu. Chemistry, Baylor University, Waco, Texas, United States*

I will discuss an experiment for the undergraduate physical chemistry laboratory in which students determine the speed of sound in various gases by finding resonant frequencies in a circular acoustic resonator. From these data, students can find the heat capacity ratio for each gas at the experimental temperature.

SWRM 2026 SW782

Reviving the Finkelstein reaction: Supramolecular chemistry in the undergraduate teaching laboratory

***Xuxian He**, xuxian.he@nicholls.edu. Chemistry & Physical Sciences, Nicholls State University, Thibodaux, Louisiana, United States*

In this two-session experiment designed for an advanced organic chemistry laboratory, students conduct parallel Finkelstein reactions of benzyl chloride with sodium iodide in the presence and absence of 15-crown-5 using separate NMR tubes. Reaction progress is monitored at multiple time points by ^{1}H NMR spectroscopy, allowing students to compare conversion profiles and relative reaction rates. The reaction produces benzyl iodide, whose benzylic methylene protons exhibit a distinct chemical shift from those of benzyl chloride, enabling students to readily distinguish starting material from product and determine percent conversion by integration. Comparison of the conversion profiles demonstrates the effect of crown ether complexation on the Finkelstein reaction. The experiment is intended for advanced chemistry students who have completed at least six semester hours of organic chemistry. By integrating concepts ranging from Le Châtelier's principle and classical S_N2 reactivity to host–guest chemistry, ^{1}H NMR reaction monitoring, and quantitative data analysis, this experiment provides a meaningful connection among general chemistry, organic chemistry, and supramolecular chemistry.

SWRM 2026 SW783

Power of alumni: Bringing real-world experiences and career pathways to students in STEM deserts

***Candice Fulton**, candice.fulton@msutexas.edu. Chemistry, Midwestern State University, Wichita Falls, Texas, United States*

In areas of the country where chemistry or STEM careers are limited, students may also have a limited view on the application of STEM knowledge possible plethora of career paths. Regional Universities may be at a distinct disadvantage due to location and resources, but utilizing successful alumni and local industry can bridge the gap. After COVID, online meetings became the new norm. For universities located hours away from industry and exposure to varied STEM career paths, online

presentations bring experience to the classroom with minimal to no cost to the university. Many alumni are eager and proud to assist their alma mater in exposing students to different journeys and career paths. Alumni from chemistry, biology, geology, computer science, and engineering employed in the public, private, and governmental sectors presented in-person or online about their positions and work at the local, state, and national levels. Through these encounters, students were able to learn from our alumni about their path to success in start-ups, graduate school, professional schools, university research, and industry. These connections influenced graduate school selection, internship opportunities while bringing perspective, new career pathway options, and encouragement.

SWRM 2026 SW784 - Withdrawn

SWRM 2026 SW785

Comparison of β-Mo2C thin film and nanoparticles as a catalyst for selective C=O bond scission: Addressing pressure and material gaps

Abdullah Ali Maruf[1]*, abdullahalimaruf@my.unt.edu, Stella C. Amagbor*[1]*, Nadiira Hassan*[1]*, Renuka Rathnayake Mudiyanselage*[1]*, Mahesh Dungana*[1]*, Anil Pudasaini*[2]*, Linxiao Chen*[1]*, Jeffry Kelber*[1]*. (1) Chemistry, University of North Texas, Denton, Texas, United States(2) Physics, University of North Texas, Denton, Texas, United States*

The selective C=O vs C-C bond scission is crucial for the synthetic fuel industry, polymer upcycling, and many other industrial and environmental processes. Beta-Mo_2C is well known for highly selective C=O and C-C bond scission. However, the important aspects, such as the temperature range over which this selectivity is maintained and the effect of surface oxidation, remain unclear. Moreover, the potential differences between well-defined thin films reacting with probe molecules under ultrahigh vacuum (UHV) conditions and practical nanoparticle (NP) catalysts interacting with polymers are still unexplored- the so-called pressure and materials gap. In this study, the temperature-dependent selectivity of 2-pentanone for β-Mo_2C thin film and polyethylene terephthalate (PET) for Mo_2C NPs was studied as probe molecules. UHV in situ XPS and mass spectrometry studies revealed that the β-Mo_2C film exposure of 2-pentanone (~10^{-5} Torr) at 250 °C showed no significant bond cleavage in the absence of H_2 but in the presence of H_2 at 250 °C, it demonstrated high selectivity towards C=O bond scission with O_2 desorption from the surface of the thin film; at the same time, significant selectivity of C-C/C-H bond cleavage was observed at 400 °C. GCMS studies showed a similar temperature dependence for Mo_2C NP reacting with PET, also demonstrating the high selectivity for C=O bond scission at 250 °C. *Ex-situ* XPS studies of β-Mo_2C thin showed oxidation to Mo^{4+} under both ambient and reaction conditions without disrupting the reactivity and selectivity, whereas. These results confirm the bond-scission selectivity of the Mo_2C thin film reacting with probe molecules under UHV conditions and the behavior of a realistic Mo_2C NP catalyst reacting with polymer under high pressure and industrial conditions.

SWRM 2026 SW786

Tuning the coordination sphere of metal-integrated two-dimensional covalent organic frameworks for selective toxic gas capture

***SAYAN MAITI**, maiti.sayan@gmail.com. Chemistry, University of North Texas, Denton, Texas, United States*

The selective capture of reactive toxic gases under realistic humid conditions remains a significant challenge. Here, we demonstrate how systematic modulation of the metal coordination environment and surrounding pore microenvironment in two-dimensional covalent organic frameworks (2D COFs) governs toxic gas capture and water tolerance. Combined gas adsorption, *in situ* spectroscopy, and density functional theory (DFT) calculations reveal that the metal coordination environment primarily controls the intrinsic gas affinity, whereas the pore microenvironment regulates competitive water adsorption and gas transformation pathways. Strategic tuning of the primary and secondary metal coordination spheres within 2D COFs enables high-capacity gas capture while maintaining exceptional humidity tolerance. These findings establish molecular design principles for developing robust porous frameworks for the selective capture of reactive and toxic gases.

SWRM 2026 SW787

Removal of uranium from water using a water-insoluble urea polymer

***Gifty Dudzilah**, gdudzilah@gmail.com, Md Mhahabubur Rhaman. Physical Science, Eastern New Mexico University, Portales, New Mexico, United States*

Contamination of groundwater with uranium is an environmental concern in parts of the southwestern United States, especially in areas where groundwater is used for drinking and agricultural purposes. The World Health Organization has recommended a guideline of 30 µg/L for uranium in drinking water. Traditional techniques such as adsorption, photocatalysis, electrocoagulation, ion exchange, and membrane filtration for removing uranium may be limited by cost, selectivity, and applicability for large volumes of water with competing mineral ions. Hence, the development of efficient, low-cost materials for removing uranium from contaminated water is necessary. In this work, a water-insoluble polymeric ligand was synthesized by reacting tris(3-aminopropyl)amine with 1,4-diisocyanatobenzene in refluxing chloroform and characterized by infrared spectroscopy. The synthesized polymer was evaluated for its ability to remove U(VI) from aqueous uranyl acetate solutions. The removal efficiency of uranium was 90% using 0.128 g of polymer and 10 mL of 0.01 M uranyl acetate solution prepared in distilled water, yielding a distribution coefficient K_d of 70. The removal of uranium was found to depend on the amount of polymeric ligand, the interaction time, and the initial uranyl acetate concentration. The results indicate the potential of the synthesized water-insoluble polymeric ligand as an adsorbent for removing uranium (VI) from aqueous systems. Further optimization and evaluation under environmentally relevant water conditions will help assess its potential for groundwater remediation applications. This project was sponsored by Eastern New Mexico University's internal grant PIRR3. Ms. Gifty acknowledges the Sponsor Project at Eastern New Mexico University for providing the graduate assistant position and travel support.

SWRM 2026 SW788

Removal of fluoride from groundwater using inexpensive biocompatible materials

***DennAsia Cordova**, dennasia.cordova@enmu.edu, Md Mhahabubur Rhaman. Physical Sciences, Eastern New Mexico University, Portales, New Mexico, United States*

Fluoride is commonly added to toothpaste to strengthen enamel, to help prevent cavities, but excessive fluoride exposure—especially through drinking water—can lead to serious health concerns such as dental and skeletal fluorosis, neurological complications, and potential links to certain cancers. In Roosevelt County, New Mexico, naturally occurring fluoride in groundwater is elevated due to the region's unique geology and prolonged drought conditions. Recent measurements show that the city water supply contains an average fluoride concentration of 2.61 ppm, exceeding the World Health Organization's recommended limit of 1.5 ppm for safe drinking water. This poses significant risks for both residents and agricultural systems, as local farming relies heavily on groundwater for irrigation. High fluoride levels in irrigation water can accumulate in soil, disrupt nutrient balance, and ultimately reduce crop yields, creating additional economic and environmental strain on rural communities. Current fluoride-removal technologies, such as reverse osmosis and activated alumina filtration, are effective but often too expensive and inaccessible for low-income households and small-scale farmers. As a result, there is an urgent need for affordable, sustainable, and locally sourced alternatives. In this study, we evaluated natural, low-cost, and biocompatible materials—including powdered eggshells, bone char, and biochar—for their ability to remove fluoride from contaminated water. Calcium-rich materials were of particular interest because fluoride binds strongly to calcium ions, forming insoluble compounds that can be separated from water. Preliminary results indicate that calcium-based materials such as bone char and eggshells show promising fluoride-removal efficiency. These findings suggest that locally available waste materials could provide an affordable and environmentally friendly option for communities in New Mexico and other regions facing similar groundwater contamination challenges. Acknowledgement: This work was supported by the 2025-2026 NM WRRI Student Grant EQ02802, along with Eastern New Mexico University for supporting the ability to conduct the experiment.

SWRM 2026 SW789

Identification of microplastic concentrations in Matagorda Bay sediments

Joseph Dulaney[1]*, joseph.dulaney@go.tarleton.edu, Rajani Srinivasan*[1]*, Adam Mitchell*[2]*, Ruaa Al Mezrakchi*[3]*, Grace Millsap*[2]*. (1) Chemistry, Geosciences, and Physics, Tarleton State University, Stephenville, Texas, United States(2) Wildlife and Natural Resources, Tarleton State University, Stephenville, Texas, United States(3) Mechanical, Environmental, and Civil Engineering, Tarleton State University, Stephenville, Texas, United States*

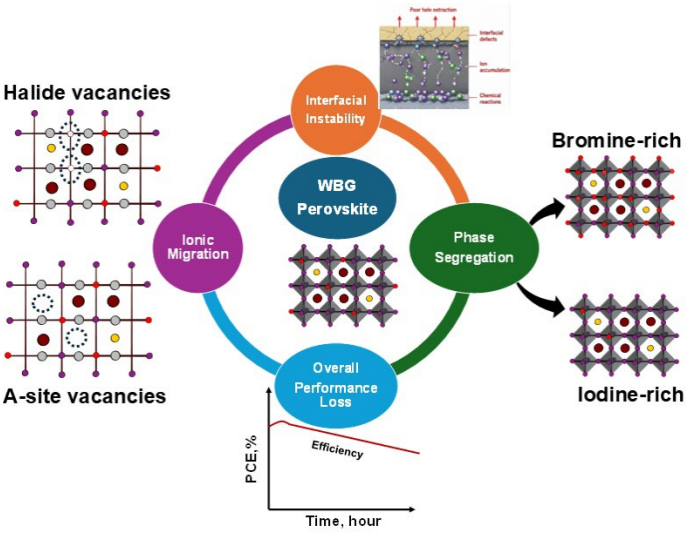
Sediment samples from the Matagorda Bay system were collected in the fall of 2024 and 2025 and analyzed to identify concentrations of microplastics (MPs) and evaluate whether quadrant counting could reduce microscopy time while retaining a high average accuracy. Dried sediments were separated with a saturated NaCl solution and decanted before being digested with 30% H_2O_2 at a 1:1 ratio in a 50°C oven. The digested samples were then vacuum filtered through a 0.45 µm filter and counted utilizing a Motic Panthera Trinocular microscope. Reported mean concentrations were 33,759 MPs/kg for the 2024 samples and 32,240 MPs/kg for the 2025 samples. The 92 quadrant-based estimates had a mean absolute percent error relative to the full-filter counts of 5.23%. One-sample t-tests also detected no significant directional bias for any quadrant, and the repeated-measures analysis found no significant difference among quadrants. These results show that MPs were consistently present at high concentrations in the sampled bay sediments and indicate that quadrant counting can provide a time-saving estimate of full-filter counts when particles are filtered evenly.

SWRM 2026 SW790

Tailored crystallization for extremely stable wide-band gap perovskite solar cell

***Nilanjana Nandi**, nandinila94@gmail.com. Chemical and Biomolecular Engineering, Rice University, Houston, Texas, United States*

The next-generation solar cell technology, tandem solar cells, offers higher efficiencies and strong potential to address the growing global energy demand. By integrating a wide-bandgap (WBG) perovskite subcell as the top layer, tandem architecture can effectively utilize a broader range of the solar spectrum and achieve enhanced power conversion efficiency. In this work, we employ an additive engineering strategy to develop highly efficient and stable WBG perovskite solar cells. The incorporation of tailored molecular additives enables improved film quality, interfacial properties, and charge extraction while mitigating defect-assisted non-radiative recombination and degradation. The additive-induced modification of the perovskite surface and buried interfaces enhances carrier dynamics and suppresses interfacial losses. Furthermore, improved control over crystallization promotes a more uniform and defect-passivated perovskite layer. These synergistic effects contribute to enhanced photovoltaic performance and operational stability under prolonged illumination and thermal stress. The developed strategy provides insights into the relationship between molecular interactions, interfacial energetics, and device stability. Overall, this work demonstrates a promising pathway for realizing durable and high-performance WBG perovskite subcells for next-generation tandem photovoltaic applications.



Problems of Wide band gap perovskite

SWRM 2026 SW791

Fluorescent sensing of per- and polyfluoroalkyl substances in water using functionalized metal–organic framework

***Danidu M. Jayasuriya**, danidu.jayasuriya@utdallas.edu, Mario Wriedt. The University of Texas at Dallas, Richardson, Texas, United States*

Per- and polyfluoroalkyl substances (PFAS) are synthetic compounds extensively used in non-stick cookware, cosmetics, food packaging, and water-resistant materials. Their remarkable chemical

stability, environmental persistence, and potential toxicity have contributed to their widespread presence, especially in aquatic environments, where they present significant risks to human and ecological health. Consequently, reliable detection of PFAS has become increasingly important. Conventional analytical techniques, such as liquid chromatography–tandem mass spectrometry (LC–MS/MS), commonly coupled with solid-phase extraction (SPE), offer excellent sensitivity and selectivity but are costly, time-intensive, and impractical for on-site monitoring. Metal–organic framework (MOF) based optical sensors have emerged as attractive alternatives because of their high surface areas, tunable pore environments, adjustable luminescent properties, and rapid response times. Nevertheless, detecting short-chain PFAS remains particularly challenging. To overcome this limitation, we investigate the synthesis and application of post-synthetically modified NH_2-MIL-68, an indium-based MOF, as a fluorescent probe for detecting short-chain perfluoroalkyl carboxylic acids (PFCAs) in aqueous media. The modified MOF demonstrates excellent water stability and distinct fluorescence quenching following PFAS interaction, generating a clear “turn-off” response. These results highlight the potential of modified NH_2-MIL-68 as a selective, rapid, and practical fluorescence sensor for short-chain PFCAs, offering an effective alternative to conventional PFAS detection approaches.

SWRM 2026 SW792

Mesoporous tin oxide-based electrochemical flow sensor for per and polyfluorinated alkyl substances (PFAS)

Andrea Razo[1]*, andrea.razo01@utrgv.edu, Yea Seul Jang*[1]*, Benjamin J. Sherman*[2]*, Chang Geun Yoo*[3]*, Mike McFarland*[4]*, Gyu Leem*[1]*. (1) The University of Texas Rio Grande Valley, Edinburg, Texas, United States(2) Chemistry, Texas Christian University, Fort Worth, Texas, United States(3) SUNY College of Environmental Science and Forestry Department of Chemistry, Syracuse, New York, United States(4) Cache Environmental Laboratories PC, Layton, Utah, United States*

Among per- and polyfluoroalkyl substances (PFASs), particularly perfluorooctanoic acid (PFOA) pose severe health and environmental risks due to the high stability of their C-F bonds which are highly resistant to degradation. Prolonged exposure to PFAS has been linked to serious health risks, including cancer and hormonal disruption, necessitating efficient detection technologies for real-time environmental monitoring. While traditional static detection techniques are often time-consuming and costly, continuous-flow electrochemical monitoring offers a transformative pathway for rapid, real-time aquatic sensing. To address this, we report on a portable continuous-flow electrochemical sensing platform engineered for high-sensitivity PFOA detection. By shifting from static sensing to a dynamic flow-based system, the platform significantly enhances analyte mass transport across mesoporous, receptor-functionalized metal oxide anodes. Coupling this in-situ continuous flow cell with electrochemical impedance spectroscopy (EIS) enables real-time, ultra-sensitive tracking of interfacial charge-transfer changes during PFOA binding, achieving detection limits down to parts-per-trillion (ppt) levels. Systematic optimization of key fluidic and surface parameters, specifically solution flow rate, metal oxide morphology, and receptor activation, ensures selective capture and rapid signal response under dynamic flow conditions. Designed for seamless integration into portable, inline water-testing systems, this continuous-flow approach eliminates sample handling delays and enables automated, real-time monitoring of persistent, fluorinated contaminants in natural and municipal water systems for public health protection.

