2026 Southwest Regional Meeting

November 16 - 19, 2026

Fort Worth, TX

Program Chairs

Mihaela Stefan

Nicolay V. Tsarevsky

Gabriele Meloni

Monday, November 16, 2026

Registration

Session Type: Registration

Time: 7:00 AM - 6:00 PM

Location: Promenade

Badge pick-up and onsite registration.

Advances in Functional Polymers and Materials

Session Type: Oral

Time: 8:00 AM - 11:35 AM

Location: Crystal B

"Advances in Functional Polymers and Materials" will highlight emerging directions in polymer and soft materials research spanning molecular design, synthesis, characterization, processing, and application-driven performance. The symposium will feature broadly themed sessions focused on polymer synthetic chemistry, sustainable and degradable polymers, functional polymers for organic electronics and bioelectronics, and emerging soft and hybrid materials with advanced optical, mechanical, and interfacial properties. By bringing together researchers from across the southwest region, the symposium aims to foster interdisciplinary discussion, strengthen connections across the regional polymer community, and showcase advances that bridge fundamental polymer science with next-generation materials technologies within the scope of ACS POLY/PMSE.

Organizer(s): Samantha L Kristufek, Mihaela C Stefan, Joshua Tropp, Nicolay V Tsarevsky

Presider(s): Samantha L Kristufek, Joshua Tropp

Presentations:

8:00 AM Opening Remarks.

8:05 AM [SW01] Employing hypervalent iodine(III) compounds in the synthesis of nitrogen-rich energetic polymers and materials. **Presented by: Nicolay V Tsarevsky**

8:30 AM [SW02] Novel imidazopyridine oligomers with manipulable backbone conformation evaluated under a probabilistic Bayesian framework. **Presented by: Octavio Miranda**

8:55 AM [SW03] Thermo-responsive desiccants for energy efficient building dehumidification. **Presented by: Chengqian Huang**

9:15 AM [SW04] N-oxyl radical-mediated electrochemical surface modification of nanocellulose toward polymer gel electrolytes for battery applications. **Presented by: Dong Hwan Nam**

9:35 AM Intermission.

9:55 AM [SW05] Elucidating the optical switching of electrochromic spiropyran copolymers. **Presented by: Robert M Pankow**

10:20 AM [SW06] Salogels design strategies for development of shape stable thermal energy storage materials. **Presented by: Kartik Kumar Rajagopalan**

10:45 AM [SW07] Perovskite solar cells with dramatically suppressed photocurrent hysteresis through conjugated organic cations with carboxyl groups. **Presented by: Xiong Gong**

11:10 AM [SW08] Solar driven catalytic degradation of renewable materials to produce value-added chemicals under mild conditions. **Presented by: Gyu Leem**

Biochemistry: Enzymes and Macromolecular Complexes

Session Type: Oral

Time: 8:00 AM - 11:20 AM

Location: Continental

Symposia will cover biochemical studies of enzyme structure and function, as well as of multi-subunit macromolecular complexes.

Presider(s): Sheena D'Arcy

Presentations:

8:00 AM [SW09] Oncogenic EGFR mutations differentially remodel receptor assembly and endocytic complex formation. **Presented by: Adam W Smith**

8:30 AM [SW10] Investigating the RNA-binding landscape of thymine DNA glycosylase. **Presented by: Victoria Shearer**

8:50 AM [SW11] Oxidized 6-guanine mediated DNA-protein cross-links block DNA replication and induce mutations. **Presented by: Peixin Wang**

9:10 AM Coffee Break.

9:30 AM [SW12] Biochemical characterization of tousled-like kinase interactions with DNA sliding clamps. **Presented by: Kirk West**

10:00 AM [SW13] MCM9 C-terminal extension is a portable regulatory module that reprograms damage specificity, RAD51 filament fate, and repair pathway choice. **Presented by: Desmond Okafor**

10:20 AM [SW14] Structural and biochemical basis of Rad34–Rad23–Rad33 in transcription-coupled repair of rDNA in yeast. **Presented by: Meenuka Dalpathadu**

10:40 AM [SW15] Structural and biochemical basis of holoTFIIH recruitment and activity in global genome nucleotide excision repair. **Presented by: Temilade Adeniran**

11:00 AM [SW16] KAT'ing edge biological activity and structural biology updates on lysine acetyltransferase (KAT) chemotypes. **Presented by: David J. Leaver**

Insight and Numbers in Quantum Chemistry

Session Type: Oral

Time: 8:00 AM - 11:30 AM

Location: Texas B

Inspired by Charles Coulson□s famous call to □give us insight, not numbers,□ and the modern reinterpretation by Frank Neese emphasizing the importance of □insight and numbers,□ this symposium will explore the evolving relationship between predictive accuracy and chemical understanding in quantum chemistry. Topics will include electronic structure theory, bonding and reaction mechanisms, machine learning, and molecular simulation, with particular emphasis on efforts to connect quantitative computation with chemical and physical interpretation. Contributions from researchers developing new theoretical frameworks, interpretable computational approaches, or applications of quantum chemistry to challenging chemical problems are welcome.

Organizer(s): Alistair Sterling

Presider(s): James Shee

Presentations:

8:00 AM Opening Remarks.

8:20 AM [SW17] Molecular orbital perspectives on relativistic effects in chemistry. **Presented by: Chad E Hoyer**

9:00 AM [SW18] Chemical bonding guided orbital spaces for ORMAS and unitary cluster Jastrow wave functions. **Presented by: Nikolay V. Tkachenko**

9:40 AM Coffee Break.

10:10 AM [SW19] Towards reliable simulations of molecular quantum devices: Projected-interacting full configuration interaction density functional theory. **Presented by: Benjamin G Janesko**

10:50 AM [SW20] Excited states and electric response properties with auxiliary field quantum Monte Carlo. **Presented by: Leon Wu Xiaoquan Otis**

11:10 AM [SW21] X-ray photoelectron spectra of halogen bonds in biochemically relevant systems. **Presented by: Daniel Devore**

Metastable, Defect-Rich, and Nanostructured Materials for Sustainable Energy

Session Type: Oral

Time: 8:00 AM - 10:00 AM

Location: Texas D

This symposium will highlight emerging chemical approaches to sustainable energy materials in which metastability, defects, dopants, nanoscale interfaces, and non-equilibrium synthesis play central roles in determining function. Topics will include materials for batteries, solid electrolytes, thermoelectrics, electrocatalysis, photocatalysis, solar fuels, and related energy-conversion and storage platforms. Particular emphasis will be placed on how synthetic control, compositional disorder, nanostructuring, interfacial chemistry, and advanced characterization can be used to tune charge and ion transport. The symposium will also welcome contributions that combine experimental materials chemistry with data-driven, machine-learning, high-throughput, or operando methods to understand structure□property relationships. By bringing together inorganic, materials, physical, analytical, and computational chemists, the session will provide a forum for discussing how chemically complex and defect-rich materials can be designed for next-generation sustainable energy technologies.

Organizer(s): Progna Banerjee

Presider(s): Progna Banerjee

Presentations:

8:00 AM [SW24] Discovery of selectively etched metastable materials for electrochemical energy storage. **Presented by: Ruocun Wang**

8:17 AM [SW22] Conductivity optimization of composite solid polymer electrolyte through additives for solid state sodium metal batteries. **Presented by: Tariq Bashir**

8:34 AM [SW23] Kinetic phase selection and defect-coupled ion transport in metastable Cu–B–Se nanocrystals. **Presented by: Progna Banerjee**

8:51 AM [SW25] Unlocking materials insights with neutrons: Techniques, applications, and user opportunities. **Presented by: Tianyu Li**

9:08 AM [SW26] Molecular insights into the MNene-electrolyte interphase for ammonia synthesis. **Presented by: David Kumar**

9:25 AM [SW27] Metal-organic framework as a new platform for heterogeneous small molecule activation. **Presented by: Shengqian Ma**

9:42 AM [SW28] Tuning excitonic and photonic transport in cavity-coupled materials. **Presented by: Arkajit Mandal**

New Instrumentation and Methods of Analysis

Session Type: Oral

Time: 8:00 AM - 12:00 PM

Location: Citizens B

Invited and open call for new and emerging analytical instrumentation, automated sample processing, and data analysis including artificial intelligence that solve critical problems in environmental, industrial, and health related applications. Advances in spectroscopic, electrochemical, and mass spectrometric detection and and separation technologies are encouraged. The application of computational tools such as machine learning and artificial intelligence for analyte detection, deconvolution, sample preparation and separations optimization, etc. are welcome.

Organizer(s): Charles Phillip Shelor

Presider(s): Charles Phillip Shelor

Presentations:

8:00 AM Opening Remarks.

8:05 AM [SW29] High-throughput cyclic voltammetry for assessment of photocatalytic C-H bond activation. **Presented by: Sydney Noell**

8:25 AM [SW30] Poly(3,4-ethylenedioxythiophene) (PEDOT)-modified microfluidic chip platform for electric- and magnetic-field-driven flow control at low ionic strength. **Presented by: Emma Greer Nordstrom**

8:45 AM [SW31] Stereolithographic 3D-printed mold processing and PDMS microfluidic pump development for a portable microsampling backpack. **Presented by: Olivia Enietan**

9:05 AM [SW32] High performance electrodialytic suppressor using 3D-printed gyroid channels for ion chromatography. **Presented by: Kalpana Dumre**

9:25 AM [SW33] Advancing 3D printed microsampling probes for neuroscience applications. **Presented by: Julie Ann Stenken**

9:45 AM [SW34] Flagellin as an internal standard for absolute quantification and automated normalization in proteomics. **Presented by: Vishal Sandilya**

10:05 AM Intermission.

10:20 AM [SW35] Advancing structural proteomics by mass spectrometry: Residue-specific covalent labeling, cross-linking, and AI analysis. **Presented by: Saiful M Chowdhury**

10:40 AM [SW36] Superficially porous particle-based stationary phases for fast LC separation of rare earths paired with direct vacuum ultraviolet detection. **Presented by: Maria Olds**

11:00 AM [SW37] Chemometric visualization of mixed-mode chromatographic selectivity induced by kosmotropic and chaotropic ions. **Presented by: Siddharth Jaya Sajeevan J**

11:20 AM [SW38] Nondestructive means for the reocovery of latent text from historical or damaged documents. **Presented by: Donald Charles Ballew**

11:40 AM [SW39] Monitoring of small-molecule pharmaceutical crystallization in microgravity with miniaturized Raman spectroscopy. **Presented by: Allison L Stelling**

SWRM Wellness Room

Session Type: Wellness

Time: 8:00 AM - 6:00 PM

Location: Keystone Room

Monday Morning Coffee Break

Session Type: Coffee Break

Time: 9:30 AM - 10:30 AM

Location: Crystal C/D

Advances in Functional Polymers and Materials

Session Type: Poster

Time: 12:00 PM - 2:00 PM

Location: Crystal C/D

"Advances in Functional Polymers and Materials" will highlight emerging directions in polymer and soft materials research spanning molecular design, synthesis, characterization, processing, and application-driven performance. The symposium will feature broadly themed sessions focused on polymer synthetic chemistry, sustainable and degradable polymers, functional polymers for organic electronics and bioelectronics, and emerging soft and hybrid materials with advanced optical, mechanical, and interfacial properties. By bringing together researchers from across the southwest region, the symposium aims to foster interdisciplinary discussion, strengthen connections across the regional polymer community, and showcase advances that bridge fundamental polymer science with next-generation materials technologies within the scope of ACS POLY/PMSE.