SWRM 2026 SW793

Toward PFAS destruction: Metal–organic frameworks for adsorption and photocatalytic degradation

***Najeeb Ullah**, nxu220007@utdallas.edu, Mario Wriedt. Department of Chemistry & Biochemistry, The University of Texas at Dallas, Richardson, Texas, United States*

Per- and polyfluoroalkyl substances (PFAS) are highly persistent environmental contaminants that pose significant concerns due to their widespread occurrence in water and resistance to degradation arising from strong carbon–fluorine (C–F) bonds. Conventional treatment methods such as activated carbon adsorption and membrane filtration primarily separate or concentrate on PFAS rather than destroy them, highlighting the need for technologies capable of effective degradation and defluorination. Metal–organic frameworks (MOFs) are promising materials for PFAS remediation because of their high surface areas, tunable pore environments, chemically versatile metal nodes and organic linkers, and potential photocatalytic activity. Incorporation of photoactive and redox-active components can enhance light absorption, charge separation, and generation of reactive species capable of initiating PFAS degradation, while the porous framework can promote adsorption and bring PFAS molecules into close proximity to catalytic sites. Despite these advantages, the use of MOFs for photocatalytic degradation of long-chain PFAS remains relatively underexplored. This work focuses on developing photoactive MOF-based materials for the synergistic adsorption and degradation of PFAS in water, with particular emphasis on understanding photocatalytic pathways, structure–activity relationships, C–F bond cleavage, and defluorination.

SWRM 2026 SW794

Photodegradation of PFAS in water by silver-based MOF–persulfate systems

***Prapti Shende**, prapti.shende@utdallas.edu, Mario Wriedt. Chemistry and Biochemistry, The University of Texas at Dallas School of Natural Sciences and Mathematics, Richardson, Texas, United States*

PFAS are synthetic chemicals widely utilized because of their high stability and hydrophobic nature. The strong C–F bonds present in PFAS contribute to their environmental persistence, resulting in widespread contamination and potential risks to human health and ecosystems. Conventional treatment techniques, including adsorption, ion exchange, and membrane filtration, can effectively remove PFAS but do not destroy these persistent compounds. Advanced oxidation processes (AOPs), particularly persulfate-assisted photocatalysis, have emerged as promising methods for PFAS degradation. In this process, photoexcited electrons generated by a suitable photocatalyst can activate persulfate to produce sulfate and hydroxyl radicals, which can promote the degradation of strong C–F bonds. However, these approaches face several limitations, including limited PFAS degradation efficiency, high energy consumption, and demanding reaction conditions that can restrict their large-scale application. Moreover, rapid recombination of photogenerated electron–hole pairs can further reduce photocatalytic efficiency. Therefore, the development of an efficient and sustainable system for PFAS degradation is highly desirable. Recent studies have highlighted the considerable potential of MOFs as photocatalytic materials. In this study, silver-based metal–organic frameworks (Ag-MOFs) are investigated for persulfate activation and enhanced photodegradation of PFAS. The redox couple in Ag-MOFs can promote charge separation and facilitate the generation of reactive oxygen species under light irradiation. In addition, the tunable band structure, high surface area, and porous framework of Ag-MOFs can enhance PFAS adsorption and facilitate interactions with reactive sites, while their structural versatility supports synergistic radical generation with persulfate. These combined features can promote the degradation of strong carbon–fluorine bonds in

PFAS and facilitate their mineralization. The Ag-MOF–persulfate system therefore represents a promising strategy for sustainable, light-driven degradation of persistent pollutants and advanced water treatment applications.

SWRM 2026 SW795

Urea-functionalized cerium metal–organic framework for fluorescent detection of PFBA and TFA

***Maryam Piroozzadeh**, mxp230063@utdallas.edu. The University of Texas at Dallas, Richardson, Texas, United States*

Herein, we report a urea-functionalized cerium-based metal–organic framework (Ce–urea MOF) as a fluorescent sensor for perfluorobutanoic acid (PFBA) and trifluoroacetic acid (TFA). The crystal structure was determined by single-crystal X-ray diffraction, and the material was further characterized by powder X-ray diffraction, FTIR spectroscopy, thermogravimetric analysis, electron microscopy, and gas sorption measurements. The Ce–urea MOF exhibited strong fluorescence responses toward PFBA and TFA in aqueous media. Concentration-dependent and selectivity studies were performed to evaluate its sensing performance and analytical sensitivity. These results demonstrate the potential of the Ce–urea MOF as a fluorescent platform for the detection of short-chain fluorinated contaminants.

SWRM 2026 SW796

Predicting contaminant transport and environmental persistence through sustainable solvation modeling

***Anika Varadharajan**, reach.anikav@gmail.com. Chemistry, University of North Texas College of Science, Denton, Texas, United States*

Pesticide contamination is a global environmental concern, affecting millions of people, plants, and animals. Agricultural pesticide use, while effective for pest control, carries unintended ecological consequences, and many phenylurea herbicides, a chemically related pesticide class, lack the solubility data needed for reliable ecological risk assessment. The Abraham Model, previously applied to model chemical partitioning in medicine and agriculture, offers a means of predicting pesticide transport and absorption into plant cuticles, but it has not been extensively parameterized for phenylurea herbicides. Monuron and diuron, two well-characterized members of this class with solubility data available in 22 and 32 organic solvents, respectively, provide a foundation for extending the model to structurally related, poorly characterized compounds.
This study integrates experimentally derived solubility data into a multi-parameter Abraham Model framework to characterize chemical transport governed by intermolecular interactions, including hydrogen bonding and dipole-dipole forces. Solubility and molar absorptivity of monuron and diuron were determined via UV-Vis spectrophotometry across a range of organic solvents (esters, alcohols, and sulfoxides). Solute descriptors representing partitioning behavior between water and gas phases were calculated from these data, and multiple linear regression (IBM SPSS) was used to derive Abraham Model solvation coefficients. Measured and predicted solute descriptors agreed to within ±0.17 log units, and predicted log SRW and log SRG (solubility descriptors for water and gas-phase partitioning) values deviated from experimental values by no more than 0.5 log units, indicating strong

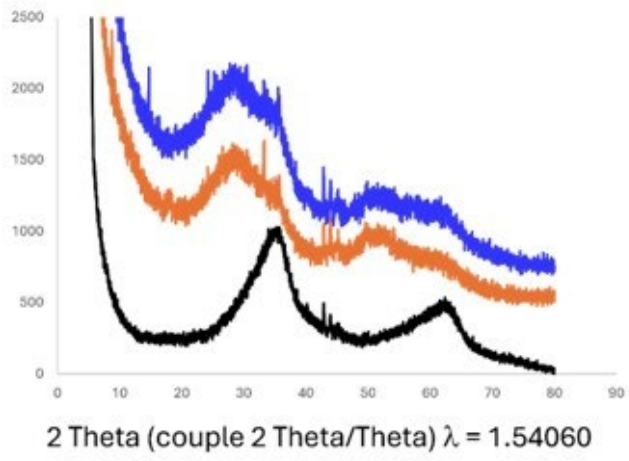
predictive accuracy. These results establish a validated framework for modeling phenylurea herbicide transport in environmental systems, offering a practical tool to support more informed, proactive agrochemical risk assessment.

SWRM 2026 SW797

Validation of iron-based oxide nanoparticles as arsenic sequestering agents for commercial fertilizers

***Leandro H. Obama**, lobamambasogo@pvamu.edu, Bre'Ayshia Perry, Gina Chairella. Chemistry, Prairie View A&M University, Prairie View, Texas, United States*

Arsenic can be found in nature in two oxidation states, arsenic V and arsenic III. Arsenic V is present in nature as arsenate and is absorbed by plants because of its similar chemical structure to phosphates. This phenomenon then allows for the introduction of arsenic V in the plant via the phosphate transport, leading to the stabilization of the chemical in the plant transport system. Due to their mineral origin and industrial preparation, commercially available fertilizers are frequently another source of arsenic. Arsenic can transfer from soil and plants to the food chain, and eventually to animals and humans, causing illnesses which include cancer, organ failure, and nerve damage. This work explores the use of five different forms of iron-based oxides as arsenic sequestrating agents, reducing the concentration of arsenic in the fertilizers. This study aims to compare the sequestrating capabilities of ferrihydrite, goethite, magnetite, iron (II)/ Iron (III) hydroxides, and nickel ferrite. These oxides were chosen due to their sustainable nature and low-cost technology. Six types of commercially available fertilizers were chosen for the study. The iron derivatives were prepared as nanoparticles using conventional methods and techniques, some of which are available in the literature, and characterized using FTIR, TGA, CV, DPV, SEM, XPS, and XRD for structure and properties confirmation. To establish a correlation and compare results among all the different nanoparticles in the study, ICP was used to offer a detailed perspective into the oxide effects and generate a view of the most effective arsenic-capturing oxide, ferrihydrite, in this case, noticed in the powder XRD as shown in the figure below. However, the effects of both the iron (II)/iron (III) hydroxide and the nickel ferrite are still under study.



Powder XRD comparison graphic. In black, pure ferrihydrite; in brown, As_2O_5 reacted with ferrihydrite; in blue, ferrihydrite with As_2O_5 and fertilizer.

SWRM 2026 SW798

Label-free impedimetric detection of perfluorooctanoic acid using silane-functionalized FTO electrodes

***QAMAR HAYAT KHAN**, qamar.hayatkhan@tcu.edu. CHEMISTRY AND BIOCHEMISTRY, Texas Christian University, Fort Worth, Texas, United States*

Per- and polyfluoroalkyl substances (PFAS), including perfluorooctanoic acid (PFOA), are persistent aqueous contaminants whose strong carbon–fluorine bonds, environmental mobility, and potential adverse health effects have created an urgent need for accessible monitoring technologies. Although established LC–MS/MS methods provide the sensitivity required for regulatory analysis, they generally require specialized instrumentation, trained personnel, and extensive sample preparation. Here, we investigate a an immittance-based approach to directly probe PFOA adsorption at a functionalized electrode–water interface. The modification of fluorine-doped tin oxide (FTO) with a self-assembled monolayer of trichloro(1H,1H,2H,2H-perfluorooctyl) silane (TCPFOS) produces a hydrophobic, fluorophilic interface to promote specific adsorption of PFOA. Unlike many electrochemical sensors that rely on redox mediators or direct faradaic reactions, this non-faradaic approach monitors adsorption-induced changes in interfacial capacitance using electrochemical impedance spectroscopy. Measurements were conducted in 0.1 M NaCl in water using a three-electrode configuration. Circuit fitting of the immittance response was used to follow changes in effective interfacial capacitance as a function of the PFOA concentration in the analyte solution. Water-droplet behavior confirmed a pronounced decrease in surface wettability following TCPFOS modification. Electrochemical characterization further demonstrated substantial surface blocking, with estimated TCPFOS coverage of 95% ± 5% by both cyclic voltammetry and impedance analysis. Preliminary PFOA measurements over the ppm range produced small but systematic changes in the interfacial capacitance, the interfacial leak resistance, and α (CPE fractional exponent). On-going studies will compare bare FTO, FTO–TCPFOS, and FTO–OTS against PFOA and octanoic acid containing solutions to validate the diagnostic ability of this approach. While the current focus is on planar electrode interfaces, subsequent work will examine mesoporous architectures with similar surface coatings.

SWRM 2026 SW799

Deep eutectic solvent-assisted synthesis of ferrocene-derived Fe-functionalized activated carbon for adsorption-assisted heterogeneous Fenton oxidation in complex dye matrices

***Sungjik Oh**[1], sungjikoh@kict.re.kr, Jiyeol Bae[1,2]. (1) Dept of Environmetal Research, Korea Institute of Civil Engineering and Building Technology, Goyang-si, Gyeonggi-do, Korea (the Republic of)(2) Korea National University of Science and Technology, Daejeon, Korea (the Republic of)*

Carbon-supported heterogeneous Fenton catalysts can integrate adsorption and oxidative degradation, but conventional synthesis often relies on organic solvents and performance is commonly evaluated in simple single-solute systems. Here, a choline chloride/glycerol deep eutectic solvent (DES) was used to immobilize ferrocene-derived Fe species on powdered activated carbon (PAC), producing GFePAC. Bulk Fe content increased from 0.0270 to 0.1992 wt%, while characterization confirmed preservation of the porous carbon framework and the presence of mixed-valent Fe(II)/Fe(III) sites. Batch experiments were conducted with methylene blue (MB) at pH 4, 7, and 9 and in synthetic textile wastewater containing MB, Congo red, and inorganic salts. At 10 mg L-1 MB, GFePAC/H2O2 exhibited apparent pseudo-first-order rate constants of 0.3731, 0.2651, and

0.2925 min-1 at pH 4, 7, and 9, respectively, compared with 0.1803, 0.1265, and 0.1111 min-1 for homogeneous FeCl2/H2O2. At 50 mg L-1 and pH 4, the kinetic advantage increased to 0.2317 versus 0.0586 min-1. Radical-scavenger tests identified hydroxyl radicals as the dominant oxidant, and Fe leaching remained negligible. In synthetic textile wastewater, GFePAC achieved 20 min degradation efficiencies of 96.8%, 88.0%, and 88.1% at pH 4, 7, and 9, respectively, consistently exceeding FeCl2. These results demonstrate that DES-mediated Fe immobilization enables stable adsorption-assisted heterogeneous Fenton oxidation under both model and complex wastewater conditions.

SWRM 2026 SW800

Arsenic removal from aqueous solutions using green synthesized Fe-Ti mixed nanoparticles

***Harshica Fernando**, hufernando@pvamu.edu. Chemistry, Prairie View A&M University, Prairie View, Texas, United States*

Heavy metal contamination in water resources presents a significant environmental and public health challenge, with arsenic being particularly concerned due to its carcinogenicity, widespread occurrence, and persistence in aquatic systems. This study reports the green synthesis of Fe-Ti mixed oxide nanoparticles (NPs) using dextrose as a renewable reducing and capping agent and investigates their effectiveness in arsenic removal from aqueous solutions. The synthesized NPs were characterized using XRD, FTIR, XPS, SEM-EDS, and BET analysis, revealing an amorphous structure with a high surface area and mesoporous characteristics. XPS analysis confirmed the presence of mixed iron valence states within a titanium rich framework, providing diverse and abundant binding sites for arsenic uptake. Sodium meta arsenite was used as the arsenic source, and arsenic concentrations were accurately quantified using an Agilent 7900 ICP-MS throughout the adsorption experiments. The material exhibited optimal arsenic removal at pH 6, with adsorption following pseudo-second-order kinetics. The maximum adsorption capacity reached 42 mg/g at 40 °C, indicating endothermic behavior. The low point of zero charge (PZC, 0.22) and abundant surface hydroxyl groups facilitated efficient arsenic binding through multiple mechanisms, including inner-sphere surface complexation and ligand exchange. The synergistic combination of iron's high affinity for arsenic species and titanium's structural stability, coupled with the environmentally benign synthesis route, yielded a highly efficient and promising material for sustainable water treatment applications.

SWRM 2026 SW801

Dynamic dye–plasmon interactions at surfactant-depleted gold nanorod interfaces: Methylene blue coupling and surfactant-like stabilization by methylene green

***Tefera Entele Tesema**, tetesema@pvamu.edu, Adela Maldonado, Inioluwa Odubanjo. Chemistry, Prairie View A&M University, Prairie View, Texas, United States*

Removal of the native surfactant layer from colloidal gold nanorods exposes a chemically responsive interface but also creates a nanoparticle system that evolves with time. We investigated the optical response of surfactant-depleted AuNR700 after exposure to methylene blue (MB) or methylene green (MG) at 1.5 and 15 μM for 1–24 h. After incubation, the samples were centrifuged, and both the supernatant and recovered nanoparticle fractions were analyzed by UV–visible spectroscopy using

time-matched AuNR controls. At 15 μM MB, the recovered AuNR fraction developed a reproducible localized line-shape deflection within the molecular–plasmon overlap region, with a principal curvature feature near 669–670 nm that was strongest at 3–6 h. A damped coupled-oscillator model yielded an effective molecular resonance at 668.7 nm and an effective coupling energy of approximately 0.094 eV, without resolved mode splitting. At 1.5 μM MB, the localized deflection was absent; instead, MB altered the non-monotonic LSPR trajectory, and differential extinction at 670 nm and at the LSPR maximum reversed sign between 6 and 12 h. MG produced a qualitatively different response. Its supernatants showed a transient, concentration-dependent redistribution within the MG electronic absorption band, quantified by changes between the 612–615 and 653–659 nm regions. The strongest departure from pure MG occurred at 1–3 h for 1.5 μM MG and at 3–6 h for 15 μM MG. The recovered AuNR–MG fractions also exhibited pronounced concentration- and residence-time-dependent changes in extinction intensity and LSPR line shape, including a strong 24 h response at 15 μM MG. Together, these observations are consistent with adsorption-driven interfacial passivation in which MG partially assumes a surfactant-like role after native-ligand removal. The results demonstrate that molecular identity, concentration, and residence time direct distinct optical pathways at dynamically evolving AuNR interfaces.

SWRM 2026 SW802 - Withdrawn

SWRM 2026 SW803

Interfacial mechanisms underlying the antibacterial activity of nano- and microscale zinc- and gallium-based oxides

Yuri Strzhemechny[1]*, y.strzhemechny@tcu.edu, John Brannon*[1]*, Joshua Humphrey*[1]*, Shauna McGillivray*[1]*, Rafal Wiglusz*[2]*, Adam Watras*[2]*, Vitalii Boiko*[2]*. (1) Texas Christian University College of Science & Engineering, Fort Worth, Texas, United States(2) Institute of Low Temperature and Structure Research, Polish Academy of Sciences, Wroclaw, Poland*

Antibiotic resistance is accelerating the need for alternative antibacterial materials. Metal oxides are promising candidates because their antibacterial effects can arise from several physicochemical processes operating simultaneously at the material–bacterium interface. These processes may involve surface-mediated production of reactive oxygen species, dissolution and release of metal ions, direct interactions with bacterial envelopes, and disruption of local ionic and osmotic stress. However, the relative contribution of these processes is strongly dependent on the physicochemical environment, making it difficult to establish clear structure–activity relationships or to predict antibacterial performance from bulk material properties alone. In this study, we examine how surface characteristics and environmental conditions influence the antibacterial behavior of ZnO-, Ga_2O_3-, and GaOOH-based materials. Hydrothermal synthesis is employed to produce nano- and microscale particles with controlled morphologies and systematically modified surface characteristics, including Fe-doped, Cu-doped and undoped compositions. The interactions of these materials with *Escherichia coli* and *Staphylococcus aureus* are evaluated under relevant growth conditions, while complementary characterization before and after exposure to bacteria provides insight into changes occurring at the oxide surface. By correlating particle morphology, surface properties, and post-assay transformations with antibacterial performance, this work aims to elucidate the surface-mediated phenomena that govern the antibacterial activity of zinc- and gallium-based oxides and to establish principles for the rational development of oxide-based antibacterial materials.

SWRM 2026 SW804

Molecular packing governs ultrafast interfacial energy flow

***Md.Shahriar Hossain Shuvo**, mshuvo@uh.edu, Nawoda Athdath Waduge, Ding-Shyue Yang. Chemistry, University of Houston System, Houston, Texas, United States*

Molecular packing at solid–molecule interface plays a critical role in nanoscale energy transport, yet its influence on ultrafast energy flow remains challenge to resolve directly. Here, we use reflection ultrafast electron diffraction to investigate energy transport across Au(111)–alkanethiol junctions with distinct molecular packing geometries. Following photoexcitation, energy flows sequentially from the Au surface layer to the molecular head groups and subsequently into the molecular backbone. Despite similar Au–S bonding, the ~30^0 tilted hydrocarbon SAM (HSAM) and the more upright fluorinated SAM (FSAM) exhibit markedly different dynamics. FSAM shows an ~15 ps delayed onset, indicating greater resistance to initial energy transfer across the interface, yet its more vertically packed CF_2 backbone thermalizes faster (~40 ps) than the tilted CH_2 backbone of HSAM (~60 ps). In contrast, the head groups of both SAMs respond on similar ~20 ps timescales. Ethanethiol, which lacks an extended ordered molecular backbone, shows substantially weaker structural effects. These observations demonstrate that molecular packing can independently regulate interfacial energy injection and subsequent energy propagation through molecular junctions.

SWRM 2026 SW805

Topological defect formation and hydrodynamic cavitation driven by asymmetric particles in nematic liquid crystals

***Xiaowei Wang**[1], xiaoweiwang@my.unt.edu, Teagan Hamlett[2], Sid Hashemi[1], Joseph E. Doebler[2], Tasha Joy[1], Giordano Tierra[1], Ying Bao[2], Xiao Li[1]. (1) University of North Texas, Denton, Texas, United States(2) Western Washington University College of Science and Engineering, Bellingham, Washington, United States*

Topological defects (TDs) emerge from disruptions in orientational order across systems spanning vastly different length scales and often adopt symmetric configurations through energy minimization. Introducing controlled symmetry breaking provides an opportunity to create unconventional defect structures and investigate self-assembly away from equilibrium. Here, we use nematic liquid crystals (LCs) as a model system to directly visualize defect formation around asymmetric tadpole-shaped particles composed of a spherical head and a long, flexible SiO2 tail. Experimental observations and numerical simulations reveal that deformation of the micrometer-scale tail strongly distorts the surrounding LC director field, producing distinctive butterfly-shaped topological defects. When the particles move through the LC under capillary forces, dynamic fluctuations at the air–LC interface can additionally generate metastable cavities. The formation and subsequent evolution of these cavities arise from hydrodynamic cavitation governed by the competition among capillary, elastic, and viscous forces, which ultimately drives cavity contraction and restoration of equilibrium. These results demonstrate how particle asymmetry and flexibility can generate unconventional defect configurations and dynamic cavitation phenomena in liquid crystals, providing new opportunities for controlling particle defect interactions in microactuators, soft robotic systems, and adaptive materials.

SWRM 2026 SW806

Solvent-mediated micellization and universal face-centered cubic ordering of Poloxamer 407

***Mostafa Tabatabaei**, smtabatabaei.76@ou.edu, Reza Foudazi. School of Chemical, Biological & Materials Engineering, The University of Oklahoma, Norman, Oklahoma, United States*

Understanding how solvent environment controls block copolymer self-assembly is important for designing tunable lyotropic liquid crystalline materials. Here, we investigate the temperature-driven self-assembly of Poloxamer 407 (P407) across the full composition range of ethylammonium nitrate (EAN)–water mixtures using small-angle X-ray scattering (SAXS), rheology, and differential scanning calorimetry (DSC). Both the critical micellization temperature and sol–gel transition temperature exhibit a nonmonotonic dependence on solvent composition, reaching a minimum at 60 wt% EAN. Structural analysis reveals a multistep micellization pathway in which micelle number density initially decreases, followed by micelle formation and growth through incorporation of free unimers. Despite pronounced solvent-dependent differences in micelle size, solvation, and transition temperatures, FCC ordering consistently occurs at a critical micelle volume fraction of approximately 0.49. Furthermore, normalization of temperature by the micellization and gelation temperatures collapses data from different solvent compositions and P407 concentrations onto a universal sigmoidal relationship between micelle volume fraction and normalized temperature. These results demonstrate that the transition from micelles to an ordered FCC structure is governed primarily by spatial packing constraints and entropic interactions rather than specific solvent–polymer interactions, providing a general framework for understanding and controlling poloxamer self-assembly.

SWRM 2026 SW807

Rapid one-pass extrusion method for the synthesis of ion-selective droplet networks

***Sneha Sinha**, snehasinha@utexas.edu, Ronald J. Vogler, Claire Baldus, Manish Kumar. The University of Texas at Austin, Austin, Texas, United States*

Droplet networks are a water-in-oil emulsion with a high concentration of water droplets, each lined with lipid monolayers. When these droplets touch, they create interface bilayers; ion channels can be inserted into these bilayers to make them selective to specific ions, allowing droplet networks to be used for ion-ion separations. Historically, droplet networks were made with a bottom up approach, allowing for precise control over composition and arrangement of the droplet networks, but the production rate is slow, ranging from 10 nL/min to 10 uL/min. Recently, droplet networks were made using a top-down approach, where an emulsion can form a network of droplets at a significantly higher pace, but this process requires a high G-force with centrifugation, which inhibits the scaling of this approach to larger volumes. In this work, we demonstrate a single step method to produce droplet networks without centrifugation. A water-in-oil emulsion consisting of aqueous buffer and monolinolein dissolved in hexadecane was loaded into a syringe equipped with a PTFE syringe filter and extruded using a syringe pump. Droplet networks only formed when at least 10 mg/mL of monolinolein was present in the oil phase and when the oil volume fraction in the emulsion was in the range of 20-30%. Extrusion rates up to 40 mL/min resulted in the successful formation of droplet networks, a rate multiple orders of magnitude higher than other, bottom-up synthesis methods for droplet networks. A confocal image of a droplet network showed a packed array of droplets that are 10 micron or less in diameter, similar to other previously-studied droplet networks. Across the droplet networks under various conditions, the lowest capacitance per area was 156 ± 24 pF/cm and the highest capacitance per area was 741±147 pF/cm, values similar to other droplet networks previously

made. Additionally, gramicidin A (an ammonium channel) was added to verify that ion selective channels can be inserted into this system. Upon adding gramicidin A, the NH4+ conductance went up from 5.0 ns/cm^2 to 5000 nS/cm^2 and, the NH4+/Na+ selectivity was 8.5, and the NH4+/Mg2+ selectivity was 910, confirming the insertion of gramicidin A into this material can have ion selective channels inserted. Altogether, this alternative synthesis method for droplet networks represents advancement in the scalability of these droplet networks.

SWRM 2026 SW808

Quinone uptake by levitated phenolic droplets: Noncovalent interactions and brown carbon light absorption

***Ahmadraza Chaudhary**, ahmadraza.chaudhary@okstate.edu, Colton T. Calvert, Holly B. Anthony, Micah R. Miles, Elijah Schnitzler. Chemistry, Oklahoma State University The College of Arts and Sciences, Stillwater, Oklahoma, United States*

Biomass burning is a significant source of light-absorbing organic aerosols known as brown carbon (BrC). These aerosols contribute to atmospheric radiation by absorbing sunlight in the near-UV and visible regions and therefore influence Earth's radiative balance. Their light-absorbing properties can also change through multiphase interactions in the atmosphere. Methoxyphenols (MPs), such as guaiacol, eugenol, and related lignin-derived compounds, are important biomass burning emissions and precursors to BrC formation. Although many MPs are themselves colorless and absorb weakly in the visible region, their interactions with other atmospheric compounds can enhance their light absorption. Here, we investigate non-covalent interactions between MPs and quinones in bulk solutions, thin films, and acoustically levitated droplets. Droplets containing donor species were suspended and exposed to different mixing ratios of gas-phase benzoquinone while visible spectroscopy was used to monitor changes in absorbance during uptake. Upon exposure to benzoquinone, the initially colorless droplets rapidly developed strong visible absorption, consistent with CT complex formation. After exposure, the system was flushed with nitrogen, which caused the absorbance to decrease and showed that the interaction was reversible. The decay in absorbance was slower than the rate of dilution, suggesting strong intermolecular interactions within the droplet and a large associated effective Gibbs partition energy. NMR spectroscopy showed no evidence for the formation of new covalent products, further supporting the presence of non-covalent intermolecular complexes. In addition to individual MPs, mixtures containing several MPs showed the same reversible trend in visible absorbance upon exposure to benzoquinone. This suggests that the interaction is not limited to individual compounds and can also occur in a more atmospherically relevant multicomponent surrogate representing the phenolic fraction of biomass-burning organic aerosol. Overall, these results suggest that non-covalent multiphase interactions between methoxyphenols and quinones may contribute to the light absorption and climate effects of BrC.

SWRM 2026 SW809

Engineering giant magnetic susceptibility in porous nanocrystal clusters for biomedical and environmental applications

***Qingbo Zhang**, qingbozhang@lsu.edu, Vicki L. Colvin. Department of Chemical Engineering, Louisiana State University, Baton Rouge, Louisiana, United States*

Magnetic nanoparticles enable remote field-driven control, moving, heating, or imaging materials at a distance, thus supporting a wide range of biomedical, environmental, and industrial applications. However, their practical utility has long been limited by intrinsically low magnetic susceptibility. Here we show that susceptibility can be greatly enhanced by engineering porous, single-crystalline iron oxide nanocrystal clusters. The clusters are synthesized via a solvothermal method that promotes oriented attachment of primary nanocrystals into porous, single-crystalline superstructures with tunable size and porosity. Giant susceptibility emerges when four structural features, shared interfaces, crystallographic alignment, internal porosity, and optimal cluster dimensions, are integrated within a single cluster. The resulting clusters exhibit an initial susceptibility up to seven times higher than that of optimally sized solid nanocrystals. Micromagnetic simulations attribute this enhancement to a moderate degree of exchange interaction between primary nanocrystals within each cluster. This giant susceptibility translates into superior performance under low magnetic fields across diverse applications, including cancer thermotherapy, magnetic particle imaging, cell targeting, and environmental remediation. These findings establish a general design strategy, tuning exchange interactions within hierarchical nanocrystal assemblies, for accessing magnetic properties previously unattainable in solid nanoparticles, opening new pathways for magnetic materials with broad technological utility.

SWRM 2026 SW810

Multichannel kinetic optical spectrometry for characterizing dynamic liquid-phase systems

***Dongmao Zhang**, dz33@msstate.edu. Chemistry, Mississippi State University, Mississippi State University, Mississippi, United States*

Dynamic liquid-phase systems, including molecular assemblies, colloids, and biomolecular condensates, undergo continuous physicochemical changes that are difficult to characterize using conventional optical spectroscopy. UV–visible extinction, light scattering, fluorescence, and polarization measurements provide complementary information about these systems but are typically acquired sequentially using different instruments or measurement configurations, making direct temporal correlation difficult for rapidly evolving samples. We have developed a multichannel kinetic optical spectrometry approach based on a multitrack linearly polarized spectrometer that simultaneously acquires reference, forward-transmission, and two polarization-resolved side-detection spectra from the same sample. This configuration enables concurrent measurement of UV–visible extinction, polarization-resolved scattering, fluorescence, and their depolarization properties with subsecond temporal resolution, generating multidimensional kinetic optical fingerprints of evolving physicochemical states. The analytical capabilities of this approach are demonstrated using two fundamentally different dynamic liquid systems. During acid-induced self-assembly of meso-tetrakis(4-sulfonatophenyl)porphyrin (TSPP), extinction, scattering, and fluorescence exhibit distinct kinetic trajectories, while the multidimensional responses distinguish assembly pathways produced by different sample-preparation histories and reveal irreversible structural reorganization during thermal perturbation. In contrast, thermally induced liquid–liquid phase separation of an elastin-like polypeptide is dominated by scattering-related changes, with simultaneous transmission and polarization-resolved scattering measurements resolving different stages of coacervation, transition kinetics, thermal hysteresis, and continued evolution of the condensed phase during isothermal incubation. Collectively, these studies demonstrate that multichannel kinetic optical spectrometry provides substantially richer information than conventional sequential measurements by directly correlating complementary optical observables throughout dynamic processes, offering a general strategy for investigating molecular assembly, phase separation, aggregation, and other evolving liquid-phase systems in chemical, materials, and biophysical research.

SWRM 2026 SW811

Using virus-like particles to develop vaccines for infectious and chronic diseases

Bryce Chackerian*, bchackerian@salud.unm.edu. Molecular Genetics and Microbiology, The University of New Mexico School of Medicine, Albuquerque, New Mexico, United States*

Many viral structural proteins have an intrinsic ability to self-assemble into virus-like particles (VLPs). VLPs physically resemble virions but are non-infectious because they lack viral genomes. Like viruses, VLPs have physical characteristics (such as their size and repetitive structure) that mediate strong immune responses. VLPs have been utilized as stand-alone vaccines, but they have also been employed as platforms for increasing the immunogenicity of diverse heterologous antigens engineered to be displayed on their surface. This ability to enhance immunogenicity applies to antigens derived from traditional targets, such as pathogens, but also to self-antigens which are normally subject to the mechanisms of B cell tolerance. In this talk, I'll describe our efforts to develop VLP-based vaccines for diverse indications. These include the development of a malaria vaccine that specifically targets a highly vulnerable epitope within the *Plasmodium falciparum* circumsporozoite protein, a vaccine targeting fentanyl that can potentially prevent the consequences of opioid overcdose, and a vaccine targeting myostatin, which may be used to prevent muscle wasting. I'll also discuss approaches for engineering VLP-based vaccines, characterisitics of the immune responses that they induce, and prospects for clinical implementation.

SWRM 2026 SW812

MOXI-214: A fully manganese-based metal-organic framework for antigen delivery and immune activation

Ziqi Wang*, ziqiwang2000@gmail.com, Alexander J. Mathai, Thomas Howlett, Emily Osborn, Shahabuddin Alam, Jeremiah J. Gassensmith. Chemistry and Biochemistry, The University of Texas at Dallas, Richardson, Texas, United States*

Activation of innate immune sensing pathways is critical for vaccines targeting intracellular pathogens, and manganese ions (Mn^{2+}) are potent activators and enhancers of these responses. However, effective and safe intracellular delivery of Mn^{2+} remains a major challenge. Here, we report MOXI-214, a fully manganese-based metal-organic framework (MOF) that functions as both an antigen carrier and immunostimulatory adjuvant. MOXI-214 exhibits tunable particle sizes: larger particles enable biomimetic mineralization of proteins and bacteria, forming protective crystalline shells, while smaller particles facilitate cellular uptake and intracellular delivery. In macrophages, MOXI-214 activates the cGAS-STING pathway and induces type I interferon production. It also promotes maturation of bone marrow-derived dendritic cells (BMDCs). Together, these findings highlight the potential of MOXI-214 as a versatile vaccine delivery and adjuvant platform.

SWRM 2026 SW813

Linker strategies for local delivery of small-molecule immunomodulators in transplantation

***Robert R. Kane**, bob_kane@baylor.edu. Chemistry & Biochemistry, Baylor University, Waco, Texas, United States*

Our lab has an ongoing interest in bioconjugation for the localized delivery of small-molcule immunomodulators in tranplantation. Much of our work is focused on customizing bioconjugation and linker chemistry for a variety of therapeutic targets. This presentation will describe the development and characterization of several drug/linker/tissue combinations.

SWRM 2026 SW814

Unlock the subdominant B cell repertoire with polymeric nanoparticle adjuvant for the next-generation vaccine development

***Qian Yin**, qian.yin@austin.utexas.edu. Biomedical Engineering, The University of Texas at Austin, Austin, Texas, United States*

Effective vaccines against rapidly mutating viruses, including influenza viruses and coronaviruses, must elicit broad, cross-reactive antibody responses. However, current vaccines often fail to provide such broad protection. A major barrier is germinal center (GC)-driven immunodominance, in which B cells recognizing variable immunodominant epitopes outcompete subdominant clones targeting conserved viral regions. To overcome this limitation, we developed a Toll-like receptor 7 agonist-conjugated nanoparticle (TLR7-NP) adjuvant designed to rescue the subdominant B cell repertoire in GC reactions. TLR7-NPs are synthesized via well-controlled, TLR7 agonist-initiated ring-opening polymerization, followed by self-assembly with mPEG-PLGA via nanoprecipitation. The resulting sub-100 nm nanoparticles (~94 nm) efficiently drain through lymphatics, accumulate in draining lymph nodes for at least three days, and provide sustained TLR7 signaling through continuous release of agonist. This persistent stimulation promotes early B cell seeding into GCs, prolongs GC reactions, and increases the T follicular helper-to-T follicular regulatory cell ratio, thereby enabling the recruitment and maturation of subdominant B cell clones recognizing conserved epitopes.
The TLR7-NP platform demonstrated robust *in vivo* efficacy across both influenza and coronavirus vaccine models. When combined with Alum-bound hemagglutinin (HA) from a single influenza strain, TLR7-NPs increased cross-reactive IgG responses, enhanced recognition of the conserved HA stem, and achieved 92.9% survival following a lethal heterologous challenge, compared to 43.8% for soluble TLR7-Alum. When formulated with the SARS-CoV-2 HexaPro spike protein, TLR7-NPs induced S2-specific antibodies in 100% of mice, produced higher neutralizing titers after a single dose than TLR7-Alum, and generated broader coronavirus-reactive antibodies than a licensed mRNA vaccine. TLR7-NPs also promoted cross-reactive long-lived plasma cells and subdominant-specific memory B cells. Altogether, these results demonstrate that TLR7-NPs present a promising strategy for developing next-generation vaccines against rapidly evolving viruses.