Organizer(s): Samantha L Kristufek, Mihaela C Stefan, Joshua Tropp, Nicolay V Tsarevsky

Presentations:

12:00 PM [SW40] Chemistry meets art: Investigating solvent dynamics and temperature-dependent solubility of shellac for art conservation. **Presented by: Anthony Vo**

12:00 PM [SW41] Withdrawn

12:00 PM [SW42] Influence of poly(3,4-ethylenedioxythiophene):poly(styrenesulfonate) (PEDOT:PSS) in organic electrochemical sensor channel. **Presented by: Javier Soliz-Martinez**

12:00 PM [SW43] Leveraging high molar mass block copolymers in salogels for thermal energy storage materials. **Presented by: Kevin Nguyen**

12:00 PM [SW44] Improving light confinement in hydrogel optical fibers using absorbing molecules. **Presented by: Sagor Biswas**

12:00 PM [SW45] Polymeric micelles for theranostic applications: Impact of polymer architecture on doxorubicin and $MnFe_2O_4$ encapsulation. **Presented by: Esmail Qasimi**

12:00 PM [SW46]*In-vitro* studies on microplastic removal from human blood products using organic plant-based polysaccharides and hydrogels. **Presented by: Addison Anderson**

12:00 PM [SW47] Telechelic all-*cis* polycyclooctene via catalytic stereoretentive ROMP for the synthesis of polylactide-based ABA triblock copolymers. **Presented by: Antoine Gravet**

12:00 PM [SW48] Synthesis and optimization of thermoresponsive polymers for reducing building energy consumption. **Presented by: Hansani Sandamali Amarasuriya Amarasuriyage**

12:00 PM [SW49] Efficient recovery of valuable chemicals from Kraft black liquor using thermo-responsive polymer absorbents. **Presented by: Leshi Feng**

12:00 PM [SW50] Self-adaptive thermal regulator for dynamic heating and cooling through coupled thermal energy storage and solar modulation. **Presented by: Jiaxiang Wen**

12:00 PM [SW51] Acid-promoted ring opening metathesis polymerization to access main-chain pyridine-containing cationic polymers. **Presented by: Vaishak Bhat**

12:00 PM [SW52] Non-native square packing and structural arrangement of ultrahigh molecular weight diblock copolymer from one-step solvent vapor annealing. **Presented by: Yuheng Wang**

12:00 PM [SW53] Zwitterionic PVA-peptide conjugate polymer (pEtN-PVA-Pep): Synthesis, characterization, and evaluation for biomedical applications with emphasis on biofilm inhibition. **Presented by: Md Tareque Hassan Mukut**

12:00 PM [SW54] Dual porphyrin-based two-dimensional π-extended covalent organic frameworks as photoactive materials. **Presented by: Jishnu Chevayil Vasudevan**

12:00 PM [SW55] Withdrawn

12:00 PM [SW56] Advanced material platforms of conductive polymer with ionic liquids for stretchable and flexible electronics. **Presented by: Fatima Abbas**

12:00 PM [SW57] Studies of the anionic ring-opening polymerization of lipoates. **Presented by: Leonel Garcia**

12:00 PM [SW58]*β*-tetra-brominated functional porphyrinic covalent organic framework. **Presented by: Nikhil Kumar**

12:00 PM [SW59] ROS-responsive gold nanoparticles for targeted methotrexate delivery. **Presented by: Niloofar Valizadeh Dana**

12:00 PM [SW60] Viscoelastic characterization of pore engineered hydrazone-linked covalent organic framework films. **Presented by: Chamila S B Rajapaksha W M**

12:00 PM [SW61] Acrylate-polyrotaxane double network hydrogels enabled by vat photopolymerization 3D printing. **Presented by: Gaveshika Rajapaksha**

12:00 PM [SW62]*In-vivo* plant-based polymers for microplastic removal from pigs. **Presented by: Jaci Youngblood**

12:00 PM [SW63] Visible light induced lignin degradation using Ir(III) polypyridyl complexes coated on metal oxide nanoparticles at room temperature. **Presented by: David Michael Martinez**

12:00 PM [SW64] Withdrawn

12:00 PM [SW65] Harnessing RAFT-based glycopolymers for sustainable heavy metal sequestration. **Presented by: Mahak Chhabra**

12:00 PM [SW66] Anionic effect on the effective saccharide hydrolysis via modified noncovalent interactions to the pore environment. **Presented by: Amena Khatoon**

12:00 PM [SW67] Actuation of polymer composites driven by the breathing of embedded metal-organic frameworks. **Presented by: Jacob Baker**

12:00 PM [SW68] Evaporation-induced assembly of paintable MXene organohydrogels for long-term skin-conformal bioelectronic interfaces. **Presented by: AAMIR IQBAL**

12:00 PM [SW69] TEMPO-functionalized copolymers for electrochemical energy storage. **Presented by: Bryn Jenkins**

12:00 PM [SW70] Controlled nanostructuring of single-ion magnets using 2D covalent organic frameworks. **Presented by: Noreen Mazhar**

12:00 PM [SW71] Sustainable drop-in alternative to PBAT: MDI chain-extended bio-based PPeAT for flexible film packaging. **Presented by: Mahdi Mazaheri**

12:00 PM [SW72] Investigating the effects of particle size on oxygen reduction reaction using MXene electrocatalysts. **Presented by: Anthony Wiederkehr**

12:00 PM [SW73] 3D-printed emulsion-templated foam composites with metal-organic frameworks for selective gas adsorption. **Presented by: Lyndsay Ayers**

12:00 PM [SW74] Structuring metal-organic framework polymer composites via polymerization induced phase separation: Towards a predictive 3D printing strategy. **Presented by: Tien M Tran**

12:00 PM [SW75] Effects of bio-based additives on the fire-retardant performance and environmental durability of phosphorus-based wood treatments. **Presented by: Chloe Qian**

Biochemistry: Enzymes and Macromolecular Complexes

Session Type: Poster

Time: 12:00 PM - 2:00 PM

Location: Crystal C/D

Organizer(s): Gabriele Meloni

Presentations:

12:00 PM [SW76] Investigating the repair of 3'-DNA-protein cross-links arising from abasic sites. **Presented by: Joel cepeda**

12:00 PM [SW77] Withdrawn

12:00 PM [SW78] Evaluating a rationally designed peptide and small-molecule compounds against *Clostridioides difficile*. **Presented by: Juan Francisco Dominguez**

12:00 PM [SW79] Watercress flavonoids as natural protectants of human serum albumin under oxidative stress: A molecular study. **Presented by: Bidisha Sengupta**

12:00 PM [SW80] Identification and characterization of a putative Fe^{2+}-ZIP transmembrane transporter in *Naegleria fowleri*. **Presented by: Prakriti Budhathoki, Gabriele Meloni**

12:00 PM [SW81] Mechanism of *Ostrinia furnacalis* PBP2 function: Role of the C-terminal tail. **Presented by: AHMAD TIJANI AZEEZ**

12:00 PM [SW82] Discovery of novel DNA–protein cross-links by mass spectrometry. **Presented by: Bingru Li**

12:00 PM [SW83] Design and synthesis of mitochondria-targeted antioxidants for improving myoglobin redox and meat color stability. **Presented by: Prabir Kumar Gharai**

12:00 PM [SW84] Analysis of the mammalian glutathione synthetase H-loop. **Presented by: Michael Marks**

12:00 PM [SW85] Withdrawn

12:00 PM [SW86] Investigation of redox-based post-translational modifications in *Arabidopsis thaliana* lipid metabolism. **Presented by: Cody King**

12:00 PM [SW87] Biochemical characterization of Rad7-Rad16 in yeast global genome nucleotide excision DNA repair. **Presented by: Chathurika Ranmini Silva Hewa Bhashithage**

12:00 PM [SW88] Impact of torsional restraint in coordinating nucleotide excision repair dual incision. **Presented by: Comfort Odunayo Alex-Samuel**

12:00 PM [SW604] Role of gating and C-terminal regions in OfurPBP2. **Presented by: Md. Ahad Khan**, **sanjana gautam**, **Smita Mohanty**

Bioinorganic Chemistry in Health, Energy, and Environment

Session Type: Poster

Time: 12:00 PM - 2:00 PM

Location: Crystal C/D

Bioinorganic chemistry lies at the interface of inorganic chemistry and biology, addressing fundamental questions about how metal ions and small molecules in biological environment mediate essential life processes. This symposium will highlight recent advances in understanding the roles of metal centers in biological systems, with particular emphasis on their impact across health, energy, and environmental applications. By bringing together diverse perspectives, the session aims to showcase how bioinorganic principles drive innovation in areas ranging from disease-related metal signaling and therapeutics to sustainable catalysis and environmental remediation.

Organizer(s): Pokhraj Ghosh, Kayla N Green

Presentations:

12:00 PM [SW89] Can a biologically relevant Fe–oxygen intermediate drive aerobic C–C bond formation. **Presented by: Tahmina Afroz**

12:00 PM [SW90] Chromatography-based investigation of the cytosolic labile iron pool of *Saccharomyces cerevisiae*. **Presented by: Salina Aryal**

12:00 PM [SW91] From Cu(II) thionitrite to N2O: Evidence for an HNO-mediated pathway. **Presented by: Anagha Kuruvayil**

12:00 PM [SW92] Hybrid copper ferrite nanomaterials for antibacterial control of *Xanthomonas* pathogens. **Presented by: Sharadie Liyanage**

12:00 PM [SW93] Electrochemical detection of gastric cancer VOC biomarkers using $Ca(OH)_2$ templated porous carbon electrodes. **Presented by: Charles Asante**

12:00 PM [SW94] Switching the heme ligand switches the chemistry: First- and second-sphere control of peroxidase reactivity in sfh5. **Presented by: Chandradeep Ghosh**

12:00 PM [SW95] Characterization of perliplasmic FtrB, a novel ferrous oxidase with a cupredoxin like fold expressed by *Brucella* spp. **Presented by: Sambuddha Banerjee**

12:00 PM [SW96] Metal–ligand cooperative electroreduction of N_2O by molecular copper complexes. **Presented by: Seif Eid**

12:00 PM [SW97] Mapping the electrostatic interface of the *Azotobacter vinelandii* MoFe protein for light-driven, bio-hybrid nitrogen reduction. **Presented by: Marguba Kamrun**

12:00 PM [SW98] Investigating structure-activity relationships of photoactive metallodrugs as antimicrobials. **Presented by: Gurleen Kaur**

12:00 PM [SW99] Investigating activity of photoactive metallodrugs as antimicrobial therapeutic agents. **Presented by: Chelsea Kimberlin**

12:00 PM [SW100] Chirality-guided design of pH-responsive self-healing peptide hydrogels. **Presented by: Umesha Subhani Kumbalathara Arachchige Dona**

12:00 PM [SW101] Minimizing H_2O_2 driven oxidative stress in immortalized human keratinocytes using a manganese catalase mimic. **Presented by: Slade Lee**

12:00 PM [SW102] Comparison of the bioelectrochemical activity of *Methylobacterium extorquens* AM1 grown with La^{3+} and Ca^{2+}. **Presented by: Chengyang Li**

12:00 PM [SW103] Transmembrane Cu(I) P-type ATPases transport Pt(II)-drugs as electrogenic uniporters. **Presented by: Nadeesha Tharangani Liyana Withanage**

12:00 PM [SW104] Synthesis and characterization of light-triggered metal complexes for cancer treatment. **Presented by: Dalton Lucas**

12:00 PM [SW105] Neuroplastics: Learning from real-world plastic particles to uncover the bioaccumulated plastics in the human brain. **Presented by: Alexis Maranan**

12:00 PM [SW106] Ligand-dependent nitroxyl generation from dinitrosyl iron complexes. **Presented by: Esther Oluwafisayomi Mosebolatan**

12:00 PM [SW107] Withdrawn

12:00 PM [SW108] Design and evaluation of photoactive metallodrugs for cancer therapy. **Presented by: Broderick Nelson**

12:00 PM [SW109] Persulfide-driven oxygen-atom transfer from copper-bound nitrate towards nitric oxide formation. **Presented by: Esther Oluwabunmi Olatunji**

12:00 PM [SW110] Cu- and Ni-based transition metal catalysts for efficient electrocatalytic CO_2 reduction. **Presented by: Snehil Patel**

12:00 PM [SW111] Assembly and characterization of human Ag(I)- and Au(I)-metallothionein metal-thiolate clusters: Comparative investigation of MT-2 and MT-3 isoforms. **Presented by: Nazer Hossain Qasimi**

12:00 PM [SW112] Synthesis and characterization of nickel(II) and manganese(III) complexes as phosphoester hydrolase mimics. **Presented by: Lorena Reyes**

12:00 PM [SW113] Life cycle of chemotherapy drugs in our environment. **Presented by: John-David Rodriguez**

12:00 PM [SW114] NO-H2S crosstalk at the zinc centre: Isolation and reactivity of zinc-perthionitrite complex. **Presented by: Yasmina Said**

12:00 PM [SW115] Photobiological applications of light-activated metallodrugs. **Presented by: Alisher Talgatov**

12:00 PM [SW116] Computational analysis of nitric oxide dioxygenase biomimicry with tetra-aza macrocycles. **Presented by: Caden-Jack Walls**

Insight and Numbers in Quantum Chemistry

Session Type: Poster

Time: 12:00 PM - 2:00 PM

Location: Crystal C/D

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theoretical frameworks, interpretable computational approaches, or applications of quantum chemistry to challenging chemical problems are welcome.