SWRM 2026 SW815

Injectable multidomain peptide (MDP) hydrogel for controlled drug delivery in the immunotherapy of oral cancer

***Arghadip Dey**[1], ad157@rice.edu, Jeffrey D. Hartgerink[1,2]. (1) Chemistry, Rice University Wiess School of Natural Sciences, Houston, Texas, United States(2) Bioengineering, Rice University, Houston, Texas, United States*

Head and neck squamous cell carcinoma (HNSCC) impacts around 890,000 patients globally each year, with oral cancer being the most common type. Combination immunotherapy has emerged as a promising strategy for oral cavity squamous cell carcinoma (OCSCC), but coordinating multiple therapeutic agents remains challenging due to differences in dosing and pharmacokinetics. Here, we developed a drug-delivery platform, multidomain peptide (MDP) hydrogel, for localized, multi-agent immunotherapy of oral cancer. MDPs are amphiphilic peptides that self-assemble into β-sheet nanofibers to form shear-thinning and shear-recovering hydrogels, allowing easy syringe delivery. The platform coordinates the release of multiple immunomodulatory agents, each with distinct release mechanisms at different timescales, from a single injectable formulation to achieve diverse therapeutic effects. In addition to controlled drug release, the peptide scaffold was also modified to provide intrinsic bioactivity, transforming its role from a passive delivery platform to an active therapeutic component. We characterize the hydrogel's properties, evaluate its multi-agent delivery behavior, and assess its biological activity in cell-based models relevant to oral cancer immunotherapy. Together, these studies demonstrate a multifunctional peptide biomaterial that integrates therapeutic delivery and material-based bioactivity on a single platform, offering a potential strategy to simplify localized combination immunotherapy for oral cancer.

SWRM 2026 SW816

Turning focused ultrasound histotripsy into an *in situ* cancer vaccine for systemic antitumor immunity

Ashish Ranjan[1,2]*, Ashish.Ranjan@UTSouthwestern.edu. (1) The University of Texas Southwestern Medical Center Department of Radiation Oncology, Dallas, Texas, United States(2) Department of Physiological Sciences, College of Veterinary Medicine, Oklahoma State University, Stillwater, Oklahoma, United States*

Focused ultrasound-based boiling histotripsy (HT) mechanically disrupts tumors and releases a rich source of tumor-derived antigens, creating an opportunity to transform local ablation into systemic cancer immunotherapy. However, antigen release alone is often insufficient to generate effective antitumor immunity, particularly in immunologically "cold" tumors. We developed biodegradable antigen-capturing microparticles incorporating an agonistic CD40 antibody (CMP) to capture HT-released tumor antigens while simultaneously promoting antigen-presenting cell activation and T-cell priming. Across murine melanoma, head and neck, and colon tumor models, combining HT with CMP enhanced antitumor immune responses following both partial (<10%) and extensive (>50%) tumor ablation. Local HT+CMP treatment increased functional immune-cell infiltration, improved control of treated tumors, and generated responses against untreated distant tumors. Importantly, the combination also sensitized otherwise resistant tumors to immune checkpoint inhibition. To further test whether HT-generated tumor material could serve as a vaccine, tumor lysates generated by HT were captured onto CMPs and administered subcutaneously. This approach similarly generated systemic antitumor activity, supporting the concept that HT can provide a personalized source of tumor antigens for therapeutic vaccination. Together, our findings demonstrate that focused ultrasound can do more than locally destroy tumors. By coupling HT-mediated antigen release with antigen capture and CD40-mediated immune activation, local tumor ablation can be converted into an in situ vaccination strategy capable of generating systemic antitumor immunity and overcoming resistance in immunologically cold tumors.

SWRM 2026 SW817

Injectable biomaterial scaffolds to prevent orthopaedic device infection

Alexander M. Tatara[1,2]*, alexander.tatara@utsouthwestern.edu. (1) Medicine, The University of Texas Southwestern Medical Center, Dallas, Texas, United States(2) Biomedical Engineering, The University of Texas Southwestern Medical Center, Dallas, Texas, United States*

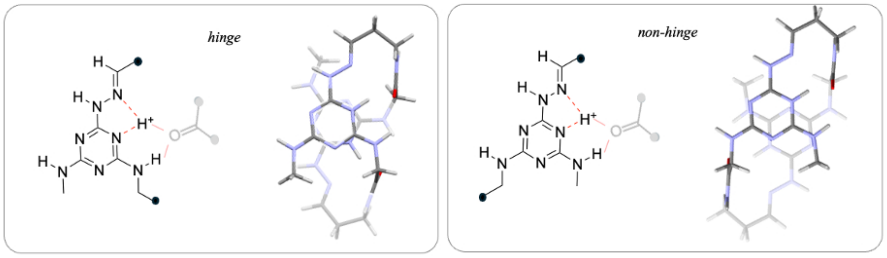
Orthopaedic devices, ranging from fracture fixation hardware to replacement joints, are becoming ubiquitous due to their ability to restore mobility and function. However, these devices are vulnerable to infection particularly by Staphylococcus aureus, a biofilm-producing virulent bacteria. S. aureus possesses a number of immune-evasive mechanisms by which it can modulate and/or mask itself from the human immune system, including toxins to destroy immune cells and proteins that act as decoys to bind and disable antibodies. Producing a vaccine to prevent orthopaedic hardware infection by Staphylococcus aureus has proven to be difficult using conventional technology. Current vaccines are short-lived liquid boluses containing antigen and adjuvant. During actual infections, antigens are presented in a specific spatial context and concentration as well as for an extended duration of time. To better mimic the natural spatiotemporal patterns of antigen presentation, we designed injectable biodegradable biomaterials as scaffold vaccine platforms. Self-assembling mesoporous silica rods serve as the backbone of the scaffold. By adsorbing antigens, adjuvants, and chemokines to the mesoporous silica rods, dendritic cells can be recruited into the injected scaffold for activation and antigen uptake. Compared to bolus injection of these reagents in a murine model, we have found that scaffold vaccines resulted in greater activation of cell-mediated immunity. In a murine model of orthopaedic hardware infection, mice that received scaffold vaccination had ~250x decreased device bacterial burden than those that received conventional liquid vaccination, and 15-25% of mice in scaffold vaccine groups had sterilizing immunity. Biomaterials for immunoengineering are an emerging frontier with great promise for infectious diseases.

SWRM 2026 SW818

Ready access to 24-atom macrocycles: Conformation, computation and application

Eric Simanek*, e.simanek@tcu.edu. Chemistry & Biochemistry, Texas Christian University, Fort Worth, Texas, United States*

Spontaneous dimerization of monomers yields 24-atom macrocycles quantitatively. The only by-products are volatile. Success is attributed to intramolecular hydrogen bond (IMHB) networks that template hydrazone formation and contribute to structure. Solution and solid-state studies indicate two dominant conformations: hinge and non-hinge. On the NMR timescale, the former conformer is dynamic, the latter static. Engineering the IMHB by removing donor and acceptor sites. These conformations are robust, tolerating substitution at multiple sites. Computation proves useful in identifying additional conformations. Libraries of these molecules have been prepared and distributed to HTS centers.



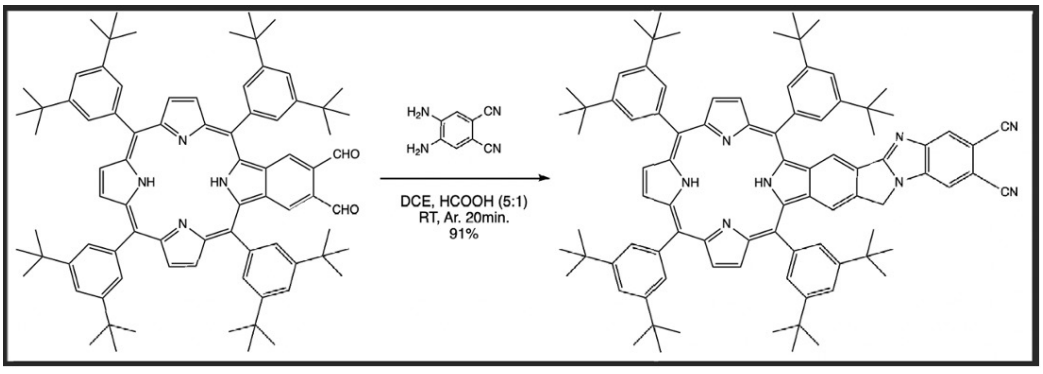
Two conformations accessible to 24-atom macrocycles with half of the macrocycle shown in atomic detail, including elements of the IMHB network.

SWRM 2026 SW819

Aromatic heterobicycle-fused porphyrins: Synthesis, characterization and study of impact on aromaticity and excited state electron transfer leading to long-lived charge separation

Joshua A. Martinez*, joshuamartinez6@my.unt.edu. Chemistry, University of North Texas, Denton, Texas, United States*

Expanding the pi-system of porphyrins improves their electrical and light-absorption capabilities. This makes them useful for biomedical imaging and organo-electronic devices. Structural modification of groups fused at the beta position are in plane of the porphyrin and have direct implications to influence electronic behavior through conjugation. This approach creates new porphyrin types and building blocks for porous materials, leads to better light-capturing systems.The pi-extension of porphyrins through the incorporation of aromatic heterocycles is rare and is synthetically more challenging. The incorporation of heteroatoms into highly pi-extended porphyrin structures can provide control of the electronic structure, and has become a critical strategy to manipulate the materials in order to endow them with desirable properties, such as electro- chemical activity, optical absorption spectra, photo- luminescence, redox behavior, charge transfer, bandgap tuning, and other characteristics. The development of new methods to introduce heteroatoms or heterocycles is very important to facilitate the growth of this field. Previous works from our group detail the fusion of benzimidazole-isoindole moiety to porphyrin at the beta position. The Zinc inserted analogue of this compound was found to promote excited state electron transfer through coordination to C_{60} fullerene bearing imidazole group. The charge separated state generated was in the order of 35ms which is quite rare in porphyrin fused systems. The formation of this long-lived charge separated state was attributed to both singlet and triplet involved excited states. Accessing porphyrin materials of this kind was thought to be a long-standing challenge in this field, and to this end, novel Benimidazole-isoindole fused porphyrin bearing 1,2 peripheral cyano groups, was synthesized. We aim to continue the investigation into the rare long-lived charge separated state found to exist within these extended aromatic porphyrin systems bearing the Benzimidazole-isoindole bridge. This methodology is high-yielding and extremely concise as it does not require lengthy purification protocols using column chromatography.

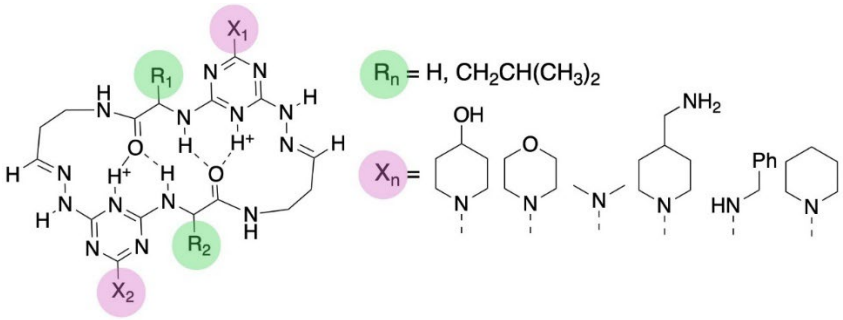


SWRM 2026 SW820

Triazine macrocycles: From library synthesis to unexpected membrane permeability

***Gretel A. Stokes**, gretel.jordan@tcu.edu, Eric Simanek. Chemistry and Biochemistry, Texas Christian University, Fort Worth, Texas, United States*

Macrocycles occupy a unique region of chemical space with potential applications in drug discovery and molecular recognition, but synthesis and prediction of physiochemical properties remain a challenge. Here, solution-phase synthesis of triazine macrocycles containing either glycine or leucine linkers with varying auxiliary amines yields a library with experimentally determined octanol-water partition coefficients (logP) values ranging from -0.3 to 5.2. Although additive algorithms for computing logP (*i.e.* AlogP) systematically underestimate hydrophobicity by a factor of 100, the correlation of computed and experimental values allows for predictions. Unexpectedly, macrocycles bearing two primary amines in the auxiliary position (outside the core of the macrocycle) possess substantially greater hydrophobicity than anticipated; the glycine homodimer exhibited a logP of 3.3 at high pH and crossed an artificial membrane approximately ten times faster than related macrocycles bearing conventionally hydrophobic substituents. CREST conformational analysis suggests that intramolecular hydrogen bonding between the two primary amines effectively glues the macrocycle in a folded conformation. Polar groups engage in an extended hydrogen-bond network within the core of the macrocycle, masking their polarity. These results demonstrate how conformationally accessible intramolecular interactions can produce nonintuitive physiochemical properties—a dimension that is especially relevant for macrocycles whose conformational space is much larger and, thus, harder to predict, than traditional small drug molecules—leading to the conclusion that triazine macrocycles are a useful model for exploring relationships among structure, lipophilicity, and membrane permeability.

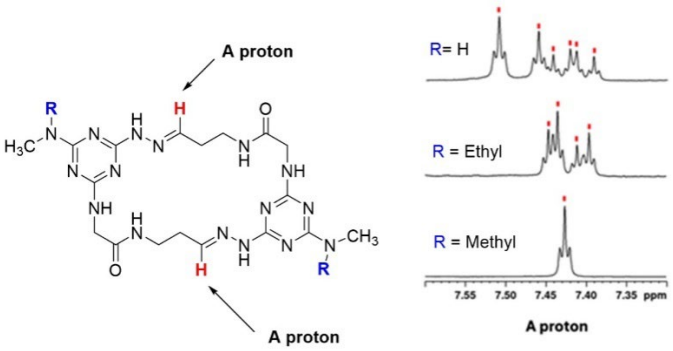


SWRM 2026 SW821

When hydrogen bonds compete: Primary amine auxiliaries reveal new conformational isomers in 24-atom triazine macrocycles

***Harsha Vardhan Reddy Kasireddy**, drharshaindia@gmail.com, Eric Simanek. Department of Chemistry & Biochemistry, Texas Christian University, Fort Worth, Texas, United States*

Intramolecular hydrogen-bond (IMHB) networks govern the conformation of 24-atom triazine macrocycles. While secondary amine auxiliaries support conserved hinge-like motifs and limited conformational ensembles, incorporation of a primary amine introduces an additional hydrogen-bond donor and a competing IMHB network. This change expands the ensemble to five persistent conformers, including a new expanded-hinge motif alongside previously established hinge and non-hinge conformations. NMR spectroscopy, H/D exchange, variable-temperature studies, and computation support the conformational assignments and hydrogen-bonding topology, with QTAIM analysis further corroborating the proposed interactions. These results demonstrate that competing IMHB networks provide a general strategy for engineering new conformational states in macrocycles.



SWRM 2026 SW822

LC–MS/MS glycomics reveals high-fat diet–modulates hemisphere-specific *N*-glycan remodeling in the thalamus following traumatic brain injury

Abiodun Adewolu[1]*, mohammedabiodun94@gmail.com, Vishal Sandilya*[1]*, Abderrahmane Koraich*[1]*, Judith Nwaiwu*[1]*, Stanley Ibeh*[2]*, Sarin Mekhjian*[3]*, Firas Kobeissy*[4]*, Yehia Mechref*[1]*. (1) Chemistry and Biochemistry, Texas Tech University, Lubbock, Texas, United States(2) Biochemistry and Neuroscience, Dalhousie University, Halifax, Nova Scotia, Canada(3) American University of Beirut, Beirut, Beirut Governorate, Lebanon*

Traumatic brain injury (TBI) initiates secondary molecular alterations that extend beyond the primary cortical lesion and contribute to progressive dysfunction in connected brain regions, including the thalamus. High-fat diet (HFD) promotes metabolic stress and neuroinflammation and may exacerbate these post-injury responses; however, whether HFD-associated glycomic remodeling after TBI is restricted to the ipsilateral hemisphere or also extends to the contralateral thalamus remains poorly understood. Here, we investigated hemisphere-specific changes in the thalamic *N*-glycome following TBI under normal chow (NC) and HFD conditions using high-resolution liquid chromatography–tandem mass spectrometry (LC–MS/MS) glycomics. Mice were maintained on NC or HFD and subsequently assigned to sham or TBI groups using a controlled cortical impact model. Ipsilateral and contralateral thalamic tissues were collected and analyzed independently. *N*-linked glycans were enzymatically released with PNGase F, reduced, permethylated, separated by liquid chromatography, and characterized by high-resolution tandem mass spectrometry. Marked *N*-glycomic remodeling was observed in the ipsilateral thalamus, with HFD-TBI producing the most extensive alterations. 32 *N*-glycans were significantly altered in HFD-TBI animals compared with 10 following TBI under normal chow conditions, indicating that HFD markedly enhances the glycomic response to injury. Diet alone also produced substantial ipsilateral remodeling, supporting an independent effect of metabolic status on thalamic glycosylation. In contrast, the contralateral thalamus exhibited comparatively limited changes, with approximately nine altered *N*-glycans detected in HFD-TBI animals and minimal changes following NC-TBI. Altered classes included complex, sialylated, and sialofucosylated *N*-glycans, which could be because of remodeling of pathways associated with inflammatory signaling, cellular stress, and tissue adaptation. Our findings demonstrate that HFD amplifies TBI-associated *N*-glycomic remodeling predominantly in the ipsilateral thalamus, revealing a strong hemisphere-dependent response to combined metabolic and traumatic injury. High-resolution LC–MS/MS glycomics provides the analytical sensitivity and structural information necessary to uncover these spatially distinct molecular signatures and may help define glycosylation pathways involved in secondary thalamic degeneration after TBI.