Organizer(s): James Shee, Alistair Sterling

Presentations:

12:00 PM [SW117] Converging electron correlation for scalar-relativistic 4-component CASSCF. **Presented by: Emmy Morrissey**

12:00 PM [SW118] Accelerating mechanistic discovery in Pd-catalyzed transformations using MLIP-driven automated workflows. **Presented by: Dev Dodiya**

12:00 PM [SW119] Understanding SiO_2 etching using HF(aq) via first-principles molecular dynamics. **Presented by: Stacie Reese Moreno**

12:00 PM [SW120] Investigating the effects of mutation on the dissociation kinetics of barnase-barstar using atomistic simulations in implicit solvent. **Presented by: Cecilia Fojut**

12:00 PM [SW121] DFT guided optimization of a general aziridine synthesis. **Presented by: Priyanka Maharana**

12:00 PM [SW122] Unraveling the importance of angular momentum symmetries in phaseless AFQMC trial wavefunctions for atoms and diatomics. **Presented by: Jackson Maxwell**

12:00 PM [SW123] Generation of polarized Hamiltonians on classical computers for simulating open quantum systems with NISQ devices. **Presented by: Abeda Sultana Shamma**

12:00 PM [SW124] Molecular dynamics simulations of BRAF kinase mutant complexes reveal variant effects and activation mechanisms. **Presented by: Daniel Pearson**

12:00 PM [SW125] Adaptive regularization of density fitting for MP2 and molecular density projection. **Presented by: Jose Marc Madriaga**

12:00 PM [SW126] Quantifying strong correlation with AFQMC. **Presented by: Saisrinivas Gudivada**

12:00 PM [SW127] Transferable force field for simulating adsorption in metal-organic frameworks with open metal sites based on the 12-6-4 Lennard-Jones potential. **Presented by: Meng Du**

12:00 PM [SW128] Robust approximation to rank-reduced $CCSD(T)_\Lambda$. **Presented by: Daniel Devore**

12:00 PM [SW129] Locally-optimal construction of pair and hybrid pair grids in LS-THC-MP2. **Presented by: Afifa Yousaf**

Metastable, Defect-Rich, and Nanostructured Materials for Sustainable Energy

Session Type: Poster

Time: 12:00 PM - 2:00 PM

Location: Crystal C/D

This symposium will highlight emerging chemical approaches to sustainable energy materials in which metastability, defects, dopants, nanoscale interfaces, and non-equilibrium synthesis play central roles in determining function. Topics will include materials for batteries, solid electrolytes, thermoelectrics, electrocatalysis, photocatalysis, solar fuels, and related energy-conversion and storage platforms. Particular emphasis will be placed on how synthetic control, compositional disorder, nanostructuring, interfacial chemistry, and advanced characterization can be used to tune charge and ion transport. The symposium will also welcome contributions that combine experimental materials chemistry with data-driven, machine-learning, high-throughput, or operando methods to understand structure□property relationships. By bringing together inorganic, materials, physical, analytical, and computational chemists, the session will provide a forum for discussing how chemically complex and defect-rich materials can be designed for next-generation sustainable energy technologies.

Organizer(s): Progna Banerjee

Presentations:

12:00 PM [SW130] Non-Markovian dynamics of exciton-polaritons. **Presented by: Rajanya Sarkar**

12:00 PM [SW131] Microscopic theory of spin-orbit interactions of light. **Presented by: Michael Fowler**

12:00 PM [SW132]*In-situ* grown metal organic framework UTSA-16 on $Ti_3C_2T_X$ MXene improves electrochemical seawater splitting. **Presented by: Eugenie Marie Pranada**

12:00 PM [SW133] Spectroelectrochemical understanding of the electronic nature of mixed-dimensional excitonic systems. **Presented by: Hyun Suk Kang**

12:00 PM [SW134] High purity titanium nitride MXene using repetition synthesis for lithium energy storage. **Presented by: Laura Hoagland**

12:00 PM [SW135] Metal clusters with well-defined nuclearity for CO_2-assisted propane dehydrogenation. **Presented by: Elmul Jamal**

12:00 PM [SW136] Selective etching strategy for unlocking ion transport in Aurivillius phases. **Presented by: Nhu Quynh Nguyen**

12:00 PM [SW137] Correlating different silver nanoparticle sizes and synthetic routes with CO_2-to-CO selectivity. **Presented by: Soundarzo Tasnim**

12:00 PM [SW138] Withdrawn

12:00 PM [SW139] Thermal and morphological control of α-CuV_2O_6 photoanodes toward enhanced photoelectrochemical water oxidation. **Presented by: Mohammad Arham Shamim**

12:00 PM [SW140] Lattice-matched RuO_2-TiO_2 interfaces enable highly active Ru/rutile-TiO_2 catalysts for NH_3 decomposition. **Presented by: Aswathi Rajeevan V V**

12:00 PM [SW141] Growing carbon on yttrium doped ceria (CeO_2) nanorods for hybrid supercapacitor application. **Presented by: S M ANYET ULLAH SHOHAG**, **Asher Grills**

12:00 PM [SW142] Tuning surface and oxidative charge through interlayer anions for enhanced OER kinetics. **Presented by: Abhirami V Krishnan**

12:00 PM [SW143] Synthesis, characterization, and testing of heteropolyacid-based carbide catalysts for chemical plastic recycling. **Presented by: Nadiira Khadar Hassan**

12:00 PM [SW144] Microscopic theory of polaron-polariton dispersion and propagation. **Presented by: Logan Perry Blackham**

12:00 PM [SW145] Many-body quantum dynamics of exciton-polaritons. **Presented by: Pritha Ghosh**

Advances in Functional Polymers and Materials

Session Type: Oral

Time: 2:00 PM - 5:40 PM

Location: Crystal B

"Advances in Functional Polymers and Materials" will highlight emerging directions in polymer and soft materials research spanning molecular design, synthesis, characterization, processing, and application-driven performance. The symposium will feature broadly themed sessions focused on polymer synthetic chemistry, sustainable and degradable polymers, functional polymers for organic electronics and bioelectronics, and emerging soft and hybrid materials with advanced optical, mechanical, and interfacial properties. By bringing together researchers from across the southwest region, the symposium aims to foster interdisciplinary discussion, strengthen connections across the regional polymer community, and

showcase advances that bridge fundamental polymer science with next-generation materials technologies within the scope of ACS POLY/PMSE.

Organizer(s): Samantha L Kristufek, Mihaela C Stefan, Joshua Tropp, Nicolay V Tsarevsky

Presider(s): Samantha L Kristufek, Joshua Tropp

Presentations:

2:00 PM [SW146] Engineering functional gelatin networks through thiol–ene chemistry for tunable 3D biomaterials. **Presented by: Melanie Ecker**

2:25 PM [SW147] Discovery and optimization of dynamic covalent polymer formulations using 3D printing. **Presented by: Ronald Smaldone**

2:50 PM [SW148] Withdrawn

3:15 PM [SW149] Coordination-enabled processing of chitosan into moldable, mechanically robust functional materials. **Presented by: Balasubramanian Rukmanikrishnan**

3:40 PM Intermission.

4:00 PM [SW150] Maleimide–enediyne-functionalized poly(ε-caprolactone) micelles for DNA-cleaving anticancer nanotherapy. **Presented by: Mihaela C Stefan**

4:25 PM [SW151] Directed self-assembly of chiral liquid crystals into biomimetic Bouligand structures in thin film for functional material design. **Presented by: Xiao Li**

4:50 PM [SW152] How backbone chirality and charge segmentation influence solution phase separation in polypeptoids and polypeptides. **Presented by: Donghui Zhang**

5:15 PM [SW153] Multifunctional nanoparticle–essential oil topical gels for synergistic antibacterial activity, hemostasis, and accelerated wound healing. **Presented by: Blessing Atim Aderibigbe**

Biochemistry: Enzymes and Macromolecular Complexes

Session Type: Oral

Time: 2:00 PM - 5:20 PM

Location: Continental

Symposia will cover biochemical studies of enzyme structure and function, as well as of multi-subunit macromolecular complexes.

Organizer(s): Sheena D'Arcy

Presider(s): Sheena D'Arcy

Presentations:

2:00 PM [SW154] Decoding chemical communication: Structural insights and gating mechanisms of pheromone-binding proteins. **Presented by: Smita Mohanty**

2:30 PM [SW155] Solution conformational changes in P_{1B}-type ATPase copper binding and Post-Albers cycle states. **Presented by: Yaamini Subramanian**

2:50 PM [SW156] Mechanistic and structural characterization of wild-type and active-site variants of F_{420}-dependent sugar-6-phosphate dehydrogenase from *Cryptosporangium arvum*. **Presented by: Lakshitha Madalagama**

3:10 PM Coffee Break.

3:30 PM [SW157] Energy transmission in ATP synthase. **Presented by: Yunxiang Li**

4:00 PM [SW158] Targeting factor XIIa: A step towards safer anticoagulant therapy. **Presented by: Jabila Mary**

4:20 PM [SW159] Functional dynamics of water in New Delhi metallo-β-lactamase catalysis. **Presented by: Palanisamy Kandhan**

4:40 PM [SW160] Metal ion substrate discrimination principles in transmembrane nickel-cobalt transporters (NiCoTs): Understanding and engineering cargo selectivity in NiCoT permeases. **Presented by: Sean Alec Lois Sunga**

5:00 PM [SW161] Structural and biophysical characterization of OfurPBP3, a pheromone-binding protein from the Asian corn borer. **Presented by: Pratikshya Paudel**

Bioinorganic Chemistry in Health, Energy, and Environment

Session Type: Oral

Time: 2:00 PM - 5:20 PM

Location: Texas A

Bioinorganic chemistry lies at the interface of inorganic chemistry and biology, addressing fundamental questions about how metal ions and small molecules in biological environment mediate essential life processes. This symposium will highlight recent advances in understanding the roles of metal centers in biological systems, with particular emphasis on their impact across health, energy, and environmental applications. By bringing together diverse perspectives, the session aims to showcase how bioinorganic principles drive innovation in areas ranging from disease-related metal signaling and therapeutics to sustainable catalysis and environmental remediation.

Organizer(s): Pokhraj Ghosh, Kayla N Green

Presider(s): Pokhraj Ghosh, Kayla N Green

Presentations:

2:00 PM [SW162] Exploring the role of the secondary coordination sphere in Ni CO_2RR. **Presented by: Shrivignesh Senthil Kumar**

2:20 PM [SW163] Nitrate reduction by thiols at Ni(II) site. **Presented by: Ayoola Ayodele**

2:40 PM [SW164] Withdrawn

3:00 PM [SW165] Investigating the impact of metal identity in complexes supported by an adaptable ligand framework on electrochemical oxygen reduction. **Presented by: Fiona Roche**

3:20 PM [SW166] Optimizing the phototherapy effects of metallodrug photosensitizers for cancer treatment. **Presented by: Ge Shi**

3:40 PM Intermission.

4:00 PM [SW167] Unveiling SNO^{1-}, $SSNO^{1-}$, and HONO intermediates in H2S-mediated nitrite reduction at zinc. **Presented by: SAIKAT MISHRA**

4:20 PM [SW168] Electrochemical and spectroelectrochemical behavior of $[Ru(tpy)(tpy\text{-}nT)]^{2+}$ as a function of thiophene chain length. **Presented by: Abbas Vali**

4:40 PM [SW169] Catalytic reduction of carbon dioxide with a bimetallic Mn(I) complex of a pyridine-based polyamine macrocycle: Applications in renewable energy. **Presented by: Md Mhahabubur Rhaman**

5:00 PM [SW170]*Ostrinia furnacalis* pheromone-binding protein 2: Role of Arg70 in ligand release. **Presented by: sanjana gautam**

Colloids, Surfactants and Interfaces

Session Type: Oral

Time: 2:00 PM - 6:00 PM

Location: Texas C

This symposium will accept papers in all areas of colloids, surfactants and interfaces. Topics include surfactant, block copolymer, lipid and other amphiphilic materials and their self-assembly, emulsions, foams, dispersions, interfacial phenomena including wetting, adhesion, colloidal glasses and gels, and colloidal and interfacial phenomena of interest to biological, environmental, material and medical technologies not covered by any of the thematic symposia.

Organizer(s): Reza Foudazi

Presider(s): Reza Foudazi

Presentations:

2:00 PM Opening Remarks.

2:05 PM [SW801] Dynamic dye–plasmon interactions at surfactant-depleted gold nanorod interfaces: Methylene blue coupling and surfactant-like stabilization by methylene green. **Presented by: Tefera Entele Tesema**

2:25 PM [SW802] Withdrawn

2:45 PM [SW804] Molecular packing governs ultrafast interfacial energy flow. **Presented by: Md.Shahriar Hossain Shuvo**

3:05 PM [SW805] Topological defect formation and hydrodynamic cavitation driven by asymmetric particles in nematic liquid crystals. **Presented by: Xiaowei Wang**

3:25 PM [SW806] Solvent-mediated micellization and universal face-centered cubic ordering of Poloxamer 407. **Presented by: Mostafa Tabatabaei**

3:45 PM Intermission.

4:15 PM [SW807] Rapid one-pass extrusion method for the synthesis of ion-selective droplet networks. **Presented by: Sneha Sinha**

4:35 PM [SW808] Quinone uptake by levitated phenolic droplets: Noncovalent interactions and brown carbon light absorption. **Presented by: Ahmadraza Chaudhary**

4:55 PM [SW809] Engineering giant magnetic susceptibility in porous nanocrystal clusters for biomedical and environmental applications. **Presented by: Qingbo Zhang**

5:15 PM [SW803] Interfacial mechanisms underlying the antibacterial activity of nano- and microscale zinc- and gallium-based oxides. **Presented by: Yuri Strzhemechny**

5:35 PM [SW810] Multichannel kinetic optical spectrometry for characterizing dynamic liquid-phase systems. **Presented by: Dongmao Zhang**

5:55 PM Closing Remarks.