SWRM 2026 SW823

Serum *N*-glycan fucosylation reveals distinct remodeling patterns across mild cognitive impairment and Alzheimer's disease

Abdulrahman Abdulmumin[1]*, ababdulm@ttu.edu, Sherifdeen Onigbinde*[1]*, Joy Solomon*[1]*, Stephen Awuku*[1]*, Abderrahmane Koraich*[1]*, Zain Zeitouni*[1]*, Fabricio Meneses*[1]*, Sofia Sepulveda*[1]*, Jie Zhang*[2]*, David M. Lubman*[2]*, Yehia Mechref*[1]*. (1) Department of Chemistry and Biochemistry, Texas Tech University, Lubbock, Texas, United States(2) Department of Surgery, University of Michigan, Ann Arbor, Michigan, United States*

Altered protein glycosylation accompanies Alzheimer's disease (AD), but how specific features of serum *N*-glycan fucosylation differ across clinical stages of cognitive impairment remains poorly defined. We investigated fucosylation remodeling across cognitively normal Controls (n=150), mild cognitive impairment (MCI; n=116), and AD dementia (n=57). Serum *N*-glycans were enzymatically released using peptide-N-glycosidase F (PNGase F), purified by solid-phase extraction, reduced with borane–ammonia complex, and permethylated using methyl iodide under basic conditions. Permethylated glycans were separated by reversed-phase nanoLC and analyzed in positive-ion mode on an Orbitrap Fusion Lumos. Full-MS spectra were acquired at 120,000 resolution over m/z 400–2000, followed by data-dependent MS/MS at 30,000 resolution using CID (35% collision energy). Following rigorous validation, 108 *N*-glycans were quantitatively evaluated. Structural resolution of serum fucosylation revealed distinct patterns associated with MCI and AD. Total fucosylation was numerically lower in both disease groups but significantly lower in AD relative to Controls. Monofucosylated glycans, the predominant fucosylated population, were significantly lower in AD, whereas bi- and trifucosylated glycans were significantly lower in MCI. Positional analysis showed a complementary distinction: core fucosylation was significantly lower in AD, while branch fucosylation was significantly lower in MCI relative to Controls. Total sialofucosylation showed a modest numerical increase in MCI and AD, although group differences were not significant. Notably, glycans unique to Control versus AD were fucosylated, whereas those unique to MCI versus AD were sialofucosylated. Collectively, MCI-associated alterations were preferentially reflected in branch and multifucosylated glycans, whereas lower total fucosylation in AD was dominated by the abundant monofucosylated population and accompanied by lower core fucosylation. Resolving fucosylation by fucose number, position, and accompanying sialylation reveals distinct glycan remodeling associated with MCI and AD, potentially reflecting disease-associated alterations in protein processing and immune regulation.

SWRM 2026 SW824

Serum N-glycome profiling identifies candidate biomarkers for genotype discrimination and severity stratification in sickle cell disease

Abderrahmane Koraich*, akoraich@ttu.edu, Joy Solomon, Sherifdeen Onigbinde, Hira Tasqeen, Abiodun M. Adewolu, Tanjina A. Suma, Yehia Mechref. Department of Chemistry and Biochemistry, Texas Tech University, Lubbock, Texas, United States*

Sickle cell disease (SCD) encompasses genotypes with markedly different clinical severities, yet current diagnostics classify genotype without reliably predicting individual severity. Protein glycosylation is highly sensitive to chronic hemolysis and inflammation, the central drivers of SCD pathophysiology, positioning serum N-glycomics as a promising source of biomarkers for genotype discrimination and severity stratification.Serum samples from the Cooperative Study of Sickle Cell Disease (CSSCD), obtained via BioLINCC, were analyzed for Control (n=47), HbSS (n=55), HbSC

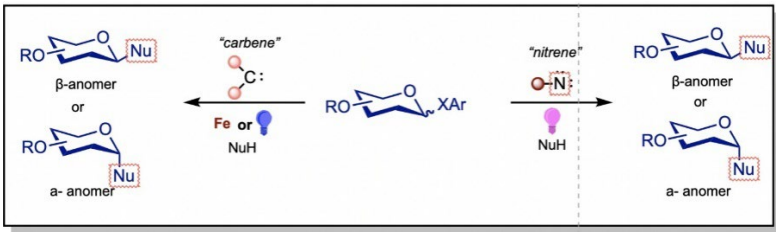
(n=34), and Sβ⁺-thalassemia (n=7) individuals. N-glycans were enzymatically released with PNGase F, purified by C18 SPE, reduced, permethylated, and analyzed by LC-MS/MS. Glycans were identified and quantified using Xcalibur, GlycoWorkbench, and Skyline. Statistical comparisons used the Kruskal-Wallis test with Dunn's post-hoc test and Benjamini-Hochberg correction. A total of 108 N-glycans were identified. Unsupervised PCA revealed clear separation between Control and disease genotypes, with HbSC and HbSS showing notable overlap, consistent with shared hemolytic and inflammatory features previously reported between these genotypes. Fucosylated glycan abundance increased, while sialylated glycan abundance decreased, with disease severity. Differential analysis identified 35–62 significantly altered glycans per pairwise comparison, converging on a 33-glycan signature shared across all three disease genotypes relative to Control, plus a 5-glycan signature specific to HbSS. ROC analysis showed strong discriminatory performance, with combined glycan panel AUCs of 0.99–1.00 across genotype comparisons. These findings show that serum N-glycosylation captures both a shared, genotype-independent SCD signature and genotype-specific alterations tied to severity, supporting glycan-based biomarkers for SCD stratification. Ongoing work will expand the Sβ⁺-thalassemia cohort for statistical power, apply targeted validation via parallel reaction monitoring (PRM), and correlate glycan signatures with clinical severity to establish clinical utility.

SWRM 2026 SW825

Earth-abundant metal-carbene/nitrene-mediated stereoselective glycosylation

Umesh Chaudhary, *umesh.c@ou.edu, Indrajeet Sharma. Chemistry and Biochemistry, The University of Oklahoma, Norman, Oklahoma, United States*

Carbohydrates are integral components of numerous biologically active molecules, yet their stereoselective synthesis remains challenging due to the intrinsic complexity of controlling anomeric selectivity. Here, we present complementary earth-abundant carbene- or nitrene-mediated neutral strategies for stereoselective glycosylation that enable efficient activation of sulfur- and selenium-based glycosyl donors. In the first approach, iron-carbene chemistry provides catalytic activation of conventional thioglycosides, enabling stereoselective glycosylation using an earth-abundant metal catalyst. This strategy offers access to challenging 1,2-cis glycosidic linkages and demonstrates the utility of carbene intermediates in modulating anomeric reactivity. Building on this concept, we developed a complementary photochemical nitrene-mediated platform for activating chalcogen glycosides. Visible-light irradiation generates a reactive nitrene species that engages thio- and selenoglycosides, enabling stereocontrolled glycosylation under mild conditions. The enhanced reactivity of selenoglycosides further enables efficient transformations with reduced dependence on additives. Together, these studies establish carbenes and nitrenes as versatile reactive intermediates for controlling glycosyl-donor activation and stereoselectivity, providing new opportunities for the synthesis of structurally complex carbohydrates.



SWRM 2026 SW826

Chemoselective monosubstitution of mono- and disaccharides

***Desiree R. Czapski**, dxc7601@mavs.uta.edu, Joseph A. Buonomo. Chemistry & Biochemistry, The University of Texas at Arlington, Arlington, Texas, United States*

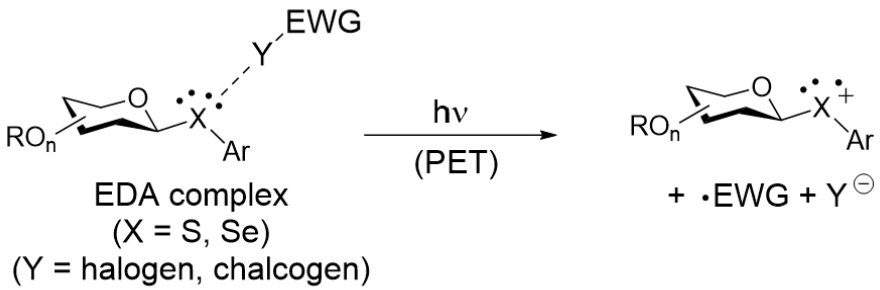
The chemoselective monosubstitution of syntehtic saccharides remains an outstanding challenge in the creation of high-value small molecules and materials. Notably, these synthetic endeavors requrire the extensive use of protecting group schemes and/or specially-designed enzyme catalysts that foster selective transformation, both of which can result in lengthy purifications and inefficient chemical transformation of base carbohydrates into functional entites that are useful in the creation of probes useful in delineating basic biology and in the creation of therapeutics. To this end, we have been delving into the creation of effective methods to yield functionalized reducing and non-reducing mono- and disaccharides that bear unique unstitutions at the primary alcohol position without the need for protecting groups. We have applied our methodolgy to create "clickable" carbohydrate probes that enable metabolic engineering and to enable the application of isotopically-labeled sugars in the real-time monitoring of enzyme activity.

SWRM 2026 SW827

***O*-Glycosylation through the photochemistry of electron-donor-acceptor complexes**

***Justin R. Ragains**, jragains@lsu.edu. Department of Chemistry, Louisiana State University, Baton Rouge, Louisiana, United States*

Chalcogenoglycosides (*e.g.* thioglycosides and selenoglycosides) are privileged electrophiles in chemical *O*-glycosylation due to their stability and reliability in multistep synthetic sequences. But it is this very stability that often necessitates the use of strong activators (*e.g.* NIS/HOTf, MeOTf, DMTST) for their eventual activation toward *O*-glycosylation. To address this challenge, we have developed visible-light-driven *O*-glycosylations based on the formation of electron-donor-acceptor (EDA) complexes between chalcogenoglycosides and species known as chalcogen-bond and halogen-bond donors. Irradiation of the EDA complexes triggers an electron transfer, and a resulting cascade of chemical events culminates in *O*-glycosylation. Thus, light provides the activation that otherwise necessitates highly reactive activators. The reactions are characterized by the use of comparatively "mild" and stable reagents and straightforward setup. Our progress in this area, including substrate scope, evidence for the formation of EDA complexes and photoinduced electron transfer, and photochemical flow methods will be discussed.



SWRM 2026 SW828

Strategies for establishing a research program at a primarily undergraduate institution

***Muhammed Yousufuddin**, myousuf@untdallas.edu. Natural Sciences, University of North Texas at Dallas, Dallas, Texas, United States*

The University of North Texas at Dallas (UNTD) is a Regional Level university and the only public, four-year university in the city of Dallas. UNTD is a Primarily Undergraduate Institution (PUI) with a student population of about 3800 students, 80% of whom identify as Hispanic or African-American. Around 250 of these students are enrolled in a Science major and about 15-20 students conduct undergraduate research every year. Undergraduate students are, therefore, a major part of my research program. Starting and sustaining a research program at a PUI comes with various challenges including lack of start-up funding, research labs, materials, and qualified students. I have employed many strategies to overcome these challenges including (1) networking, (2) securing institutional support, (3) securing external support, (4) recruiting students, (5) and finding time to write up results for publication. In this presentation I will review these strategies as well as discuss how I was able to leverage a successful research program to secure a brand-new 110,000 square ft STEM building with nine teaching labs and three dedicated research labs.

SWRM 2026 SW829

Undergraduate research into predicting pK_a using machine learning, quantum mechanical workflows with explicit solvation

*Alphonsus Nguyen, Matthew Petroff, Madison Meduna, **Prajay Patel**, pmpatel@udallas.edu. Chemistry, University of Dallas, Irving, Texas, United States*

The Statistical Assessment of Proteins and Ligands (SAMPL) series of blind predictive challenges has tasked computational scientists worldwide to blindly predict protein-ligand binding interactions, host-guest binding interactions, as well as thermodynamic properties of smaller drug and drug-like molecules to develop robust protocols for computer-aided drug design. Cheminformatic approaches have been at the center of the approaches through combining results obtained through quantum mechanics (QM), molecular mechanics (MM), and machine learning (ML) to obtain quantitative structure-property relationships (QSPR). The first iteration of the European SAMPL (euroSAMPL) competition continues this effort through examining the prediction of pK_a values of 35 monoprotic complexes including phenols, carboxylic acids, amines, and thiols. This work compares machine learning (ML) and quantum mechanical (QM) approaches for predicting pK_a. The ML workflow uses one-dimensional SMILES strings as inputs to three supervised regression models, while the QM workflows examine the effects of molecular conformational sampling and explicit solvation. Rather than relying on a single optimized structure, ensemble-based calculations account for the thermodynamic contributions of multiple conformers identified from freely rotatable bonds. Explicit solvent molecules were subsequently incorporated into ensemble-based calculations to evaluate the influence of local solvation on predicted pK_a values. Comparison with the experimental euroSAMPL data demonstrates that both conformational sampling and solvation treatment lowered the root mean square error (RMSE) by 1.7 pK_a units compared to the single conformer approach, highlighting limitations of single conformer approaches for flexible molecules. Undergraduate researchers contributed to the development, execution, and analysis of both workflows, making extensive use of Python to automate computational workflows, data analysis, and visualization.

SWRM 2026 SW830 - Withdrawn

SWRM 2026 SW831 - Withdrawn

SWRM 2026 SW832

From growing environment to geographic origin: HPLC-based phenolic profiling of Sri Lankan and global teas

***Felicity Gomez**, felicity.godwins@cameron.edu, Lydia Park, Kandalama Priyasantha. Chemistry, Physics and Engineering, Cameron University, Lawton, Oklahoma, United States*

Tea is one of the most widely consumed beverages worldwide and contains a chemically diverse mixture of phenolic compounds associated with its sensory characteristics and potential biological properties. The phenolic composition of tea may be influenced by multiple factors, including elevation, climate, geographic origin, cultivar, and processing. Understanding this chemical variation requires comparisons both within individual tea-producing regions and across teas originating from different parts of the world. This study uses high-performance liquid chromatography (HPLC) to investigate phenolic diversity in Sri Lankan teas grown under contrasting environmental conditions and white teas originating from different geographic regions.
Tea samples were extracted using standardized hot-water extraction procedures and analyzed using reversed-phase HPLC with photodiode array (PDA) detection. Reference phenolic standards were used to establish chromatographic retention times and calibration curves for the identification and quantitative comparison of selected phenolic compounds. The first component of the study compared Sri Lankan teas grown in warm, low-elevation environments with teas from traditional cooler, high-elevation growing regions. The second component expanded the investigation to white teas representing different geographic origins. Chromatographic fingerprints and concentrations of selected phenolic compounds were compared across the sample groups.
The resulting chromatographic profiles demonstrate substantial chemical diversity among tea samples and provide evidence that both growing environment and geographic origin may contribute to variation in phenolic composition. Differences in individual compounds and overall chromatographic patterns provide a chemical basis for distinguishing teas produced under different conditions. Together, these findings demonstrate the value of HPLC-based chemical profiling for investigating environmental and geographic influences on tea composition and provide a foundation for future studies linking individual phenolic compounds with antioxidant capacity and other biologically relevant properties.

SWRM 2026 SW833

Cell-mediated delivery of liposomal nanoparticles for tumor-targeted therapy

***Mina Poursharifi**, mina.poursharifi@untdallas.edu. Chemistry, University of North Texas at Dallas, Dallas, Texas, United States*

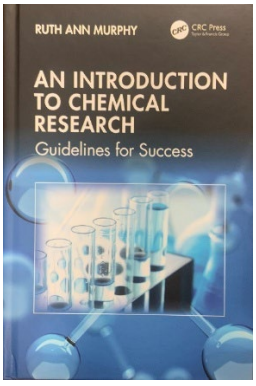
Current cancer therapies are limited by poor tumor specificity, systemic toxicity, and drug resistance. Although liposomal nanoparticles can improve the solubility, stability, and delivery of anticancer agents, their accumulation through the enhanced permeability and retention (EPR) effect is variable and can result in off-target exposure. To overcome this limitation, we propose a cell-mediated nanodelivery strategy that combines the tumor-homing properties of mesenchymal stem cells (MSCs) with the high drug-loading capacity of liposomes. Specifically, anticancer agents such as doxorubicin (DOX) will be encapsulated within liposomes and loaded into MSCs, which will serve as cellular carriers to facilitate delivery of the therapeutic payload to tumor tissue. We hypothesize that this integrated approach will enhance tumor-specific accumulation of anticancer agents while reducing their exposure to healthy tissues. This work aims to establish a targeted drug delivery platform that integrates cell-based targeting with nanotechnology and may provide a more precise and effective strategy for cancer therapy.

SWRM 2026 SW834

Introduction to chemical research: Guidelines for success

Ruth A. Murphy*, rmurphy@umhb.edu. Chemistry, University of Mary Hardin-Baylor, Belton, Texas, United States*

An A-to-Z exposition of proven, tested chemical research strategies for the novice, the experienced researcher, and mentoring faculty. This novel presentation fills a gap by addressing not only project selection, development, and communication, but basics such as ordering supplies, obtaining grants, and working as a team member in the lab. Actual case studies clearly illustrate principles. Beginning with the "5W's" and the "how" of chemical research, the essential matters of ethics, safety, and hazardous waste management are also described. Graduate school is discussed so that prospective researchers can be armed with the facts when they decide whether "To Go or Not to Go?" Topic selection, the scientific method, and resarch project design follow, providing expert guidance. Methods of obtaining support for chemical research are presented with literature search methods, financial support avenues, and procurement processes (including types of orders such as rush, sale, and trial). Data management is treated with laboratory notebook essentials, and strategies for data collection. Teamwork in chemical research is highlighted and explained for its invaluable role. Next, communication of chemical research provides guidance on sharing research results with a discussion of data analysis, and considerations for both written and oral presentations. A listing of power phrases assists the researcher in making their point with clarity and tact, knowing "what to say when" in challenging situations. In closing, the impact of chemical research, public perception, and final reminders outline an inspiring frontier for future chemical research. A chemical research course - in a nutshell!



SWRM 2026 SW835

Abraham solvation parameter model: Experiment based solute descriptor values for potential medicinal candidates, dietary healthcare supplements and pharmaceutical formulation ingredient

Andrew Evans[2]*, andrewfevans0001@gmail.com, William E. Acree*[1]*, Chelsi Wilson*[1]*, Ananya Jamdagneya*[1]*, Nitya Damera*[1]*, Amber Gallimore*[1]*. (1) University of North Texas, Denton, Texas, United States(2) Natural Sciences, University of North Texas at Dallas, Dallas, Texas, United States*

Recently published mole fraction solubility data was used to determine experiment-based Abraham model solute descriptors for oxibendazole, meglumine, 3,3'-diindolylmethane, N-acetyl-L-phenylalanine, and Tranilast. The calculated values were reasonably accurate differing from the measured values by only ±0.17 log units. The Abraham model successfully calculated solute descriptors of the 5 medicinal compounds. Calculated solute descriptors describe experimental solubility data within ± 0.17 log units. The expectation is that the calculated values would allow one to calculate solubility in additional solvents

SWRM 2026 SW836

Multi-generational inheritance of plastic degradation traits in superworms and mealworms

Sophia Flores-Arguello*, SophiaFlores-Arguello@my.untdallas.edu, Mehdi Eslamieh. Natural Sciences, University of North Texas at Dallas, Dallas, Texas, United States*

Plastic pollution has become a defining environmental challenge that threatens many different ecosystems, yet current waste-management strategies remain insufficient for persistent polymers such as polystyrene (PS) and polyethylene (PE). The discovery that mealworms (Tenebrio molitor) and superworms (Zophobas morio) can biodegrade these plastics in their gut microbiota happens through enzymatic hydrolysis and oxidation of polymer chains has generated considerable interest in their use for insect-based bioremediation. However, most research has focused on their short-term degradation performance, leaving unanswered questions about whether these capabilities can be inherited across generations, improve through adaptation, or impose physiological costs that limit their long-term use. This study explores plastic degradation as an evolutionary and ecological trait by examining multiple generations of mealworms and superworms maintained on PS- and PE-containing diets through different periods of time. By comparing selectively bred high-performing degraders, unselected laboratory populations, and wild-derived colonies, the project investigates whether enhanced degradation capacity is heritable and whether repeated exposure to plastics drives measurable changes in performance, fitness, and microbiome composition. The study also evaluates the accumulation of plastic-derived metabolites and associated indicators of oxidative stress to determine whether chronic plastic consumption produces hidden transgenerational health effs genetics toxicology microbiology and selective breeding to address the gaps in our understanding of insect medicated plastic bioremediation. The results will help determine whether plastic degrading traits can be strengthened through selective breeding, whether biological trade-offs have increased degradation efficiency, and how host-associated microbial communities contribute to adaptation. By addressing these questions, the project advances a critical but largely unexplored area of insect-mediated bioremediation and provides foundational knowledge for the development of a scalable and sustainable approach to plastic waste management. In addition, the work establishes a framework for

integrating genetics, toxicology, and microbiome research in the study of emerging biodegradation systems.

SWRM 2026 SW837

Proposed synthetic strategy for a thioether-linked bis-quaternary ammonium compound: An undergraduate research collaboration between a PUI and research-intensive institution

***Gustavo Gomez**, Gustavo.Gomez@untdallas.edu. Natural Sciences, University of North Texas at Dallas, Dallas, Texas, United States*

Primarily undergraduate institutions (PUIs) face challenges in providing undergraduate research opportunities due to limitations in laboratory infrastructure, instrumentation, and faculty research capacity. Collaborative research models can help overcome these barriers while providing students with authentic experiences in scientific inquiry. This project presents a proposed synthetic strategy for the development of a thioether-linked bis-quaternary ammonium compound using (10-bromodecyl) triethylammonium bromide as a key synthetic intermediate. The proposed approach utilizes the terminal bromide of (10-bromodecyl) triethylammonium bromide as a functional handle for attachment to a second quaternary ammonium-containing component through formation of a thioether linkage. Rather than reporting a completed synthesis, this project focuses on the development and evaluation of a feasible synthetic pathway through literature research, retrosynthetic analysis, reagent selection, reaction planning, and consideration of purification and characterization methods. Experimental implementation has been limited by laboratory availability and resource constraints, highlighting challenges commonly encountered by undergraduate researchers at teaching-focused institutions. This project represents a collaborative research effort between The University of North Texas at Dallas (UNT Dallas) and UNT Health, demonstrating how partnerships between institutions with different research infrastructures can expand undergraduate research opportunities. By developing a chemically meaningful project that can be advanced through collaboration and future experimental validation, this work illustrates how undergraduate researchers at PUIs can participate in research despite resource limitations. The project ultimately provides a framework for translating a proposed synthetic design into future experimental work while developing undergraduate skills in organic synthesis, chemical literature analysis, and research problem-solving.

SWRM 2026 SW838

Sustainable olefin functionalization reactions

***Kami Hull**, 32763513@acs.org. Chemistry, The University of Texas at Austin College of Natural Sciences, Austin, Texas, United States*

Given our current knowledge, synthetic chemists have the ability, granted unlimited time and resources, to make almost any organic scaffold. Thus, the fundamental motivations in the field have shifted toward developing efficient processes that accelerate synthesis and reduce associated waste. Research in the Hull group focuses on the development and mechanistic evaluation of transition metal-catalyzed methodologies with the direct goal of reducing the time and waste associated with chemical synthesis. This seminar will describe our recent efforts toward the development of Cu-catalyzed carbofunctionalization of alkenes. We will discuss the design principles guiding catalyst and

substrate selection, mechanistic studies that inform our understanding of the key bond-forming steps, and the scope of this methodology for rapidly accessing structurally diverse products.

SWRM 2026 SW839

Biocatalysts for selective functionalization: A sustainable approach to small molecule oxidation

***Meagan E. Hinze**, meh066@shsu.edu. Chemistry, Sam Houston State University, Huntsville, Texas, United States*

In the past decade, biocatalysis has emerged as an alternative to compliment traditional chemical methods. Employing enzymes results in a greener process by utilizing naturally biodegradable catalysts and decreases the reliance on hazardous reagents or reaction byproducts. In recent years, biocatalysts have been increasingly explored and leveraged in redox transformations for small molecule synthesis. Research in our lab focuses on Baeyer-Villiger monooxygenases, and the potential of these flavin-dependent enzymes for achieving oxidations with chemo- and stereo-selectivity. This presentation will disclose our current efforts toward the development of oxidative chiral resolutions along with a comparison to chemical methods.

SWRM 2026 SW840

Designing molecular copper catalysts for sustainable chemistry: Oxidation and C–N bond formation

***Anne E. Gorden**, anne.gorden@ttu.edu, Xander Duke, Xiaoyu Huo. Chemistry and Biochemistry, Texas Tech University, Lubbock, Texas, United States*

Catalysis offers an opportunity to reduce the environmental impact of chemical synthesis by minimizing waste, energy consumption, and the use of hazardous reagents. This research explores how ligand design can be used to develop more sustainable copper catalysts for oxidation and C–N bond formation. Here, we have developed Cu(II) Schiff-base catalysts that use earth-abundant copper and tunable ligand environments to promote selective oxidative transformations under mild conditions. A water-soluble imidazolium-functionalized Cu(II) catalyst enables allylic and benzylic oxidation in water at moderate temperature and can be recovered and reused for up to eight reactions, highlighting the benefits of catalyst recovery and an aqueous reaction medium. Building on this work, Cu(II) 2-quinoxalinol salen complexes catalyze the direct oxidative coupling of alcohols and amines to form imines, avoiding the use of preformed aldehydes and producing water as the main byproduct. Together, these studies illustrate how ligand architecture, catalyst recovery, solvent selection, and reaction design can be combined to address key principles of Green Chemistry.

SWRM 2026 SW841

Direct carboxylation and esterification of terminal alkynes by Cu-CNC complexes: The role of metal ligand cooperativity

***Laleh Tahsini**, tahsini@okstate.edu. Chemistry, Oklahoma State University, Stillwater, Oklahoma, United States*

CO_2 utilization is a significant and emerging field in catalysis, playing a crucial role in reducing atmospheric CO_2 and mitigating climate change. In this work, we report on Cu(I) complexes that utilize atmospheric CO_2 for the direct carboxylation and esterification of terminal alkynes. The Cu(I) complexes bear ligands of the type 2,6-bis(3-alkyl/arylimidazol-2-ylidene) methylpyridine $I(R)^{C\wedge N\wedge C}$, where R = ^{i}Pr, Me, 2,6-^{i}Pr$_2$Ph (Dipp), 2,4,6-Me$_3$Ph (Mes), and 4-CF$_3$Ph, and a handful of them have been previously reported by our group [1,2]. While copper-catalyzed carboxylation reactions are not unprecedented, this work presents the first example of metal-ligand cooperativity (MLC) through a dearomatization-aromatization process used in the direct carboxylation of terminal alkynes [3]. It also presents the first dearomatized Cu-CNC complexes that have been characterized by crystallography and spectroscopy. Further investigation using UV-Vis spectroscopy revealed the enthalpy and entropy of formation, as well as the activation parameters for the dearomatized $[Cu^{I}(I(^{i}Pr)^{C\wedge N\wedge C})*]$ complex. This marks the first time such data have been reported for dearomatized-metal-CNC systems. To elucidate the mechanistic details of the reaction, we performed stoichiometric reactions and characterized the products using a variety of NMR methods. Combined with supporting computational studies, the work yields several new CNC-supported copper intermediates, including copper-styrenyl, copper-acetylide, and copper-propiolate. While the reactive and labile nature of some of these intermediates precludes their solid-state characterization, DFT-computed structures are consistent with spectroscopic characterization.

SWRM 2026 SW842 - Withdrawn

SWRM 2026 SW843

Advancing water and energy catalysis by controlling electrochemical properties through confinement

***Noemie Elgrishi**, noemie.elgrishi@gmail.com. Chemistry, Louisiana State University System, Baton Rouge, Louisiana, United States*

Molecular transition-metal catalysts have emerged as promising candidates for solar fuel production, enabling the conversion of energy-poor feedstocks into fuels through either photochemical processes or electrochemical reactions in the dark. Molecular containers have also shown considerable promise for encapsulating a wide range of organic and inorganic molecules, with increasing attention now directed toward their ability to host molecular catalysts. As molecular electrocatalysts continue to gain importance, particularly for energy-storage applications, our work focuses on evaluating key performance metrics of molecular metal–organic cages to modulate the secondary coordination sphere of fuel-producing molecular electrocatalysts. In this study, redox-active guests are employed as probes to assess how confinement influences electrochemical properties.

SWRM 2026 SW844

Leveraging computational tools to reduce experimental burden in the optimization of organic transformations

***Jacquelyne Read**, jacquelyne.read@utsa.edu. Chemistry, The University of Texas at San Antonio, San Antonio, Texas, United States*

Considerable time, cost, and materials are dedicated to the optimization of organic reactions in industry and academia alike. Computational tools such as quantum chemical calculations, data science, and machine learning can serve as resources to accelerate reaction development while reducing the experimental burden. This talk will highlight the application of these approaches to the design of chiral organocatalysts for enantioselective transformations, with additional applications in supramolecular chemistry. A computational tool for identifying cation−π, anion−π, CH−π, and π−π interactions in noncovalently driven processes will also be presented.

SWRM 2026 SW845

Study of cationic micelle-mediated reaction of small aromatic molecules using MD simulations

***Archana Mishra**, archana.mishra@uafs.edu, Rahul Yadav, Soneika Carby. Physical Science, University of Arkansas Fort Smith, Fort Smith, Arkansas, United States*

Surfactants play an important role in the solubilization, and localization of reactants and ligands by providing a pseudo phase that is different from the bulk solvent. Cetyltrimethylammonium (CTA^+) and cetylpyridinium (CP^+) surfactants form cationic micelles in water and have wide pharmaceutical and industrial applications. In this project, we have studied the effect of these surfactant head groups on the interactions of selected small molecules such as para and ortho -hydroxyl benzene using molecular dynamics (MD) simulations. The small molecules are selected with aromatic rings and with symmetric and asymmetric geometries to understand the orientation of the molecule with the surfactant head group. We have used the analytical tools in the GROMACS package to study the changes in the structural and dynamic properties such as size, shape, surface behavior, and spatial distribution of solvent around the micelle and surfactant head group to predict the types of interactions. The results of MD simulations show differences in the orientation of symmetric vs asymmetric molecules in both micelles without a significant effect on the overall assembly of the micelle. The orientation of the aromatic ring shows some stacking with the pyridinium ring of the CP+ surfactant head group in the CPB micelle, which is not seen in the case of the CTA+ surfactant.

SWRM 2026 SW846

Impacts of brown carbon deposition from wildfires on solar cell performance

***Tasnim Mahzabin Tanha**, ttanha@okstate.edu, Sithumi Liyanage, Elijah Schnitzler. Oklahoma State University, Stillwater, Oklahoma, United States*

Wildfires are a significant source of organic aerosol, called brown carbon (BrC). BrC gets its name for its characteristic color, resulting from preferential absorption at near ultraviolet wavelengths, and the absorptivity at a particular wavelength can change through atmospheric irradiation or oxidation. Since BrC is light-absorbing, soiling of solar panels by BrC downwind of wildfires may reduce the amount of sunlight reaching the surface, impacting power output. Consequently, understanding the evolving absorptivity of deposited BrC is critical for understanding the effects of wildfire emissions on solar energy generation. In this project, we investigate the influence of BrC thin films on solar cell photovoltaic performance by monitoring changes in voltage output upon deposition of laboratory-

generated BrC coatings onto polysilicon solar cell surfaces. Laboratory-generated BrC from the thermal degradation of eastern red cedar was deposited as a thin film, using an airbrush, and irradiated in a xenon-lamp solar simulator. Photovoltaic performance was evaluated through continuous voltage measurements under a known resistive load for 24 h using a PicoLog data acquisition system to quantify changes in photovoltaic response before and after coating. Initial results demonstrate that BrC coatings modify the voltage output, with changes in voltage response over irradiation time. The magnitude of these effects is influenced by film thickness and coating uniformity. These findings provide insight into the potential impact of biomass burning organic aerosol deposition on solar panels.

SWRM 2026 SW847

Deep-UV fluorescence of ethers: Mechanisms, characterization, and high-sensitivity liquid chromatography detection

***Alanah Junge**, jungealanah@gmail.com, Charles P. Shelor. Chemistry and Biochemistry, The University of Texas at Arlington, Arlington, Texas, United States*

Ethers are essential solvents, surfactants, and synthetic intermediates across chemical and industrial processes, yet many lack intrinsic chromophores for conventional optical detection. Here, I report that ether-based compounds natively fluoresce under deep-UV excitation (<220 nm). Characterization of a broad spectrum of structures including simple aliphatic ethers, polyether surfactants, crown ethers, carbohydrates, alcohols, and peroxides reveal universal excitation below 220 nm with peak emissions spanning 290-320 nm. Aliphatic ethers and polyether surfactants exhibit high fluorescence intensity, whereas crown ethers demonstrate a characteristic dual emission peak shifted to slightly longer wavelengths. In contrast, alcohols and peroxides show no detectable fluorescence under identical conditions, and dissolved oxygen acts as an efficient quencher. Leveraging this native fluorescence, we developed a Liquid Core Waveguide (LCW) cell utilizing broadband deep-UV excitation from a deuterium lamp with unfiltered off-axis collection for online post-column liquid chromatography detection. This system provides high sensitivity while simultaneously capturing UV absorbance data. Compared to destructive or high-maintenance alternatives like aerosol-based detectors, this LCW approach offers a low-cost, robust, and non-destructive detection platform holding significant promise for carbohydrate analysis and label-free detection of non-chromophoric species.

SWRM 2026 SW848

Nanoscale confinement, fusion–fission dynamics, and ice nucleation in reverse micelles

***Romana A. Shathy**[1], rshathy@g.syr.edu, Alexandria Guinness[1,3], John M. Franck[2]. (1) Chemistry, Syracuse University, Syracuse, New York, United States(2) Chemistry, Cornell University, Ithaca, New York, United States(3) Lotte Biologics USA LLC, East Syracuse, New York, United States*

Water confined within nanoscale environments exhibits structural, dynamical, and phase behavior distinct from bulk water. Reverse micelles (RMs) provide a controlled colloidal platform for investigating these effects by enabling precise manipulation of water-pool size and the extent to which individual pools can interact through fusion–fission processes. Understanding this behavior can provide important insights across fields ranging from biophysics and protein dynamics to nanomaterials. Electron spin resonance (ESR) spectroscopy is used to probe molecular dynamics

within RMs from room temperature to deeply supercooled conditions. Time-resolved ESR measurements combined with feedback-guided temperature control enable monitoring of molecular dynamics and the slow kinetics of cold-shedding over a broad temperature range. Variation of the dispersant surrounding the RMs enables investigation of how colloidal mobility and fusion–fission dynamics regulate cold-shedding and ice nucleation. When the dispersant suppresses fusion–fission between RM aggregates, ESR reveals transient signatures consistent with the formation of unstable ice embryos consistent with the classical nucleation theory. Together, these results provide critical insight into how nanoscale confinement, RM mobility, and fusion–fission dynamics affect the stability and phase behavior of confined water. More precise insights into the dynamics and thermodynamic transitions within confined aqueous systems advances the understanding of nucleation and ice formation and has broader relevance to fields ranging from biophysics and protein dynamics to the development of nanomaterials.

SWRM 2026 SW849

Investigating how charge influences the spontaneous formation of hydrogen peroxide in electrospray and suspended water microdroplets

***Emery Hamilton**, emmyhamilton04@gmail.com, Michael Jacobs. Chemistry and Biochemistry, Texas State University, San Marcos, Texas, United States*

The proposed mechanism for the formation of hydrogen peroxide (H2O2) in aqueous microdroplets is a contested topic amongst researchers, with theories spanning charge-activated radical chemistry at the air-water interface, strong interfacial electric fields, and oxygen (O2) driven pathways at metal-water interfaces. Recent studies have established that the net charges on microdroplets influence production of H2O2. For example, negatively charged electrospray droplets produced micromolar concentrations of H2O2 in anaerobic conditions, whereas neutral and positively charged droplets produced minimal amounts of H2O2 under the same conditions. These findings suggest a pathway that is net-charge-polarity specific, in which electrons are ejected from hydroxide groups (OH-) during droplet fission and surface impact, leading to hydroxyl radical formation (OH.) which combines to form H2O2. This work investigates how droplet charge influences H2O2 production in electrospray and levitated microdroplets. Specifically, we aim to determine if droplet fission or impact is required for H2O2 formation in negatively charged droplets. In this work, Amplex Red is used as a quantitative probe to detect H2O2 formation in microdroplets. In preliminary data, electrospray measurements demonstrate that negatively charged droplets produce significantly more resorufin than positively or neutrally charged droplets. However, we observe that a significant fraction of H2O2 formation results from gas phase or heterogeneous chemistry driven by the electrospray source. To quantify its importance, we are probing the formation of H2O2 in suspended droplets with net charges that approach the Rayleigh limit using a quadrupole electrodynamic trap (QET). By measuring H2O2 formation as a function of net droplet charge, we are determining whether similar charge-dependent reactivity emerges in the absence of dynamic droplet fission events and surface contact. Ultimately, understanding the mechanism driving the generation of oxidants like H2O2 from droplets will support emerging research and the development of analytical and synthesis methods within the realms of atmospheric chemistry, redox chemistry, and microdroplet chemistry.