Insight and Numbers in Quantum Chemistry

Session Type: Oral

Time: 2:00 PM - 5:30 PM

Location: Texas B

Inspired by Charles Coulson□s famous call to □give us insight, not numbers,□ and the modern reinterpretation by Frank Neese emphasizing the importance of □insight and numbers,□ this symposium will

explore the evolving relationship between predictive accuracy and chemical understanding in quantum chemistry. Topics will include electronic structure theory, bonding and reaction mechanisms, machine learning, and molecular simulation, with particular emphasis on efforts to connect quantitative computation with chemical and physical interpretation. Contributions from researchers developing new theoretical frameworks, interpretable computational approaches, or applications of quantum chemistry to challenging chemical problems are welcome.

Organizer(s): James Shee

Presider(s): Alistair Sterling

Presentations:

2:00 PM Opening Remarks.

2:20 PM [SW171] From numbers to insight: A chemical interpretation of phonon band structures. **Presented by: Elfi Kraka**

3:00 PM [SW172] Benzene in the excited state: A playground for photochemical transformations. **Presented by: Judy Wu**

3:40 PM Coffee Break.

4:10 PM [SW173] Pauli exclusion, electron (de)localization, and the origin of the transition state barrier in the $H_2 + H^{\bullet}$ hydrogen atom transfer reaction. **Presented by: Shehan Hemantha Fernando**

4:30 PM [SW174] Chemically informed pruning of unitary cluster Jastrow ansätze using localized orbitals. **Presented by: Aradhika Paul**

4:50 PM [SW175] Assessing the stability of metal-organic frameworks with local vibrational mode theory. **Presented by: Sophia Trejo**

5:10 PM [SW176] Machine learning prediction of gas solubility in deep eutectic solvents using electrostatic potential-derived descriptors. **Presented by: Sahar Heidari**

Metastable, Defect-Rich, and Nanostructured Materials for Sustainable Energy

Session Type: Oral

Time: 2:00 PM - 4:00 PM

Location: Texas D

This symposium will highlight emerging chemical approaches to sustainable energy materials in which metastability, defects, dopants, nanoscale interfaces, and non-equilibrium synthesis play central roles in determining function. Topics will include materials for batteries, solid electrolytes, thermoelectrics, electrocatalysis, photocatalysis, solar fuels, and related energy-conversion and storage platforms. Particular emphasis will be placed on how synthetic control, compositional disorder, nanostructuring, interfacial chemistry, and advanced characterization can be used to tune charge and ion transport. The symposium will also welcome contributions that combine experimental materials chemistry with data-driven, machine-learning, high-throughput, or operando methods to understand structure□property relationships. By bringing together inorganic, materials, physical, analytical, and computational chemists, the session will provide a forum for discussing how chemically complex and defect-rich materials can be designed for next-generation sustainable energy technologies.

Organizer(s): Progna Banerjee

Presider(s): Progna Banerjee

Presentations:

2:00 PM [SW177]*Operando* EIS for probing interfacial evolution in lithium metal batteries. **Presented by: Tariq Bashir**

2:17 PM [SW178] Withdrawn

2:34 PM [SW179] Electrode surface modification with conductive carbon support for enhanced porphyrin electrocatalyzed oxygen reduction reaction. **Presented by: Justin Ratliff**

2:51 PM [SW180] One-step synthesis of highly active and conductive transition metal nitride for oxygen evolution in alkaline anion exchange membrane electrolysis. **Presented by: Scott Folkman**

3:08 PM [SW181] Modification of the active site microenvironment for enhanced direct oxidation of methane to methanol. **Presented by: Frederick Michael MacDonnell**

3:25 PM [SW182] From lattice to Lorentz: Programming metal-free water splitting with donor–acceptor COF junctions. **Presented by: Sreeprasad Sreenivasan**

3:42 PM [SW183] Solvent-free mechanochemical passivation of Ti3C2Tx MXene surfaces guided by machine learning. **Presented by: Julie P Vanegas**

New Instrumentation and Methods of Analysis

Session Type: Oral

Time: 2:00 PM - 6:00 PM

Location: Citizens B

Invited and open call for new and emerging analytical instrumentation, automated sample processing, and data analysis including artificial intelligence that solve critical problems in environmental, industrial, and health related applications. Advances in spectroscopic, electrochemical, and mass spectrometric detection and and separation technologies are encouraged. The application of computational tools such as machine learning and artificial intelligence for analyte detection, deconvolution, sample preparation and separations optimization, etc. are welcome.

Organizer(s): Charles Phillip Shelor

Presider(s): Charles Phillip Shelor

Presentations:

2:00 PM Opening Remarks.

2:05 PM [SW184] GC-PID determination of BTEX in foods and food extracts. **Presented by: Jennifer L Maclachlan**

2:25 PM [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. **Presented by: Hala Muhiar**

2:45 PM [SW186] Oxygenate characterization of waste plastic pyrolysis oils (WPPO) using total oxygen analysis, simulated distillation, and GC-MS. **Presented by: Amey Gonzalez**

3:05 PM [SW187] Imaging microplastics single-particles via laser-assisted micro-pyrolysis FAPA ambient mass spectrometry. **Presented by: Gerardo Gamez**

3:25 PM [SW188] Admittance detector with fast Fourier transform signal processing in suppressed ion chromatography. **Presented by: Joisha Girme**

3:45 PM [SW189] Immittance-based sensing for perfluorooctanoic acid. **Presented by: Ben Sherman**

4:05 PM Intermission.

4:20 PM [SW190] Supercritical water reaction (SCWR) as a rapid digestion method for total organic fluorine (TOF) analysis. **Presented by: Arya Mojahed Naghi**

4:40 PM [SW191] Fluorine-free conjugated polymer-based optical nanosensor arrays for trace PFAS detection and discrimination. **Presented by: Joshua Tropp**

5:00 PM [SW192] Sensor for inline chemical monitoring for water and wastewater. **Presented by: Chase Hazboun**, **Katy Roodenko**

5:20 PM [SW193] Continuously rejuvenated copper electrode for carbohydrate analysis. **Presented by: Shane Wilson**

5:40 PM [SW194] Electrochemical profiling of beef sarcoplasm: From meat quality monitoring to native electron-transfer kinetics. **Presented by: Silan Bhandari**

Monday Afternoon Coffee Break

Session Type: Coffee Break

Time: 3:30 PM - 4:30 PM

Location: Crystal C/D

Plenary Lecture: The Future of Chemistry: Innovation, Education, and Opportunities in a Changing World by Dr. H. N. Cheng

Session Type: Plenary

Time: 6:30 PM - 7:30 PM

Location: Crystal A/B

Dr. H. N. Cheng: (Retired) Southern Regional Research Center, USDA Agricultural Research Center, New Orleans, LA 70124, USA. Abstract: Chemistry is entering a transformative era in which scientific discovery, technological innovation, and societal needs are becoming increasingly interconnected. Global challenges—including climate change, sustainable energy, environmental stewardship, food security, and human health—are creating unprecedented opportunities for chemistry to develop innovative solutions that improve quality of life and support a more sustainable future. This presentation explores emerging research frontiers, including sustainable materials, green chemistry, artificial intelligence, biotechnology, advanced manufacturing, and the circular economy, while highlighting the growing importance of interdisciplinary collaboration. Equally critical are the future directions of chemical education, workforce development, and career opportunities as chemists prepare to work in an increasingly digital, data-driven, and globally connected environment. The knowledge, skills, and adaptability required of future chemists are evolving rapidly, emphasizing lifelong learning, effective communication, and flexible leadership. Thus, the future of chemistry is not defined solely by the molecules we discover or the materials we create. It is equally defined by the people we educate, the partnerships we build, and the societal challenges we choose to address. The next generation of chemists will not simply advance chemistry—they will help shape a healthier, more sustainable, and more prosperous world.

ACS 150th Anniversary Celebration / Welcome Reception

Session Type: Networking Event

Time: 7:30 PM - 9:00 PM

Location: Promenade

Tuesday, November 17, 2026

Registration

Session Type: Registration

Time: 7:00 AM - 7:00 PM

Location: Promenade

Badge pick-up and onsite registration.

Advancing Sustainable, Safer, and Responsible Chemistry: Innovations in Research & Teaching

Session Type: Oral

Time: 8:00 AM - 11:40 AM

Location: Continental

Advances in sustainable, safe, resource-efficient and responsible chemistry are essential to transforming how we conduct research, educate future scientists, and address global challenges in energy, advanced materials, environmental remediation, and human health. This symposium highlights these core values as guiding principles in modern chemical research, innovative teaching, and interdisciplinary collaboration. Ultimately, it showcases how these principles drive scientific discovery, curriculum development, and workforce preparation for a more sustainable future.

Organizer(s): John D. Beatty, Ting Han, Shiru Lin, Nasrin Mirsaleh-Kohan, Manal Rawashdeh-Omary

Presider(s): Ting Han, Manal Rawashdeh-Omary

Presentations:

8:00 AM [SW195] Drag-and-drop PowerPoint slides for digital quizing and active learning in organic chemistry. **Presented by: Robert Comito**

8:13 AM [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. **Presented by: Yonghong Zhang**

8:26 AM [SW197] Geometry-governed symmetry-breaking charge separation and photocatalysis of benzoperylenetriimide dimers. **Presented by: Ram Ratan Kaswan**

8:39 AM Intermission.

8:47 AM [SW198] Withdrawn

9:00 AM [SW199] Atomistic structures of a sustainable polymer: AI-accelerated *ab initio* bottom-up polymer structure prediction of amorphous. **Presented by: Yizhi Song**

9:13 AM [SW200] Unveiling the exceptional electron-acceptor ability of C_{60} in phenothiazine-C_{60}-based multi-modular donor-acceptor conjugates. **Presented by: Chamari Viyanga Kusalani Ileperuma**

9:26 AM [SW201] Diffusional effects on Langmuirian kinetics in heterogeneous catalysis. **Presented by: Paulo Morgado**

9:39 AM Intermission.

9:49 AM [SW202] Towards sustainable computing: Kubernetes for efficient security and portability for computational chemistry. **Presented by: Kriti Alam**

10:02 AM [SW203] Examining long-lived excited charge separation in silicon(IV) phthalocyanine with axially bound C_{60} incorporated via azobenzene linkers. **Presented by: Andrew Dawson**

10:15 AM [SW204] Intramolecular charge transfer in phosphorus(V) porphyrin-based push-pull systems for efficient charge transfer. **Presented by: Hasanka Rathnayaka**

10:28 AM [SW205] Screening of potentially toxic elements in children's toys across the USA–Mexico border region using X-ray fluorescence spectroscopy. **Presented by: Abraham Dagda Torres**

10:41 AM [SW206] Effects of polyethylene branch structure and zeolite framework on catalytic pyrolysis. **Presented by: K SADASHIVA PATIL**

10:54 AM Intermission.

10:59 AM [SW207] Structure determination in the classroom: Investigating supramolecules using NMR. **Presented by: Lakshmi Chockalingam Kasi Viswanath**

11:12 AM [SW208] From single-ligand binding to multicomponent flavor recognition: A computational study of protein–volatile interactions. **Presented by: Saranya Yamunan**

11:25 AM [SW209] Sustainable recovery of lithium from discarded lithium-ion battery black mass using hydrometallurgical leaching and electrodialysis. **Presented by: Kalpana Dumre**

Bioinorganic Chemistry in Health, Energy, and Environment

Session Type: Oral

Time: 8:00 AM - 11:40 AM

Location: Crystal B

Bioinorganic chemistry lies at the interface of inorganic chemistry and biology, addressing fundamental questions about how metal ions and small molecules in biological environment mediate essential life processes. This symposium will highlight recent advances in understanding the roles of metal centers in biological systems, with particular emphasis on their impact across health, energy, and environmental applications. By bringing together diverse perspectives, the session aims to showcase how bioinorganic principles drive innovation in areas ranging from disease-related metal signaling and therapeutics to sustainable catalysis and environmental remediation.

Organizer(s): Pokhraj Ghosh, Kayla N Green

Presider(s): Pokhraj Ghosh, Kayla N Green

Presentations:

8:00 AM Opening Remarks.

8:05 AM [SW210] Radical SAM enzymes: Generating and controlling the 5'-deoxyadenosyl radical. **Presented by: Broderick Joan**

8:30 AM [SW211] Characterization of the cytosolic labile iron pool in *Saccharomyces cerevisiae*. **Presented by: Paul Alan Lindahl**

8:55 AM [SW212] Chemistry at and beyond the oxo-wall. **Presented by: Jason Shearer**

9:20 AM [SW213] Radical chemistry of metal–alkyl bonds. **Presented by: Kurtis Carsch**

9:45 AM Intermission.