SWRM 2026 SW850

Tuning proton donor molecular architecture to control interfacial microenvironment for enhanced nonaqueous electrochemical CO_2 reduction

***Asitha Gihan Aberathna Ariyathunga Pathiranage**, aaberathna@tulane.edu. Department of Chemistry, Tulane University, New Orleans, Louisiana, United States*

Tuning the electrode-electrolyte interfacial microenvironment enables precise control over the selectivity and efficiency for electrochemical conversions. At the electrode-electrolyte interface, electrochemical conversions take place through a series of electron transfers and are mostly coupled with proton transfers, necessitating the presence of active and abundant proton donors to achieve optimal reaction rates. However, high proton activity triggers competing H_2 formation and compromises the selectivity of the target reactions, highlighting the need for strategic optimization of interfacial proton activity. This requires tuning of the proton donor behavior at the interface to decouple its chemical activity from electrochemical activity. In this study, using nonaqueous electrochemical CO_2 reduction as a model, we demonstrate that the molecular architecture of active proton donors can be leveraged to control the interfacial microenvironment and direct them toward the proton-coupled electron transfer (PCET) pathway to enhance the target reaction, rather than toward H_2 formation. Here, we use a series of tertiary ammonium proton donors with near-identical pK_a but varied structures to show that increasing the steric hindrance around the proton center suppresses H_2 formation kinetics and favorably shifts proton transfer toward CO_2 reduction. We further identify structural rigidity as an independent, complementary factor by examining cyclic tertiary ammonium proton donors, which exhibit a distinct enhancement of CO selectivity at more cathodic potentials, attributed to restricted reorientation of the N-H bond at the electrode-electrolyte interface. Our findings establish proton donor molecular architecture as a design lever to tune the interfacial microenvironment for electrochemical conversions involving PCET

SWRM 2026 SW851

Optimizing high throughput formulation of lipid nanoparticles with robotic liquid handlers

***Pavan Ramesha**[1], pavan.ram.64sqrd@gmail.com, Hassan Tajarenejad[2], Alexandro DeAnda[4], Shuguang Wei[3], Bruce Posner[3], Zhenpeng Qin[2,4]. (1) Department of Biological Sciences, The University of Texas at Dallas, Richardson, Texas, United States(2) Department of Mechanical Engineering, The University of Texas at Dallas, Richardson, Texas, United States(3) Department of Chemistry, The University of Texas Southwestern Medical Center, Dallas, Texas, United States(4) Department of Bioengineering, The University of Texas at Dallas, Richardson, Texas, United States*

Lipid nanoparticles (LNPs) are a promising platform for targeted nucleic acid-based drug delivery. Achieving reproducible, uniform, and high-quality formulations is essential, because even subtle changes in preparation can significantly alter their physicochemical properties and delivery performance. The primary goal of this project is to systematically identify and vary the conditions that influence three critical LNP characteristics: particle diameter, polydispersity index (PDI), and nucleic acid encapsulation efficiency (EE). LNPs were synthesized using a high-throughput screening (HTS) workflow with a Biomek i7 liquid handler, which enables automated mixing of the organic (lipid) and aqueous (nucleic acid) phases. LNP formulations were prepared in 384-well plates, followed by dynamic light scattering (DLS) measurements to assess particle size and PDI. Encapsulation efficiency was quantified using a RiboGreen assay. Five formulation and processing parameters were evaluated: (i) number of mixing cycles, (ii) total sample volume, (iii) organic-to-aqueous phase ratio, (iv) mixing speed, and (v) molar ratios of lipid components. Our results indicate that six mixing cycles at an organic-to-aqueous ratio of 1:3 and a mixing speed of 300 µL/s produce highly uniform LNPs

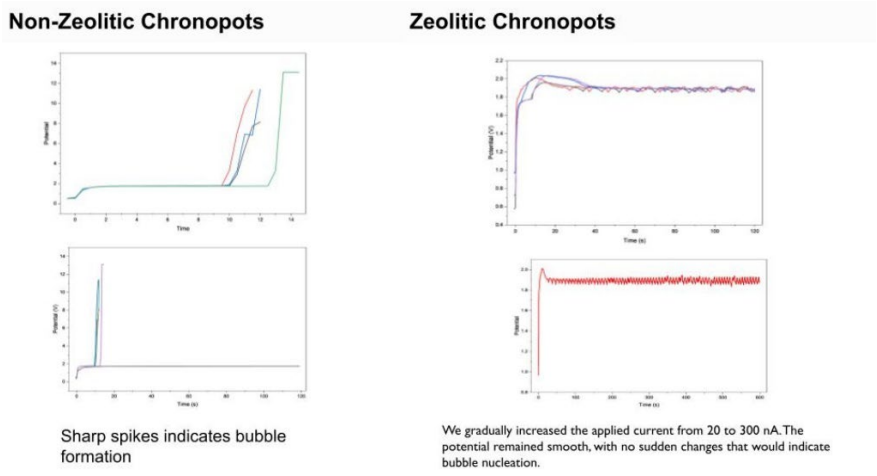
with DNA encapsulation efficiency above 80%. Additionally, formulations prepared at volumes greater than 60 µL exhibited improved consistency. In regards to lipid components, we observed that formulations incorporating the helper lipid DOPE produced smaller particles than those with the helper lipid DSPC. Overall, this optimization of LNP preparation conditions provides a framework for generating LNPs with consistent physicochemical characteristics, therefore supporting more reliable and effective in vivo delivery in future studies.

SWRM 2026 SW852

Probing bubble nucleation with microporous materials

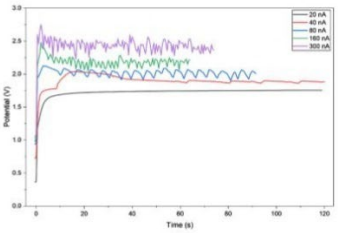
Andrei O. Santos[1,2]*, dreisantos@unm.edu. (1) Chemistry and Chemical Biology, Harvard University, Cambridge, Massachusetts, United States(2) Chemistry and Chemical Biology, University of New Mexico Centennial Science and Engineering Library, Albuquerque, New Mexico, United States*

Gas bubble formation plays an important role in many aqueous systems, particularly in gas-evolving reactions where bubbles can affect gas transport and release. Previous work has shown that stable aqueous suspensions of silicalite-1, a microporous zeolite with nanometer-sized pores, can significantly increase the gas-carrying capacity of water. However, while these materials can change how much gas is stored in solution, much less is known about how they influence the onset of bubble nucleation. Understanding this process is important for developing materials that can eventually control bubble formation, with potential applications in systems such as decompression sickness, where dissolved gases form expanding bubbles as pressure decreases. This work focuses on developing experimental methods to probe the onset of bubble nucleation in aqueous silicalite-1 suspensions. Electrochemical gas-evolving reactions are used to intentionally generate oxygen bubbles under controlled conditions, while chronopotentiometric measurements are used to identify the onset of bubble nucleation. These methods provide a way to investigate how silicalite-1 influences bubble formation and to distinguish potential effects associated with changes in gas transport and gas solubility. Alongside these electrochemical studies, silicalite-1 is surface-functionalized with an N-oxide zwitterionic species to improve particle stability in aqueous environments. This coating is designed to reduce particle aggregation while maintaining the material's hydrophilic exterior. Together, this work establishes experimental approaches for studying bubble nucleation in microporous water and provides a foundation for understanding how microporous materials influence gas storage, transport, and bubble formation.

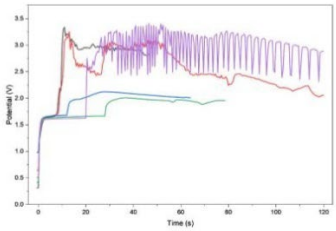


Non-zeolitic vs. zeolitic chronopotentiometry

Attempting to "Race" this Effect **Using a Deeper Electrode**



We gradually increased the applied current from 20 to 300 nA. The potential remained smooth, with no sudden changes that would indicate bubble nucleation.



Deeper electrode etching produced an initial feature, but no bubble nucleation onset was observed.

Method development

SWRM 2026 SW853

Machine-learning-guided size control in the thermal decomposition synthesis of iron oxide nanoparticles

Md Yeasin Kabir[1]*, mkabi11@lsu.edu, Jaspreet Kaur*[2]*, Jhonattan David D. Manosalvas Mora*[4]*, Soundarzo Tasnim*[4]*, Md Sohag Hossain*[1]*, Qingbo Zhang*[4]*, Dong Lao*[3]*, Vicki L. Colvin*[1,2,4]*. (1) Department of Chemistry, Louisiana State University, Baton Rouge, Louisiana, United States(2) Department of Chemistry, Brown University, Providence, Rhode Island, United States(3) Division of Computer Science and Engineering, Louisiana State University, Baton Rouge, Louisiana, United States(4) Cain Department of Chemical Engineering, Louisiana State University, Baton Rouge, Louisiana, United States*

Iron oxide nanoparticles are widely used in magnetic imaging, separation, and heating, but their magnetic behavior is strongly influenced by core size and dimensional uniformity. Iron–oleate thermal decomposition is one of the most widely applied synthetic routes to these materials. Many factors, including precursor chemistry, surfactant loading, iron concentration, and heating profile, are known to affect particle size and quality, and many of these are tightly coupled. Because published syntheses report predominantly successful outcomes, mechanistic understanding of the reaction remains incomplete, and condition combinations that could lead to unique outcomes may be overlooked. We report a machine-learning framework trained on a systematically designed experimental dataset rather than literature data. From the synthesis conditions alone, it predicts the core diameter and a four-class quality score: uniform, nonuniform, aggregated, or no reaction. Two hundred sixty-two reactions were performed across 155 conditions at 320 °C in 1-octadecene at fixed volume. Most syntheses used iron(III) oxyhydroxide converted to iron(III) oleate in situ; a smaller set used pre-synthesized iron(III) oleate to test whether the same trends hold for a second precursor. Both routes are described by total iron [Fe] (15–3608 mM), total oleate [OA] (28–3000 mM), and [Fe]/[OA] (0.03–4.0). Failed reactions were scored and kept, so the model learns where nanoparticles form and, most importantly, the shape of the phase space that yields the best materials. An open-source workflow combining TEM image denoising with edge-based segmentation measured at least 500 cleanly segmented particles per batch, 12× faster than manual ImageJ analysis with a mean bias of 0.14 nm. An early neural network trained on an initial 207 reactions guided the selection of 55 more at sparsely sampled or uncertain conditions. In ten condition-grouped 80/20 splits, a two-head neural network gave the best average performance of five models, predicting the quality score with 73% accuracy (78% balanced accuracy) and mean diameter with a mean absolute error of 2.6 nm. The

resulting phase landscape reveals a narrow window of conditions for uniform nanoparticle formation, in which the iron-to-oleate balance plays a central role, and helps identify conditions for a desired diameter. Its shape suggests a possible surfactant self-assembly process that involves a non-classical nucleation pathway.

SWRM 2026 SW854

Development of a droplet counter system for ultra-low flow-rate measurement

Nur Jafira Akhter Chowdhury[2]*, nxc2705@mavs.uta.edu, Mahmudul Hasan*[1]*, Purnendu K. Dasgupta*[2]*. (1) Department of Chemistry and Biochemistry, Utah State University, Logan, Utah, United States(2) Department of Chemistry and Biochemistry, The University of Texas at Arlington, Arlington, Texas, United States*

Accurate measurement and control of ultra-low liquid flow rates are important in microfluidics, analytical chemistry, and controlled liquid-delivery applications. We described a digital droplet flow counter that relies on forming and counting drops as small as ~60 pL. flow exits through a hydrophobic tip stainless-steel (SS) capillary, with the receiving SS tube ~80 μm below. We have developed strategies for accelerating drop formation and detachment. Reproducible droplet formation and counting were achieved. Like thermal mass flow meters, the system behavior depends on the liquid composition. We are exploring the exact dependence of drop formation on fluid composition (that affects surface tension, density and viscosity) should this dependence be large enough, it would be possible to use such a device as a detector in isocratic HPLC and may be particularly useful in detecting olefinic polymers or carbohydrate macromolecules where sensitive optical absorption is often not present.

SWRM 2026 SW855

Synthesis and characterization of carbazole-based porphyrinoid-metal complexes

Biswash Guragain *, twentywash67.bg@gmail.com. Chemistry and Biochemistry, Texas Tech University System, Lubbock, Texas, United States*

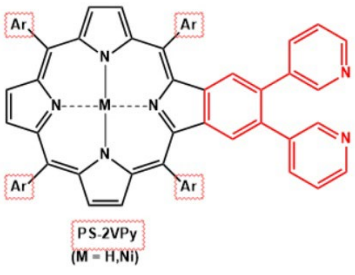
Porphyrins are key biological chromophores involved in respiration and photosynthesis. Inspired by nature, chemists have synthesized porphyrins, expanded porphyrins, and porphyinoid analogs for decades. Recent studies have focused on their potential applications in solar cells and photodynamic therapy. Metal complexes incorporating main-group and transition metals have been investigated extensively; however, analogous complexes with f-block elements remain uncommon. Previously, we reported the synthesis of 2:3 metal-to-ligand sandwich complexes of naphthylsalophen that exhibit erbium-centered upconversion emission in the solid state, as well as water-soluble salophen-based lanthanide complexes that exhibit erbium-centered upconversion in both solid and solution states. Carbazole-based lanthanide complexes are of interest because carbazole antennae could perhaps support one- and two-photon excitation and upconversion processes. Our research aims to develop new porphyrinoids to explore their emission properties and potential applications. In this work, we report the synthesis of a porphyrinoid bearing carbazole moieties to study its emission properties and compare them with those of its metal complexes. The synthesis begins with alkylation at the 3,6-positions of carbazole and halogenation at the 1,8-positions, followed by borylation at the 1,8-positions and, finally, a fourfold Suzuki-Miyaura cross-coupling with a dibromopyridine linker.

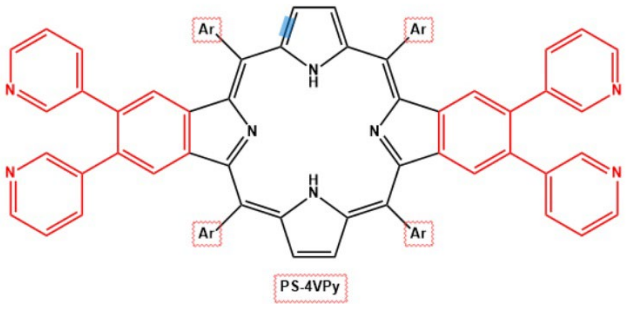
SWRM 2026 SW856

Synthesis and study of optical properties of aromatic heterocycle π-extended porphyrin

***Prabha Sharma**, prabha.sharma@unt.edu, Hong Wang. Chemistry, University of North Texas, Denton, Texas, United States*

The π-extension of porphyrins enhances their electrical and photophysical properties, making them suitable for biomedical imaging and organoelectronics. Their properties can be tuned by structural modification. For instance, linearly extending conjugation via β-β' pyrrolic positions and meso positions. Introducing aromatic heterocycles to a π-conjugated structure could be another possible strategy for modifying the electrical and aromatic characteristics of organic compounds. This strategy opens a new direction to novel porphyrin derivatives and building blocks for porous organic materials, ultimately advancing more efficient porphyrin-based light harvesting systems. In a previous work, thiophenes, F2VTP and its isomeric structure F3VTP were fused to the porphyrin periphery, giving a unique set of optical and electronic properties that resulted in ~20% and ~30% increase in fluorescence lifetime, respectively. A more than two-fold decline in emission quantum yield for F2VTP and a 1.5-fold increase in fluorescence quantum yield for F3VTP were observed, suggesting an unusual trend. In addition, other examples of water soluble heterocycle π-extended tetrabenzoporphyrins have been reported. The other potential application of this type of porphyrin is photochemical CO_2 reduction to CO. Matlachowski et. al. has investigated the photochemical CO_2 reduction of phenanthroline extended porphyrin complex with Rhenium(I) tricarbonyl unit. In this work, mono- and dibenzo porphyrins bearing pyridyl groups were synthesized and characterized. We have investigated how structural modifications affect their optical and electronic properties. Furthermore, this type of porphyrins can serve as a ligand to form heterodinuclear complexes with Rhenium such as: $Re(L)(CO)_3Cl$ [L is porphyrin periphery].



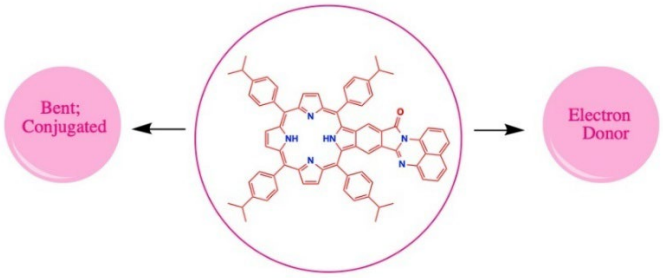


SWRM 2026 SW857

Enhancing π-conjugation in perimidine-fused porphyrins: Exploring their distinct optical and electronic properties

Thi Nguyen *, sangthinguyen1996@gmail.com. Chemistry, University of North Texas College of Science, Denton, Texas, United States*

Macrocyclic porphyrin derivatives are widely studied as photosensitizers in photodynamic therapy due to their unique property of absorbing light in the red and near-IR regions. On the other hand, perimidines serve as scaffolds for various antiproliferative agents, such as anti-prostate cancer and anti-leukemia agents. However, traditional porphyrins have limited tissue penetration because they absorb primarily in the blue spectrum, and their strong π–π stacking reduces hydrophilicity in aqueous systems, which diminishes their ability to detect tumors in deeper tissues. Additionally, perimidines are highly toxic, poorly soluble, and exhibit low selectivity. The objective of this project is to overcome these limitations while enhancing their advantages. In this study, 5,10,15,20-tetrakis(2,4,6-triisopropylphenyl)porphyrin (TIPP) will be used as the core, substituted at the β,β'-positions with 12H-isoindolo[2,1-a]perimidin-12-one. According to preliminary data, fusion of porphyrins with electron-rich perimidine heterocyclic subunits results in a red-shifted absorption. Importantly, TD-DFT calculations demonstrate the conjugation of the porphyrin complex, show that this complex can serve as an electron donor, and show that the perimidine-porphyrin structure slightly bends, which is expected to increase its water solubility. Therefore, further comprehensive characterizations, including electrochemical and optoelectronic studies, such as fluorescence spectroscopy and differential pulse voltammetry, will be conducted to reveal the full potential of this versatile compound. A disubstituted porphyrin analogue will be employed to enable comparison, maximize its potential, and explore the subtle differences of these compounds. These findings may open new areas in medical and optoelectronic applications.