10:00 AM [SW214] Harnessing the oxidizing power of nitric oxide at copper. **Presented by: Timothy H Warren**

10:25 AM [SW215] Know your NO: Managing health with reactive oxygen and nitrogen species. **Presented by: Alex R Lippert**

10:50 AM [SW216] Role of scaffold ligand dynamics to modulate electron transfer activation parameters in dinuclear copper(I/II) complexes. **Presented by: Michael J Rose**

11:15 AM [SW217] Interception of Cu(II)-SNO and HONO intermediates in H_2S-mediated reduction of Cu(II)-nitrite. **Presented by: Pokhraj Ghosh**

Communication Skills in Preparing, Presenting, and Publishing Papers

Session Type: Oral

Time: 8:00 AM - 11:50 AM

Location: Citizens B

This symposium will highlight essential practices that help chemists communicate their work clearly and effectively. It will cover the full communication arc from writing well-structured manuscripts and designing strong visuals to delivering engaging presentations and navigating peer review. Key themes include historical developments, audience-focused writing, visual storytelling, and the growing role of digital and AI-based tools. The objective is to equip researchers, especially early career chemists and chemical engineers, with practical strategies that strengthen their communication skills and enhance the visibility and impact of their work.

Theme: Education

Organizer(s): Benjamin Eric Blass, H.N. N. Cheng

Presider(s): Benjamin Eric Blass, H.N. N. Cheng

Presentations:

8:00 AM Opening Remarks.

8:05 AM [SW218] Paving the road to publications in scientific periodicals: Lessons from the past. **Presented by: Nicolay V Tsarevsky**

8:35 AM [SW219]*Caveat emptor*: Advice and tips for preparing scientific publications and presentations. **Presented by: Ronald Smaldone**

9:05 AM [SW220] Do's and don'ts of effective presentations. **Presented by: Frank Dennis Blum**

9:35 AM [SW221] Communicating science to the outside world: Lessons on style, substance, and presentation. **Presented by: Benjamin Eric Blass**

10:05 AM Intermission.

10:20 AM [SW222] Brave enough to be visible: Personal branding and the confidence to communicate your chemistry. **Presented by: Jennifer L Maclachlan**

10:50 AM [SW223] Balancing innovation protection and scientific publication: Challenges and opportunities for industrial researchers. **Presented by: MASUD MONWAR**

11:20 AM [SW224] Use of artificial intelligence to facilitate scientific communication. **Presented by: H.N. N. Cheng**

Functional Solid State Materials

Session Type: Oral

Time: 8:00 AM - 12:00 PM

Location: Texas A

This symposium brings together chemists to advance the frontiers of solid-state chemistry, with an emphasis on the experimental and computational discovery and design of new functional materials for energy and sustainability applications. The scope encompasses the synthesis of novel inorganic, hybrid, and complex solid-state materials, alongside the determination and analysis of crystal structures using

modern diffraction and spectroscopic techniques. One of the central objectives is to explore the mechanistic underpinnings of solid-state reactions from thermodynamic driving forces to kinetic pathways and phase transformations. Equally important is elucidating structure property relationships that govern the behavior of solid-state materials in applications such as energy storage and conversion, thermoelectrics, photocatalysis, ionic conductors, and sustainable chemical processes.

Organizer(s): Shruti Hariyani, Tianyu Li

Presider(s): Shruti Hariyani, Tianyu Li

Presentations:

8:00 AM [SW225] Synthesis, modification, and control of quantum materials using electrochemistry. **Presented by: Joshua Bocarsly**

8:40 AM [SW226] Strong, yet split hydrogen bonding with ice rules in delafossite (H/D)RhO_2. **Presented by: Matthew Wright**

9:00 AM [SW227] Mixed ligand *f*-element coordination polymers with 2-bromoterephthalate and aliphatic dicarboxylate spacers. **Presented by: Ralph A Zehnder**

9:30 AM [SW228] Ultrafast energy flow in supported TMDC heterostructures. **Presented by: Md Shaikot Alam Shakil**

9:50 AM Coffee Break.

10:10 AM [SW229] Packing pentagons. **Presented by: Tomce Runcevski**

10:40 AM [SW230] Synthesis-enabled discovery and crystal chemistry of rare earth silicon pnictides. **Presented by: Gayatri Viswanathan**

11:00 AM [SW231] Reversible and asymmetric phase-transition pathways in MnSb conversion-type anodes revealed by synchrotron X-ray diffraction. **Presented by: Jason Jiale Zhou**

11:20 AM [SW232] Chirality transfer to the magnetic sublattice in the hybrid perovskite (R)-/(S)-3-fluoropyrrolidinium copper(II) chloride. **Presented by: Daniel B. Straus**

Hyperpolarized Magnetic Resonance - from Chemistry and Applications

Session Type: Oral

Time: 8:00 AM - 11:50 AM

Location: Texas B

Magnetic resonance is a versatile method that has driven various research fields in analytical chemistry, structure determination of proteins and even biomedical imaging. Hyperpolarization is an approach that overcomes the sensitivity limitations of magnetic resonance and amplifies signals by orders of magnitude. This enables to study chemical and biochemical questions in unprecedented ways. We are proposing to bring the hyperpolarization community together as part of the regional meeting and hold three sessions on the topics of hyperpolarization method development, developing molecular probes and imaging and studying biomolecules. The ACS meeting will serve as an ideal platform to inform and discuss developments in the field with a general chemistry oriented audience that can benefit from hyperpolarization approaches. The Dallas Fort Worth area has a particular large hyperpolarization community from which we can expect high attendance.

Organizer(s): Kendra Frederick, Stefan Gloeggler, Mai Huynh

Presider(s): Kendra Frederick, Stefan Gloeggler, Mai Huynh

Presentations:

8:00 AM Opening Remarks.

8:05 AM [SW233] Early adventures in hyperpolarized metabolic imaging. **Presented by: A. Dean Sherry**

8:25 AM [SW234] Opportunities for new probes in clinical ^{13}C imaging. **Presented by: Craig Malloy**

8:45 AM [SW235] Hyperpolarized ^{13}C MRI for imaging brain metabolism. **Presented by: Jae Mo Park**

9:05 AM [SW236] Quantitative analysis of pyruvate delivery and spatial characteristics in hyperpolarized [1-13C]pyruvate cardiac MRI. **Presented by: Fatemeh Khashami**

9:20 AM [SW237] HyperCEST NMR reveals size-selective guest binding in hidden diastereomers of paramagnetic MOPs. **Presented by: Leif Schröder**

9:35 AM [SW238] Cucurbit[6]uril-tethered DNA conjugates as potential ^{129}Xe hyperCEST biosensors. **Presented by: SOUMEN PRADHAN**

9:50 AM Intermission.

10:20 AM [SW239] Optimization of dissolution dynamic nuclear polarization-enhanced NMR and MRI signals. **Presented by: Lloyd Laporca Lumata**

10:40 AM [SW240] Accessible metabolic 13C magnetic resonance with rapid parahydrogen-based hyperpolarization. **Presented by: Andreas Benjamin Schmidt**

11:00 AM [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. **Presented by: Eduard Y Chekmenev**

11:15 AM [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. **Presented by: Devyn Ericksen**

11:20 AM [SW243] DNP NMR reveals environment-dependent conformational ensemble of disordered proteins. **Presented by: Rupam Ghosh**

11:25 AM [SW244] Structural context modulates the conformational ensemble of the intrinsically disordered amino terminus of α-synuclein. **Presented by: Rania Dumarieh**

11:30 AM [SW245] Study of T_1 and T_2 relaxation times of water in the presence of bimetallic complexes of a furan-based polyamine macrocycle. **Presented by: Alesha Foster**

11:35 AM [SW246] Investigating thiol-containing biomolecules in parahydrogen-induced hyperpolarization at low-field NMR. **Presented by: Gabriel Rocha**

11:40 AM [SW247] Exploring new PHIP-SAH precursor for real-time metabolic magnetic resonance spectroscopy. **Presented by: Leander Konstantin Konstantin May**

11:45 AM [SW248] Reaction-encoded hyperpolarized ^{15}N molecular probes for glutathione detection. **Presented by: Guoshu Xie**

Organic and Chemical Biology Young Investigator Symposium

Session Type: Oral

Time: 8:00 AM - 12:00 PM

Location: Texas C

This symposium will highlight assistant professors in organic and chemical biology from throughout the Southwest.

Organizer(s): Kami Hull, Uttam K Tambar

Presider(s): Kami Hull, Uttam K Tambar

Presentations:

8:00 AM [SW249] Building the spliceosome: Molecular control of RNA–protein complex assembly in gene expression and disease. **Presented by: Byung Ran So**

8:30 AM [SW250] Structure-guided design of amido cyanines (AmCy) for high-performance near-infrared imaging. **Presented by: Syed Usama**

9:00 AM [SW251] Quantifying and controlling beta-strand hydrogen bonds in peptides and proteins. **Presented by: Robert W Newberry**

9:30 AM Intermission.

10:00 AM [SW252] Chemical reactivity as a quantitative readout of RNA molecular recognition in cells. **Presented by: Lauren Hagler**

10:30 AM [SW253] Boron chemistry in organic synthesis, bioconjugation, and drug discovery. **Presented by: Shiqing Xu**

11:00 AM [SW254] Chemical investigations inspired by unusual alkaloids. **Presented by: Myles Smith**

11:30 AM [SW255] Strategy-driven complex bioactive molecule synthesis. **Presented by: Filippo Romiti**

Senior Chemists Breakfast

Session Type: Networking Event

Time: 8:00 AM - 9:30 AM

Location: Crystal A

Supramolecular Chemistry and Functional Molecular Materials

Session Type: Oral

Time: 8:00 AM - 12:00 PM

Location: Texas D

This symposium will bring together researchers developing supramolecular systems that enable new functions through molecular recognition, self-assembly, and noncovalent interactions. Presentations will span macrocyclic chemistry, host□guest systems, supramolecular polymers, crystal engineering, charge-transfer materials, molecular machines, biomolecular assemblies, and functional organic materials for applications in energy, sustainability, catalysis, sensing, and biomedicine. The symposium seeks to promote interactions across traditionally separate research areas while highlighting emerging directions in functional supramolecular materials.

Organizer(s): Yuanning Feng

Presider(s): Yuanning Feng

Presentations:

8:00 AM [SW256] Patterns within patterns: Shaping light and chemistry in space and time. **Presented by: Alex R Lippert**

8:20 AM [SW257] Bright NIR-II/SWIR emissive polymer-based nanoassemblies. **Presented by: Joshua Tropp**

8:40 AM [SW258] Low-energy excitation leading to symmetry-breaking charge separation in near-infrared-absorbing bisstyryltriphenylamine–BODIPY dimers. **Presented by: Swatej Sabbarwal**

8:55 AM [SW259] Evolution of push-pull donor-acceptor systems for NIR-active optoelectronic applications. **Presented by: Sainyam Sikka**

9:10 AM [SW260] Supramolecular control of lanthanide coordination in multinuclear sandwich complexes for two-photon upconversion. **Presented by: Anne Elizabeth Vivian Gorden**

9:30 AM [SW261] Circularly polarized luminescent cyanostilbenes: Efficient design strategies to tune self-sorting and chiral amplification in self-assemblies. **Presented by: Bhawani Narayan**

9:50 AM Coffee Break.

10:10 AM [SW262] Aromatic heterocycle-fused porphyrins: Synthesis and impact on photophysical properties. **Presented by: Hong Wang**

10:30 AM [SW263] Structural modulation of metalloporphyrins for electrocatalytic conversion of nitrate and carbon dioxide pollutants into value-added products. **Presented by: Alankar Kafle**

10:45 AM [SW264] Symmetry breaking charge separation in zinc phthalocyanine dimers self-assembled via hydrogen bonding. **Presented by: Ram Ratan Kaswan**

11:00 AM [SW265] Functional rotaxanes in lipid membranes: From photoswitchable membrane modulation to ion transport, neuromorphic behavior, and antibacterial activity. **Presented by: Jeremy Smith**

11:20 AM [SW266] Tellurium-based strategies for ion transport across biological membrane mimics. **Presented by: You Jiang**

11:40 AM [SW267] Highly selective ionophore-based bilayer emulsion membranes. **Presented by: Ronald J Vogler**

SWRM Wellness Room

Session Type: Wellness

Time: 8:00 AM - 6:00 PM

Location: Keystone Room

Exposition

Session Type: Expo

Time: 9:00 AM - 5:00 PM

Location: Crystal C/D

Tuesday Morning Coffee Break

Session Type: Coffee Break

Time: 9:30 AM - 10:30 AM

Location: Crystal C/D

Graduate Recruitment Fair

Session Type: Special Event

Time: 11:00 AM - 3:00 PM

Location: Promenade

High School Research in Chemistry

Session Type: Poster

Time: 12:00 PM - 2:00 PM

Location: Crystal C/D

Organizer(s): Gabriele Meloni, Mihaela C Stefan, Nicolay V Tsarevsky

Presider(s): Gabriele Meloni

Presentations:

12:00 PM [SW268] Predicting and controlling which mefenamic acid crystal forms appear in organic crystallization: Crystal growth and design. **Presented by: Zainab Khokhar**

12:00 PM [SW269] Theoretical determination of substituent effects for chromium complexed arenes. **Presented by: Daniyal Khan**

12:00 PM [SW270] Withdrawn

12:00 PM [SW271] Influence of sonication media on the particle size of Ti_3CNT_x MXene. **Presented by: Hasan Faiaz Zubaer**

12:00 PM [SW272] Time-dependent breakdown of MNenes to facilitate a sustainable future. **Presented by: Lauren Page**