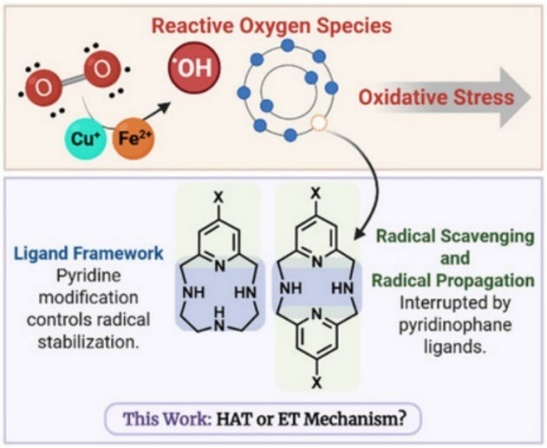
SWRM 2026 SW858

Metal-free ligand-centered radical scavenging in pyridine-modified tetraaza macrocycles

Hannah K. Pyle*, h.k.pyle@tcu.edu. Chemistry and Biochemistry, Texas Christian University, Fort Worth, Texas, United States*

Pyridine-modified tetraaza macrocycles are widely studied as ligand platforms for metal coordination, yet their intrinsic redox and radical reactivity in the absence of metals remains unclear. Here, we report the unexpected finding that pyridinophane Py_2N_2 and PyN_3 macrocycles act as efficient metal-free radical scavengers toward the stable free radical 2,2-diphenyl-1-picrylhydrazyl (DPPH). Systematic evaluation of substituent effects reveals distinct structure–reactivity relationships. PyN_3 derivatives exhibit a linear dependence on electronic parameters, consistent with a donor-controlled

regime, whereas Py_2N_2 macrocycles show a pronounced parabolic dependence on resonance and inductive effects, indicative of cooperative stabilization. ^{1}H NMR spectroscopy supports the formation of a transient ligand–DPPH encounter complex, followed by a rapid hydrogen-atom transfer (HAT). Density functional theory identifies the β-C–H position on the macrocyclic backbone as the thermodynamically preferred hydrogen-donor site. The resulting ligand-centered radical is formed with the Py_2N_2 and stabilized through delocalization across the macrocyclic framework, enabling a captodative-like electronic environment that is inaccessible to the PyN_3 scaffold. Together, these findings establish a ligand-centered HAT mechanism governed by macrocyclic topology rather than metal coordination and highlight a previously unrecognized design principle for electronically tunable, metal-free macrocyclic radical scavengers.

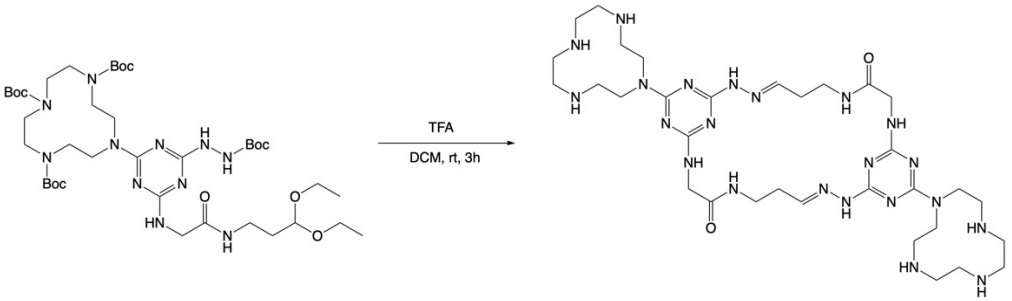


SWRM 2026 SW859

Creating libraries of macrocycles with engineerable conformations

***Andrea E. Rangel**, andrearangel@sandiego.edu, Eric Simanek. Chemistry and Biochemistry, Texas Christian University College of Science & Engineering, Fort Worth, Texas, United States*

Chemotherapy relies on two therapeutic paradigms. The classic approach employs small molecules to specifically target enzyme active sites, as represented by the new generation of kinase inhibitors. A secondary approach relies on interfering with protein-protein interactions thus requiring the use of larger compounds. While this latter strategy is garnering the attention of the pharmaceutical community, the rules for the design of these larger molecules, which are often cyclic, are not understood. The compact shape of small molecules leads to predictable behaviors including oral availability and cell uptake. For larger molecules that adopt multiple shapes, understanding the factors that control their shape and dynamic motion provides opportunities to predict similar behaviors that are critical for rational drug design. Here, the synthesis and characterization of a library of macrocycles is described. The macrocycles of interest result from the dimerization of triazine-based monomers. A total of 50 functionalized monomers containing both hydrazine and glycine linkers were synthesized. Reaction of a single monomer yields a homodimer, while combination of two different monomers leads to a 1:1:2 mixture of homodimers and a heterodimer. This reaction is quantitative and all byproducts are volatile. Combination of all monomers resulted in a library of 1,275 unique macrocycles. Liquid chromatography-mass spectrometry confirms that >99.9% of the reactions were successful. To investigate the biological activity of these compounds, this library was sent to high throughput drug-screening facilities at Vanderbilt University and Scripps Florida. Building off this library, macrocyclic compounds with pendant azamacrocyclic ligands have become of interest for their inherent biological activity as well as their ability to bind metal ions.



Cyclization reaction of cyclen-containing monomer to form cyclen-containing macrocycle.

SWRM 2026 SW860

Utilization of rings to increase blood-brain barrier permeability

Nathaniel McKinney*, nathanielmckinney15@gmail.com, Killian Lyon, Davis Wagnon, Jack Bonnell, Kayla N. Green. Texas Christian University College of Science & Engineering, Fort Worth, Texas, United States*

Oxidative stress is a contributing factor to the development of neurodegenerative diseases such as Alzheimer's, Parkinson's, and amyotrophic lateral sclerosis. It results from an imbalance between the production of reactive oxygen species (ROS) and the ability of cells and tissues to neutralize them. Excessive ROS can cause oxidative damage to cellular components, ultimately leading to cellular dysfunction and death. The Green Group aims to synthesize pyridinophane-based compounds capable of reducing ROS levels through antioxidant activity and metal ion chelation. For these compounds to be effective therapeutic candidates for neurodegenerative diseases, they must possess antioxidant activity, strong metal ion chelation, and the ability to cross the blood-brain barrier. Current pyridinophanes demonstrate antioxidant capabilities and strong binding affinities for specific metal ions but lack sufficient blood-brain barrier permeability. To address this limitation, a phenyl group was introduced at the 4-position of the pyridinophane scaffold to increase the lipophilicity of the compound and potentially enhance blood-brain barrier permeability. Synthetic methods and results will be presented.

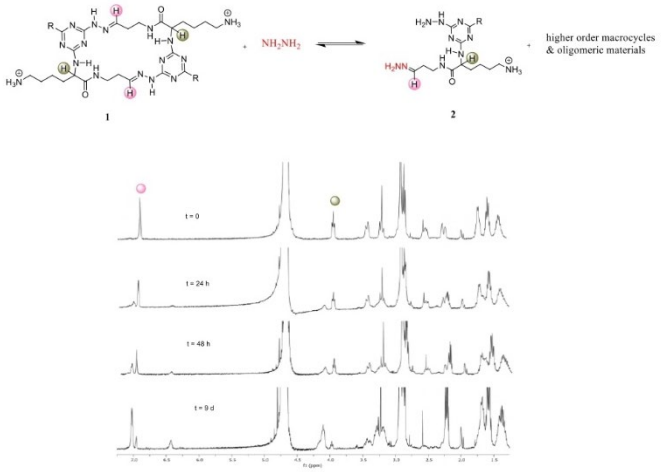
SWRM 2026 SW861

Using nucleophilic catalysis to probe stability and exchange in 24 atom triazine macrocycles comprising bishydrazones

THIRUPATHI REDDY*, thirureddy36@gmail.com, Eric Simanek. CHEMISTRY, Texas Christian University, Fort Worth, Texas, United States*

Using nucleophiles to catalyze hydrazone formation and exchange has been adopted widely—from investigations in basic science to practical applications in bioconjugation, peptide ligation, medicinal chemistry. Here, nucleophilic catalysis is used to probe the origins of the quantitative yields of macrocycles. These macrocycles derive from dimerization of monomers containing an acetal and hydrazine masked with a BOC group. Under strongly acidic conditions, the resulting bishydrazone macrocycle appears inert. Mixing homodimeric macrocycles in organic solvents does not lead to exchange reactions to introduce heterodimers. To afford water solubility across a broad pH range,

lysine macrocycles have been prepared. In the presence of an excess of hydrazine and across a limited pH range, an equilibrium between macrocycle, **1**, and other species, presumably including the monomeric adduct, **2**, can be revealed by NMR spectroscopy. This observation establishes that the cooperativity engendered by the bishydrazone macrocycle can be overcome, and that macrocycle-macrocycle exchange reactions facilitated by nucleophilic catalysis should be possible. The environmental conditions required for exchange and the role of hydrazine and other nucleophilic catalysts in promoting hydrazone exchange will be discussed.



SWRM 2026 SW862

Intranasal delivery of NanoSTING confers broad protection against seasonal and highly pathogenic influenza strains

Ankita Leekha[1]*, aleekha@central.uh.edu, Kate Reichel*[1]*, Brett Hurst*[2]*, Navin Varadarajan*[1]*. (1) Department of Chemical & Biomolecular Engg., University of Houston, Houston, Texas, United States(2) Institute for Antiviral Research, Utah State University, Logan, Utah, United States*

Influenza continues to pose a major global health threat because of its zoonotic potential, rapid antigenic drift, limited vaccine effectiveness, and the emergence of antiviral-resistant strains. A long-standing goal in the field is a broad-spectrum treatment approach capable of protecting at-risk groups, speeding up recovery, and lowering death rates. Here, we developed NanoSTING, a STING pathway agonist (cGAMP) packaged in liposomes, designed as a single intranasal dose for treating influenza. Mechanistically, NanoSTING upregulates locoregional interferon-dependent and interferon-independent pathways within the myeloid cell populations and diverse epithelial cell subsets in the nasal compartment. NanoSTING remained stable under refrigerated conditions for up to one year without degradation of encapsulated cGAMP. In therapeutic challenge studies, NanoSTING protected mice from influenza A viruses, including H1N1 and highly pathogenic H5N1, as well as influenza B. Its therapeutic efficacy was comparable to or greater than that achieved with 10 doses of oseltamivir treatment. Importantly, NanoSTING remained effective when treatment was initiated 48–72 h post-infection, indicating a broad therapeutic window. NanoSTING also induced robust interferon responses in the nasal tissues of aged and immunocompromised mice. Together, these findings support NanoSTING as a promising host-directed intranasal therapy with broad-spectrum antiviral activity and potential utility for treating influenza in vulnerable populations.

SWRM 2026 SW863

Ready, aim, MOF: A metal–organic framework gun for needle-free delivery

Nithish Agamendran*, nithish.agamendran@utdallas.edu, Ziqi Wang, Thomas Howlett, Emily Osborn, Jeremiah J. Gassensmith. Chemistry and Biochemistry, The University of Texas at Dallas, Richardson, Texas, United States*

For many people, the fear and discomfort associated with needles can make even routine injections unpleasant, creating a strong motivation for alternative delivery approaches. Metal organic frameworks (MOFs) offer a useful way to protect and carry biological cargo, but getting that across tissue barriers remians a challenge. Here, we introduce the MOF Gun, a biolistic platform designed to deliver cargo-loaded ZIF-8 particles without the use of needles. Using pressurized gas, the system accelerates MOF particles toward biological targets, offering a different route for delivering biomolecular cargo through the skin. Computational fluid dynamics was combined with experimental testing to understand particle movement through the device and to guide improvements in nozzle geometry and operating conditions. The delivery behavior of the MOF Gun was evaluated using tissue-mimicking substrates and then extended to murine skin models. Pressure and particle loading are being varied to understand how these parameters influence penetration and deposition across biological barriers. By combining the protective properties of MOF-based carriers with a tunable biolistic platform, the MOF Gun provides a flexible approach for needle-free delivery.

SWRM 2026 SW864 - Withdrawn

SWRM 2026 SW865

Adjuvants affect the quality and quantity of neutralizing antibodies stimulated in response to *Alphavirus* protein antigens

Catherine H. Schein*, chschein@utmb.edu. Biochemistry and Molecular Biology, The University of Texas Medical Branch at Galveston, Galveston, Texas, United States*

The adjuvant required for presentation to the immune system can vary with the type of protein. In additon to expressing our Alphavirus physicochemical property (PCP) consensus antigens as part of whole viruses, we have compared a variety of adjuvants,for inoculation of the isolated proteins. Emulsions used for other proteins proved to have limited efficacy with our broad spectrum, PCP consensus proteins The Freund's adjuvants used in rabbit inoculation and Adda SO3 for mice required multiple doses of 100-300 micrograms protein to obtain virus neutralizing antititers, although total antibodies to the antigens, measured by ELISA or dotspots, were quite high. Much less protein was needed to obtain superior neutralizing and absolute antibody titers when the same antigens were incorporated into CPQ-nanoparticles. Cobalt porphyrins in the nanoparticles bound the his-tagged antigens, shortening the purification process by several steps. The isolated his tag did not induce significant amounts of antibodies according to ELISA, and using a double his tag did not improve results. Stable protein antigens induced antibodies with broader viral neutralizaiton capacity. The ability to tether proteins to the nanoparticle through an expressed his tag greatly simplifies using this immunization method for rapidly comparing multiple protein antigens.

SWRM 2026 SW866

Iron-catalyzed ethylene dimerization in the absence of a cocatalyst

Nir Kadosh[1]*, kadosh2018@gmail.com, Shourya Gupta*[1]*, Daniel Najera*[2]*, Elizabeth March*[1]*, Alison R. Fout*[1]*. (1) Chemistry, Texas A&M University, College Station, Texas, United States(2) Chemistry, University of Illinois Urbana-Champaign, Urbana, Illinois, United States*

The (^{Mes}CCC)FeH(Py) complex (^{Mes}CCC = bis(2,4,6-trimethylphenyl-benzimidazol-2-ylidene)phenyl, Py = pyridine), is a competent catalyst for the hydrogenation of terminal olefins to alkanes. Expanding on terminal olefin hydrogenation activity, we investigated the reactivity of (^{Mes}CCC)FeH(Py) with ethylene. Surprisingly, introduction of ethylene to a J. Young NMR tube containing a degassed C_6D_6 solution of the iron complex at room temperature resulted in an immediate reaction. ^{1}H NMR spectroscopy revealed the rapid dimerization of ethylene to 1- and 2-butenes, with complete ethylene consumption. Product analysis was further investigated via vacuum transfer of the volatiles and GC-MS analysis, which also indicated the formation of ethane and hexenes in the reaction mixture. Deuterium labeling of the iron hydride enabled observation of ethane-d_2 *via* ^{2}H NMR spectroscopy. Furthermore, gas rapid injection NMR studies showed that ethylene is initially converted to 1-butene, concurrent with the loss of the characteristic hydride resonance of the (^{Mes}CCC)FeH(Py) complex. Additionally, observable resonances for a putative (^{Mes}CCC)Fe-alkyl intermediate species appear. Once the injection of ethylene is stopped, the characteristic hydride resonances return, alongside slow isomerization of 1-butene to both *Z*- and *E*-2-butenes. Oligomerization could ensue as long as the hydride resonance of (^{Mes}CCC)FeH(Py) remains, even after several rounds of ethylene addition. Furthermore, mechanistic investigations support the linear binding of the ethyl and butyl chains to the iron center, with facile and reversible insertion and β-hydride elimination. Overall, these investigations elucidate the complex mechanistic landscape of iron-catalyzed ethylene oligomerization.

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EPA-based method for the quantification of primary inorganic chemical contaminants of drinking water along the Gulf Coast in South Texas

Ayesha Khalid*, akhalid1@islander.tamucc.edu. Chemistry, Texas A&M University System, Corpus Christi, Texas, United States*

South Texas regions along the Gulf Coast are experiencing extreme drought conditions, bringing water supply and water quality to the forefront of urgent state measures. The water shortage is the result of frequent natural and anthropogenic stressors such as contaminants, extreme weather events, and outdated sewage infrastructures. For example, the combined water storage levels of the city of Corpus Christi, where authors reside, have reached 8.2% as of March 27th, 2026. Corpus Christi houses the third-largest crude oil port in the country and is a hub for petrochemical manufacturing. Corpus Christi was declared a federal flood disaster at least 18 times and reached a Clean Water Act settlement with U.S. Environmental Protection Agency (EPA) in 2020. If current trends continue, the city estimates that demand will outpace supply by June 2027. Herein, this pressing socioeconomic and public health need is addressed through the development and validation of an EPA-based method for the quantification of primary inorganic chemical contaminants in local public drinking water (i.e., As, Ba, Be, Cd, Cr, Cu, Hg, Pb, Sb, Se, and Tl). These pollutants can cause severe human health effects including cancers and organ damage if present in water above the maximum contaminant levels (MCLs of 0-2,000 ppb or µg/L) imposed by the EPA. First, 50+ water samples were collected from public fountains at public Corpus Christi parks and buildings on

our university campus. Samples were then filtered (0.45 μm) and acidified/matrix-matched to standards (2% nitric and hydrochloric acid). Last, multielement analysis was conducted using inductively coupled plasma-optical emission spectrometry (ICP-OES) down to a low ppb range. Results were validated in accordance with EPA Methods 200.3, 200.7, and 6010D. Arsenic was detected in all samples but was below the MCL. Public parks such as Palmetto Park showed high levels of Cd (> 10x MCL of 5 ppb), Hg (> 20x MCL of 2 ppb), and Pb (> 85x MCL of 10 ppb). This analytical chemistry study emphasizes the importance of monitoring drinking water quality in South Texas cities prone to severe water shortages like Corpus Christi.