12:00 PM [SW273] Effect of sonication time on MXene particle size and agglomeration. **Presented by: Saim Karim**

12:00 PM [SW274] Decoding biophysical fragility in MYC/MAX condensate networks in MYC-driven cancer states. **Presented by: Alexander Nam Nguyen**, **Yuvraj Rathore**

12:00 PM [SW275] Disentangling inner filter, dilution, and quenching effects on the native fluorescence of albumin. **Presented by: Han Vo**

12:00 PM [SW276] Molecular glues: Computational modeling of a PROteolysis TArgeting Chimeras (PROTACs) targeting Aurora kinase A for diffuse large B-cell lymphoma. **Presented by: Gaurav Sharma**

12:00 PM [SW277] Shuriken: Computational design of a multispecific hexabody targeting surface glycoproteins of six pathogenic viruses. **Presented by: Rithvik Kamesh**

12:00 PM [SW278] Evaluating the efficacy of aggregation propensity as a predictor of oligopeptide dimerization in redox-active conditions. **Presented by: Pranav Kolli**

12:00 PM [SW279] Studying the effect of calcium on the growth, viability, and inflammation induced by H2O2 of *Lactiplantibacillus plantarum* using *in-vitro* assay and minibioreactor. **Presented by: Aliyah Odunowo**

12:00 PM [SW280] Effect of chiral nanoparticles in biomolecule polymorphism. **Presented by: jacqueline lam**

12:00 PM [SW281] Withdrawn

12:00 PM [SW282] $Mn_{1-x}Fe_xSb$ as a conversion anode material for lithium-ion batteries. **Presented by: Aran Pirouzan**

12:00 PM [SW283] Withdrawn

12:00 PM [SW284] Synthesis of layered oxide cathodes materials for lithium-ion batteries. **Presented by: Shwetha Jayakumar**

12:00 PM [SW285] Synthesis and characterization of polymer-coated iron oxide nanoparticles as potential templates for guiding organic compound crystallization. **Presented by: Hy Kim**

12:00 PM [SW517] Computational identification of microRNAs as potential biomarkers and follistatin-targeting therapeutic candidates in ischemic heart disease. **Presented by: Nethania Ajan**

Undergraduate Research in Chemistry

Session Type: Poster

Time: 12:00 PM - 2:00 PM

Location: Crystal C/D

Organizer(s): Gabriele Meloni, Mihaela C Stefan, Nicolay V Tsarevsky

Presider(s): Gabriele Meloni, Mihaela C Stefan, Nicolay V Tsarevsky

Presentations:

12:00 PM [SW286] ICP-MS determination of selected trace metals in commercial instant noodles using hot plate and microwave-assisted acid digestion. **Presented by: Victor Tran**, **Shawnise Gregory**, **Tuan Phan**

12:00 PM [SW287] Withdrawn

12:00 PM [SW288] Comparison of hot plate and microwave-assisted acid digestion for ICP-MS determination of trace elements in honey. **Presented by: Victoria Tran**, **Morgan Clark**, **Aliya Broadway**, **Tuan Phan**

12:00 PM [SW289] Biosorption of copper and cadmium using hydrochar derived from *Chlorella* and rice hull. **Presented by: Ben Jang**

12:00 PM [SW290] Plastics as heavy metal vectors in landfill-mined soil: A rapid *in-situ* handheld XRF assessment from Bhalswa dumpsite, New Delhi. **Presented by: Rhea Kochhar**

12:00 PM [SW291] Assessment of heavy metal contamination in playground dust using atomic absorption spectrometry (AAS). **Presented by: Jessica Meza**

12:00 PM [SW292] Through the lens of chirality: Breakdown of single-walled carbon nanotubes into graphene quantum dots. **Presented by: Alyssa Dickens**

12:00 PM [SW293] Gold nanoparticle-based biosensors for targeted detection of HPV E6 and E7 oncoproteins. **Presented by: Louie Tapia**

12:00 PM [SW294] ROS-responsive gold nanoparticles for targeted methotrexate delivery in inflammatory diseases. **Presented by: Elaina HEath**

12:00 PM [SW295] Withdrawn

12:00 PM [SW296] Exploring Mn-based MOF, MOXI-214, as a vaccine adjuvant candidate. **Presented by: Alexander James Mathai**

12:00 PM [SW297] Nanoscale characterization of co-assembled peptide fibers. **Presented by: Erwin Kingston**

12:00 PM [SW298] Withdrawn

12:00 PM [SW299] From bacteria to cancer therapy: Self-assembled virus-like particles for targeted enzyme delivery. **Presented by: Y Nguyen**

12:00 PM [SW300] Effect of benzalkonium halide chain length on magnetic cellulose nanocrystal stability. **Presented by: Thatcher Bentley**

12:00 PM [SW301] Synthesis of gallium-based liquid metal nanoparticles. **Presented by: Benjamin Thomas Lopez**

12:00 PM [SW302] Withdrawn

12:00 PM [SW303] Enzymatic construction of chiral 2D/3D fused heterocyclic ring scaffolds. **Presented by: Quoc Hoa Ngo**

12:00 PM [SW304] Establishing a malate dehydrogenase (MDH) drug screening assay for the discovery of MDH selective inhibitors with anticancer potential. **Presented by: Nicholas Aidan Furman**

12:00 PM [SW305] Biochemical studies of the avocado (*Persea americana*) pit. A potential remedy for the control of diabetes. **Presented by: Arnulfo Mar**

12:00 PM [SW306] Expression and activity profiling of recombinant PhoX from *Shewanella oneidensis* MR-1. **Presented by: Isabella Ibanez**

12:00 PM [SW307] Examination of antimicrobial production by a *Pseudomonas donghunesis* strain isolated from Sorcerer's Cave. **Presented by: Amy Osborn**, **Jessica Leach**

12:00 PM [SW308] Genetic modification of designer DNA for glial cell targeting. **Presented by: Yanelisse Mariel Luiggi Garcia**

12:00 PM [SW309] Withdrawn

12:00 PM [SW310] Inhibition of human islet amyloid polypeptide aggregation by the ATP-independent molecular chaperone cpSRP43. **Presented by: Bismah Ahmed**, **Aayan Ahmed**

12:00 PM [SW311] Comprehensive biochemical analysis of defective high-density lipoprotein (HDL) via cardiovascular-associated oxidative damage. **Presented by: Haylie Tran**

12:00 PM [SW312] Withdrawn

12:00 PM [SW313] Exploring the expression and reactivity of Baeyer-Villiger monooxygenases from *Thermobifida fusca* and *Acinetobacter caloaceticus*. **Presented by: Daniela Guerrero**

12:00 PM [SW314] Comparative investigation of zinc binding in two isomeric peptides using experimental and computational approaches. **Presented by: Rawan Siddig**

12:00 PM [SW315] Synthesis and characterization of dearomatized Cu(I)-C^N^C complexes: Intermediates in catalysis. **Presented by: Emylie Guthrie**

12:00 PM [SW316] Data-driven mapping of backbone conformational space across all 400 dipeptides. **Presented by: Adair Oropeza**

12:00 PM [SW317] Withanolides targeting H5N1 bird flu: *In silico* screening via pharmacokinetic and molecular dynamics studies. **Presented by: Siwar Kefi**

12:00 PM [SW318] Anti-fouling strategy using triple pulse amperometry for electrochemical detection of xylazine at modified electrodes. **Presented by: Ella Saltstein**, **Sarah Leiva**

12:00 PM [SW319] Synthesis and study of PDI derivatives for organic semiconductor applications. **Presented by: Paula Andrea Sanchez Rendon**

12:00 PM [SW320] Stepwise chemical construction of functional interfaces on mica through covalent surface modification. **Presented by: Abigail Bellucci**

12:00 PM [SW321] Uncovering the factors directing the mechanochemical degradation of polythiophenes. **Presented by: Andrea Mena**

12:00 PM [SW322] Tracking stepwise mica surface functionalization using FTIR-GATR: A rapid and accessible characterization strategy. **Presented by: Scarlett Deluna**

12:00 PM [SW323] Synthesis of amino and hydroxyl-group modified polymers using ring-opening metathesis polymerization (ROMP). **Presented by: Monique Faith Boodram**

12:00 PM [SW324] Sustainable and chromatography-free synthesis of trityl ether tosylates from glycols and diols. **Presented by: Khanh Nguyen**

12:00 PM [SW325] Twist to upconvert: Conformational control of DSA governs photon upconversion properties. **Presented by: Parker Jia**

12:00 PM [SW326] Automatic matching of excited states through orbital overlap. **Presented by: Mollie Hamman**

12:00 PM [SW327] Deep unrolling AI model for compressed sensing reconstruction in GDOES snapshot multi-elemental mapping. **Presented by: HYUNMO GOO**

12:00 PM [SW328] Compositional and morphological effects on phase stability and the shock response of AlCoCrFeNi high-entropy alloys. **Presented by: Luke Radich**

12:00 PM [SW329] Training machine learning models with experimental NMR and quantum chemical descriptors to predict Hammett σ constants. **Presented by: Isabel McLeod**

12:00 PM [SW330] Exploring single-site heterogeneity with Universal Models for Atoms. **Presented by: Marcus Alphonse Broussard**

12:00 PM [SW331] 18 electron rule and metal-metal bonding. **Presented by: Andrea Joglar**, **Jimena Martinez-Olivares**

12:00 PM [SW332] Machine learning-guided prediction of optical properties in naphthopyran photochromic dyes for next-generation photovoltaics. **Presented by: Ruben Nunez**

12:00 PM [SW333] Predicting pK_a of drug-like molecules in aqueous solution via thermodynamic conformers and explicit solvation. **Presented by: Alphonsus Nguyen**

12:00 PM [SW334] Catalytic activity of Kuratowski-type clusters in hydrogenation reactions. **Presented by: Giovanni Antonio Bartolozzi**

12:00 PM [SW335] Redox-controlled reactivity of dinitrosyl cobalt complexes. **Presented by: Krish Pudu**

12:00 PM [SW336] Understanding the role of S-nitrosothiols as NO carriers at iron. **Presented by: Kalkidan Abebe**

12:00 PM [SW337] Synthesis of Ni-Co catalysts for dry reforming of methane. **Presented by: Ben Jang**

12:00 PM [SW338] Development of a colorimetric portable sensor for heavy metals. **Presented by: Andrew Do**

12:00 PM [SW339] Evaluation of dopant retention in carbothermally synthesized ZnO tetrapods. **Presented by: Joshua Humphrey**

12:00 PM [SW340] Host-guest complexation of pillar[6]arenes towards PFAS. **Presented by: Gavin Duke Harman**

12:00 PM [SW341] pH-dependence of reduced graphene oxide membrane-based osmotic batteries. **Presented by: Rayyah Shah**

12:00 PM [SW342] Electrophoretic deposition of barium titanate on carbon electrodes. **Presented by: Meggan Amber Collicelli**

12:00 PM [SW343] Investigation of pH-dependent static quenching of fluorescein by graphene oxide (GO) using steady-state and time-resolved techniques. **Presented by: Daniel Kim**

12:00 PM [SW344] Development of chemoselective reactions for amino acid sidechain for applications in protein sequencing. **Presented by: Cannon Casey**

12:00 PM [SW345] Investigation of an alternative zinc binding affinity tag by experimental and computational methods. **Presented by: Jessica Dall**

12:00 PM [SW346] Molecular docking and microwave-assisted synthesis of imidazole derivatives as potential CYP51B inhibitors in *Aspergillus fumigatus*. **Presented by: Mollie Felicity Wheeler**

12:00 PM [SW347] Development and protection of functionalized aminophenols for oxazaborole-based macrocycle synthesis. **Presented by: Carlos Rea**

12:00 PM [SW348] Development of a SPE-UPLC-MS/MS method for detection of steroid sex hormones in wastewater samples from wastewater treatment plants. **Presented by: Ben Lewis**

12:00 PM [SW349] Synthesis and characterization of β-functionalized porphyrin liquid crystals. **Presented by: Imad Al Naqeeb**

12:00 PM [SW350] Synthesis of β-ketoester substrates and biocatalytic oxidations to access to α-acyloxy ketone scaffolds through biocatalytic Baeyer-Villiger oxidation. **Presented by: Samantha Shannon**

12:00 PM [SW351] Analysis and extraction of pesticides from biosolids. **Presented by: Kefa K Onchoke**, **Joe Kinnear-Meza**

12:00 PM [SW352] Varying linear solvation energy relationship descriptors using fentanyl surrogates and analogs for supercritical fluid chromatography. **Presented by: Elijah Danysix Almanza**

12:00 PM [SW353] Total phenolic content and antioxidant capacity of white teas from different geographic origins. **Presented by: Graciela Gonzalez**

12:00 PM [SW354] Influence of growing environment on the phenolic profile of Sri Lankan tea: An HPLC study. **Presented by: Felicity Gomez**

12:00 PM [SW355] Comparative HPLC analysis of phenolic compounds in white teas from different geographic origins. **Presented by: Lydia Park**

12:00 PM [SW356] Harnessing microalgal functionality in cellulose nanofiber films for sustainable functional materials. **Presented by: Ning Zhang**

12:00 PM [SW357] Determination of phosphate in soil extracts in Lower Barnett Shale: A green chemistry enzymatic method. **Presented by: Elsie Kambili Okoye**

12:00 PM [SW358] Metal-ion-mediated assembly of ambient-dried cellulose nanofiber–spirulina biofoams. **Presented by: Isabelle Maki**

12:00 PM [SW359] Synthesis, characterization, and cytotoxic assessment of dinuclear copper(II) complexes targeting triple-negative breast cancer. **Presented by: Isaac Borrego**

12:00 PM [SW360] Synthesis and characterization of palladium(II) complexes with phenanthroline and bipyridine ligands for selective cytotoxicity against triple-negative breast cancer. **Presented by: Natalia Aguilar**

12:00 PM [SW361] Design and characterization of heteroleptic copper complexes for enhanced antitumor activity with reduced side effects. **Presented by: Stefina M Cortese**

12:00 PM [SW362] Preparation of very pure osajin and pomiferin for testing against cultured pancreatic cancer cells. **Presented by: Garrett Heimann**, **Jacob Rasmussen**

12:00 PM [SW363] Extraction, isolation, and cytotoxic evaluation of gaillardin from West Texas *Gaillardia pulchella*. **Presented by: Sophia Peltier**

12:00 PM [SW364] 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. **Presented by: Evan Capuccio**

12:00 PM [SW365] Stereochemically defined cyclohexylamide scaffolds as chiral peptidomimetics for mimicking α-helical surfaces. **Presented by: Julia Floyd**

12:00 PM [SW366] Optimization of ZnO electrodeposition on stainless steel mesh for photoelectrochemical applications. **Presented by: Charles Bonagura**

12:00 PM [SW367] Unlocking edge-site activity in MNenes for green electrochemical ammonia production. **Presented by: Joshua Ferguson**

12:00 PM [SW368] Evaluation of a Cu(II) salophen complex for Chan-Lam C-N coupling. **Presented by: Ansh Chugh**

12:00 PM [SW369] Towards the synthesis of Zn-Oxy-DPA-Diiodo-BODIPY photosensitizer for intracellular photodynamic therapy. **Presented by: Michael P.**

12:00 PM [SW370] Bridging the gap: Ligand-directed assembly of dinuclear palladium phenanthroline complexes. **Presented by: Muqtadir Musharaf**

12:00 PM [SW371] Photopolymerization, characterization and aquatic toxicity of PEDOT. **Presented by: Neetika Sainju**

12:00 PM [SW372] Synthesis of porphyrin-based receptors for perfluoroalkyl substances (PFAS). **Presented by: Kharese Alexander**

12:00 PM [SW373] Synthesis of square planar pincer ligand transition metal complexes. **Presented by: Alexander Jimenez**, **Leah Autry**

12:00 PM [SW374] To condense the diffused light of a page. **Presented by: Emily Ruby Carrizales**

12:00 PM [SW375] Design and synthesis of self-assembling peptides for the formation of coacervates. **Presented by: Raniyah Ali**

12:00 PM [SW376] Cajun Country POGIL: Supporting student success and college preparedness in general chemistry. **Presented by: Nelson Eguizabal**, **Theodore Emmanuel Gatmaitan Alivio**

Women Chemists Committee Luncheon

Session Type: Networking Event

Time: 12:00 PM - 1:30 PM

Location: Crystal A

Advancing Sustainable, Safer, and Responsible Chemistry: Innovations in Research & Teaching

Session Type: Oral

Time: 2:00 PM - 5:15 PM

Location: Continental

Advances in sustainable, safe, resource-efficient and responsible chemistry are essential to transforming how we conduct research, educate future scientists, and address global challenges in energy, advanced materials, environmental remediation, and human health. This symposium highlights these core values as guiding principles in modern chemical research, innovative teaching, and interdisciplinary collaboration. Ultimately, it showcases how these principles drive scientific discovery, curriculum development, and workforce preparation for a more sustainable future.

Organizer(s): John D. Beatty, Ting Han, Shiru Lin, Nasrin Mirsaleh-Kohan, Manal Rawashdeh-Omary

Presider(s): Ting Han, Shiru Lin, Manal Rawashdeh-Omary

Presentations:

2:00 PM [SW377] Nanospace engineering for sustainability. **Presented by: Shengqian Ma**

2:20 PM [SW378] Guest binding in cyclobenzoin derivatives. **Presented by: Ognjen Miljanic**

2:40 PM [SW379] "Genuine" vs "fake news" DNA metallointercalation via planar coordination spheres in green aqua systems. **Presented by: Mohammad A Omary**

3:00 PM Intermission.

3:15 PM [SW380] Real-world digital chemistry: Putting quantum simulation, machine learning, AI, and big data into practicing chemists' hands. **Presented by: Benjamin G Janesko**

3:30 PM [SW381] From C-H bonds to functionalities: Toward more practical and sustainable catalysis. **Presented by: Xin Cui**

3:45 PM [SW382] Development of an intrinsic tryptophan FRET platform for studying GAG-protein interactions. **Presented by: Daniel Kwame Afosah**

4:00 PM Intermission.

4:12 PM [SW383] Sustainably enabling computational chemistry in the condensed phases by combining the SeA high-throughput hybrid DFT engine and Deep Potential molecular dynamics. **Presented by: Hsin-Yu Ko**

4:27 PM [SW384] Degradation behavior of polyethylene of different densities under reactive extrusion process. **Presented by: MASUD MONWAR**

4:42 PM [SW385] Data-driven insights into machine learning–accelerated density functional theory for catalytic materials discovery. **Presented by: Shiru Lin**

4:57 PM [SW386] Incorporating responsible chemistry and sustainability across the curriculum: Transforming teaching, research, and student engagement. **Presented by: Manal Rawashdeh-Omary**

Bioinorganic Chemistry in Health, Energy, and Environment

Session Type: Oral

Time: 2:00 PM - 5:15 PM

Location: Crystal B

Bioinorganic chemistry lies at the interface of inorganic chemistry and biology, addressing fundamental questions about how metal ions and small molecules in biological environment mediate essential life processes. This symposium will highlight recent advances in understanding the roles of metal centers in biological systems, with particular emphasis on their impact across health, energy, and environmental applications. By bringing together diverse perspectives, the session aims to showcase how bioinorganic principles drive innovation in areas ranging from disease-related metal signaling and therapeutics to sustainable catalysis and environmental remediation.

Organizer(s): Pokhraj Ghosh, Kayla N Green

Presider(s): Pokhraj Ghosh, Kayla N Green

Presentations:

2:00 PM Opening Remarks.

2:05 PM [SW387] Interactions of hydroxylamines and aldoximes with synthetic metalloporphyrins. **Presented by: George B Richter-Addo**

2:30 PM [SW388] Tuning product selectivity in nonheme iron-catalyzed nitrogen oxyanion reduction. **Presented by: Alison R Fout**

2:55 PM [SW389] Low oxidation state metallocorroles: Bioinspired motifs with applications in catalysis and energy. **Presented by: Zachary J Tonzetich**

3:20 PM [SW390] Multifunctional antioxidant macrocycles as small-molecule mimics of endogenous defense systems. **Presented by: Kayla N Green**

3:45 PM Intermission.

4:00 PM [SW391] Investigation of the DSF/Cu reaction using LC HDMS and reactivity studies. **Presented by: Patrick Joseph Farmer**

4:25 PM [SW392] Configurational isomers with a CB-TE2A core. **Presented by: Paul Jurek**

4:50 PM [SW393] Control of secondary coordination spheres of nickel(II) dithiolate complexes through sulfur functionalization: Effects on electrochemistry and the HER. **Presented by: Marcetta York Darensbourg**

Functional Solid State Materials

Session Type: Oral

Time: 2:00 PM - 5:30 PM

Location: Texas A

This symposium brings together chemists to advance the frontiers of solid-state chemistry, with an emphasis on the experimental and computational discovery and design of new functional materials for energy and sustainability applications. The scope encompasses the synthesis of novel inorganic, hybrid, and complex solid-state materials, alongside the determination and analysis of crystal structures using modern diffraction and spectroscopic techniques. One of the central objectives is to explore the mechanistic underpinnings of solid-state reactions from thermodynamic driving forces to kinetic pathways and phase transformations. Equally important is elucidating structure property relationships that govern the behavior of solid-state materials in applications such as energy storage and conversion, thermoelectrics, photocatalysis, ionic conductors, and sustainable chemical processes.

Organizer(s): Shruti Hariyani, Tianyu Li

Presider(s): Shruti Hariyani, Tianyu Li

Presentations:

2:00 PM [SW394] Lamellar hybrid metal chlorides A_2MCl_4 for thermal energy management: Alkyl cation engineering of 2D and 0D hybrids. **Presented by: Kyle McCall**

2:40 PM [SW395] Surface sp^2 carbon elimination and hydroxylation of polycrystalline diamond. **Presented by: Renuka Rathnayake Mudiyanselage**

3:00 PM [SW396] Synthesis, characterization, and photothermal effect of CuS nanoparticles deposited on MXene. **Presented by: Gururaj Neelgund**

3:20 PM Coffee Break.

3:40 PM [SW397] Bismuth vanadate-based photoanodes for photoelectrosynthetic biomass conversion. **Presented by: Ben Sherman**

4:10 PM [SW398] Electrocatalytic and magnetic properties of porous iron phosphide nanorods. **Presented by: Yolanda Vasquez**

4:30 PM [SW399] Withdrawn

4:50 PM [SW400] Synthesis and phase evolution of MAX phases to multimetal MNenes. **Presented by: Abdoulaye Djire**

Hyperpolarized Magnetic Resonance - from Chemistry and Applications

Session Type: Oral

Time: 2:00 PM - 5:45 PM

Location: Texas B

Magnetic resonance is a versatile method that has driven various research fields in analytical chemistry, structure determination of proteins and even biomedical imaging. Hyperpolarization is an approach that overcomes the sensitivity limitations of magnetic resonance and amplifies signals by orders of magnitude. This enables to study chemical and biochemical questions in unprecedented ways. We are proposing to bring the hyperpolarization community together as part of the regional meeting and hold three sessions on the topics of hyperpolarization method development, developing molecular probes and imaging and studying biomolecules. The ACS meeting will serve as an ideal platform to inform and discuss developments in the field with a general chemistry oriented audience that can benefit from hyperpolarization approaches. The Dallas Fort Worth area has a particular large hyperpolarization community from which we can expect high attendance.

Organizer(s): Kendra Frederick, Stefan Gloeggler, Mai Huynh

Presider(s): Kendra Frederick, Stefan Gloeggler, Mai Huynh

Presentations:

2:00 PM [SW401] High frequency dynamic nuclear polarization in rotating solids. **Presented by: Robert G. Griffin**

2:20 PM [SW402] Mapping protein hydration and exchange dynamics by cross-polarization from hyperpolarized water. **Presented by: Olivia Chatterjee**

2:35 PM [SW403] Studying hydrogen-bound states of hydrogenases under turnover conditions by parahydrogen-enhanced NMR. **Presented by: Julius Frederik Frederik Matz**

2:50 PM [SW404] High-field liquid-state Overhauser DNP: From sub-picosecond dynamics to high-resolution spectroscopy. **Presented by: Tomas Orlando**

3:05 PM [SW405] Characterization of nitroxides multi-radicals and their effects on DNP enhancement. **Presented by: Emmanuel Ameh**

3:20 PM [SW406] Developing HP 15N-MRI probes targeting aberrant metabolism for cancers. **Presented by: Qiu Wang**

3:35 PM Intermission.

4:05 PM [SW407] Low-field NMR with sensitivity enhancement by parahydrogen and applications in chemistry and biochemistry. **Presented by: Christian Hilty**

4:25 PM [SW408] Hyperpolarized magnetic resonance at low magnetic fields enables assessment of drug-protein binding *in vivo*. **Presented by: Charlotte von Petersdorff-Campen**

4:40 PM [SW409] Parahydrogen hyperpolarization with a reusable MOF catalyst: Applications in ligand binding. **Presented by: Ashes Roy**

4:55 PM [SW410] Revealing hyperpolarized 2-methylsuccinic acid for dual applications: Anti-bacterial drug discovery and renewable feedstocks. **Presented by: Quy Son Luu**

5:10 PM [SW411] Leveraging millitesla SABRE dynamics to hyperpolarize ^{13}C in proximity to quadrupolar ^{14}N. **Presented by: Loren Smith**

5:25 PM [SW412] Synthesis and application bench-stable, mildly-reducible cobalt catalysts for PHIP. **Presented by: Brennan McCoy Vaught**

5:40 PM Closing Remarks.

Lessons and Inspiration from the Past

Session Type: Oral

Time: 2:00 PM - 5:55 PM

Location: Citizens B

Organizer(s): Nicolay V Tsarevsky

Presider(s): Christine Hahn

Presentations:

2:00 PM Opening Remarks.

2:05 PM [SW413] Holleman, Wiberg, and a textbook of inorganic chemistry that has lasted more than a century. **Presented by: Christine Hahn**

2:40 PM [SW414] Facts, ideas, and words: Lavoisier's lesson on chemistry communication. **Presented by: Eszter Trufan**

3:15 PM [SW415] Pioneers of chemical nomenclature: Torbern Bergman, his predecessors, and his followers. **Presented by: Nicolay V Tsarevsky**

3:50 PM Intermission.

4:10 PM [SW416] Determination of magnesium levels in natural waters by conductometric titration. **Presented by: Linda Dalquest Schultz**

4:45 PM [SW417] From chemistry to iconic scents: The history of perfumes built on aldehydes, lactones, and damascones. **Presented by: Mihaela C Stefan**

5:20 PM [SW418] Elemental rhymes and tunes: Using poetry and music to convey chemical ideas. **Presented by: Nicolay V Tsarevsky**

Organic and Chemical Biology Young Investigator Symposium

Session Type: Oral

Time: 2:00 PM - 6:00 PM

Location: Texas C

This symposium will highlight assistant professors in organic and chemical biology from throughout the Southwest.

Organizer(s): Kami Hull, Uttam K Tambar

Presider(s): Kami Hull, Uttam K Tambar

Presentations:

2:00 PM [SW419] Toward predictive organic chemical physics: From automated quantum chemistry and machine learning to fundamental reactivity. **Presented by: Alistair Sterling**

2:30 PM [SW420] Integrated platform for experimental discovery and predictive modeling of electron donor–acceptor complexes. **Presented by: Jacquelyne Read**

3:00 PM [SW421] Mechanism-driven advances in synthetic organic chemistry. **Presented by: Connor Patrick Delaney**

3:30 PM Intermission.

4:00 PM [SW422] Photocatalytic C–F functionalization: Mechanism and methodology. **Presented by: Dennis Chung-Yang Huang**

4:30 PM [SW423] Biocatalytic oxa-Pictet-Spengler reactions. **Presented by: David C. Miller**

5:00 PM [SW424] Bifunctional boron/phosphorus organocatalysts for amide bond formation. **Presented by: Christopher Sandford**

5:30 PM [SW425] Cross-coupling of abundant C(sp3) electrophiles by first-row transition metal catalysts. **Presented by: Reginald Mills**

Polymers and Sustainability Challenges

Session Type: Oral

Time: 2:00 PM - 6:05 PM

Location: Texas D

The goal of Polymer and Sustainability Challenges symposium is to emphasize the pivotal role of polymers in confronting sustainability challenges and to explore methods of engineering and design that enable these materials to effectively tackle such issues. This symposium will cover the spectrum of research on bio-based polymers, biodegradability, and polymers aimed at mitigating the carbon footprint across various processes and industrial applications.

Organizer(s): Reza Foudazi

Presider(s): Reza Foudazi

Presentations:

2:00 PM Opening Remarks.

2:05 PM [SW426] Decoding molecular mechanisms underpinning helium separation using halogenated polymer blends. **Presented by: Michele Galizia**

2:30 PM [SW427] Lanthanide-based optical unclonable anticounterfeit features embedded in additively manufactured polymer parts. **Presented by: Kyungtae Kim**

2:55 PM [SW428] Oxidation-mediated pathways for upcycling legacy plastics into value-added chemicals. **Presented by: Hyunjin Moon**

3:20 PM [SW429] Probing the influence of fixed charge chemistry on selective ion transport in cation exchange membranes. **Presented by: Everett Zofchak**

3:45 PM [SW430] Cellulose biomass sustainability through cellulose fiber reproduction. **Presented by: Jonathan Chen**

4:10 PM Intermission.

4:25 PM [SW431] Sugar, polyphenolic, and catechol motifs for polymeric materials. **Presented by: Samantha L Kristufek**

4:50 PM [SW432] Growing the future of sustainable materials with multifunctional bacterial cellulose. **Presented by: Muhammad Rahman**

5:15 PM [SW433] Elasticity dominated surface segregation in formulated products. **Presented by: Buddhapriya Chakrabarti**

5:40 PM [SW434] Polymerized lyotropic liquid crystal membranes for monoclonal antibody concentration. **Presented by: Shirin Tahazadeh**

6:00 PM Closing Remarks.

Tuesday Afternoon Coffee Break

Session Type: Coffee Break

Time: 3:30 PM - 4:30 PM

Location: Crystal C/D

ACS Governance Reception

Session Type: Networking Event

Time: 5:00 PM - 6:30 PM

Location: Crystal A

Elemental Rhymes and Tunes: Chemistry in Poetry and Music

Session Type: Special Event

Time: 6:30 PM - 7:30 PM

Location: Crystal B

Poems about the elements and their history by Atto Rex Vincent, read by the author. With music by Christine Hahn and Emmeline Miles, performed by The Savon Duo (Yvon Arseneault on cello and Sam Domzella on piano) and Emmeline Miles (piano, guitar, and voice).

Advancing Sustainable, Safer, and Responsible Chemistry: Innovations in Research & Teaching

Session Type: Poster

Time: 8:00 PM - 10:00 PM

Location: Crystal C/D

Advances in sustainable, safe, resource-efficient and responsible chemistry are essential to transforming how we conduct research, educate future scientists, and address global challenges in energy, advanced materials, environmental remediation, and human health. This symposium highlights these core values as guiding principles in modern chemical research, innovative teaching, and interdisciplinary collaboration. Ultimately, it showcases how these principles drive scientific discovery, curriculum development, and workforce preparation for a more sustainable future.

Organizer(s): John D. Beatty, Ting Han, Shiru Lin, Nasrin Mirsaleh-Kohan, Manal Rawashdeh-Omary

Presentations:

8:00 PM [SW435] Development of an interpretable machine learning framework for food additive toxicity prediction. **Presented by: Sara Castillo**

8:00 PM [SW436] Surrogate reference standards for RP-HPLC quantification of paracetamol: Influence of structural variability on assay values. **Presented by: Japhat Opoku Ofosu**

8:00 PM [SW437] First-principles computational investigation of structural characteristics, electronic properties, and interactive coupling behavior of 12-5-12 cationic gemini surfactant. **Presented by: Saima Tabassum Bristi**

8:00 PM [SW438] Chirality-induced spectral changes in multi-walled carbon nanotubes: Computational and experimental analysis. **Presented by: Maya Schwickert**

8:00 PM [SW439] Withdrawn

8:00 PM [SW440] Octa- and tetra- Heck reaction, a novel porphyrin synthesis. **Presented by: Nicholas Starrett**

8:00 PM [SW441] Novel metalated porphyrin synthesis: Tuning photochemical properties for functionality. **Presented by: Ireland LaBass**

8:00 PM [SW442] Development and characterization of BSA-functionalized PNVCL particles with tunable thermoresponsive behavior for biomedical applications. **Presented by: Gabriel ReCalderon**

8:00 PM [SW443] Investigation of newly synthesized Cu(I) complex interactions with deoxyguanosine monophosphate as a model for copper and DNA interactions. **Presented by: Jose Eduardo Paniagua**

8:00 PM [SW444] Learning biochemistry: Student challenges and strategies for success. **Presented by: Natalie Caracena**, **Rafaela Dominguez**

8:00 PM [SW445] Integrating competency based assessment and sustainable practices into hands-on separation methods instruction. **Presented by: John D. Beatty**

8:00 PM [SW446] Discovery of selective factor XIa inhibitors as potential anticoagulant agents. **Presented by: Catherine Ortiz**, **Savannah Bryant**, **Simran Pereira**

8:00 PM [SW447] Switching luminescence through solvent effects and mechanochemistry in copper(I) chloride–niacinamide complexes. **Presented by: Manal Rawashdeh-Omary**

8:00 PM [SW448] Mixed-ligand design of sustainable luminescent Cu(I) halide complexes: Synthetic control of structure and photophysical properties. **Presented by: Manal Rawashdeh-Omary**

8:00 PM [SW449] Automating and standardizing green microplastic extraction from terrestrial soil matrices. **Presented by: Jay Payne**

8:00 PM [SW450] Target-responsive nanointerfaces for amplified optical and electrochemical biosensing. **Presented by: Sicheng Wang**

8:00 PM [SW451] Enhancing ionic conductivity and electrochemical stability of zinc-ion batteries via optimized PAM hydrogel matrix. **Presented by: Chaekyung Kim**

8:00 PM [SW452] Get involved with the ACS Division of Chemical Education. **Presented by: Alena Moon**

8:00 PM [SW453] Design, synthesis, and characterization of functional Zr(IV) and Eu(III) macrocycle-based metal–organic frameworks for sensing applications. **Presented by: Habiba Abigail Ouattara Kouadio**

8:00 PM [SW454] Biocompatible polymer–gold nanoparticle composites for photothermal therapy and controlled drug delivery. **Presented by: Anna Ilundu**

Colloids, Surfactants and Interfaces

Session Type: Poster

Time: 8:00 PM - 10:00 PM

Location: Crystal C/D

This symposium will accept papers in all areas of colloids, surfactants and interfaces. Topics include surfactant, block copolymer, lipid and other amphiphilic materials and their self-assembly, emulsions, foams, dispersions, interfacial phenomena including wetting, adhesion, colloidal glasses and gels, and colloidal and interfacial phenomena of interest to biological, environmental, material and medical technologies not covered by any of the thematic symposia.

Organizer(s): Reza Foudazi

Presentations:

8:00 PM [SW845] Study of cationic micelle-mediated reaction of small aromatic molecules using MD simulations. **Presented by: Archana Mishra**

8:00 PM [SW846] Impacts of brown carbon deposition from wildfires on solar cell performance. **Presented by: Tasnim Mahzabin Tanha**

8:00 PM [SW847] Deep-UV fluorescence of ethers: Mechanisms, characterization, and high-sensitivity liquid chromatography detection. **Presented by: Alanah Junge**

8:00 PM [SW848] Nanoscale confinement, fusion–fission dynamics, and ice nucleation in reverse micelles. **Presented by: Romana Akter Shathy**

8:00 PM [SW849] Investigating how charge influences the spontaneous formation of hydrogen peroxide in electrospray and suspended water microdroplets. **Presented by: Emery Hamilton**

8:00 PM [SW850] Tuning proton donor molecular architecture to control interfacial microenvironment for enhanced nonaqueous electrochemical CO_2 reduction. **Presented by: Asitha Gihan Aberathna Ariyathunga Pathiranage**

8:00 PM [SW851] Optimizing high throughput formulation of lipid nanoparticles with robotic liquid handlers. **Presented by: Pavan Ramesha**

8:00 PM [SW852] Probing bubble nucleation with microporous materials. **Presented by: Andrei Ocampo Santos**

8:00 PM [SW853] Machine-learning-guided size control in the thermal decomposition synthesis of iron oxide nanoparticles. **Presented by: Md Yeasin Kabir**

8:00 PM [SW854] Development of a droplet counter system for ultra-low flow-rate measurement. **Presented by: Nur Jafira Akhter Chowdhury**

Functional Solid State Materials

Session Type: Poster

Time: 8:00 PM - 10:00 PM

Location: Crystal C/D

This symposium brings together chemists to advance the frontiers of solid-state chemistry, with an emphasis on the experimental and computational discovery and design of new functional materials for energy and sustainability applications. The scope encompasses the synthesis of novel inorganic, hybrid, and complex solid-state materials, alongside the determination and analysis of crystal structures using modern diffraction and spectroscopic techniques. One of the central objectives is to explore the mechanistic underpinnings of solid-state reactions from thermodynamic driving forces to kinetic pathways and phase transformations. Equally important is elucidating structure property relationships that govern the behavior of solid-state materials in applications such as energy storage and conversion, thermoelectrics, photocatalysis, ionic conductors, and sustainable chemical processes.

Organizer(s): Shruti Hariyani, Tianyu Li

Presentations:

8:00 PM [SW455] Isomorphous series of lanthanide adipate 2-bromoterephthalate coordination polymers, $Ln_2(Adip)(TPBr)_2(H_2O)_2$. **Presented by: Vinson Ratcliffgardy**, **Megan Walsh**, **Sophia Nguyen**

8:00 PM [SW456] Switching emission pathways via molecular engineering in hybrid metal halides for scintillation and neutron detection. **Presented by: Muhammad Sani Muhammad**

8:00 PM [SW457] Unveiling the factors governing structural evolution in entropy-stabilized cation-disordered Li_2TiO_3. **Presented by: Wolalorm Makafui Zudor**

8:00 PM [SW458] Elucidating mechanisms of chirality transfer in circularly polarized luminescent phosphors. **Presented by: Victor Caycedo**

8:00 PM [SW459] Synthesis of low-dimensional metal tellurides from boron-mediated flux mixtures. **Presented by: Chirantha Pramod Edirisinghe**

8:00 PM [SW460] How incorporating Zn into $Sn_2Nb_2O_7$ affects structure and properties for pigment applications. **Presented by: Mariah Carrillo**

8:00 PM [SW461] Rare earth metal (Ce and Pr) doped lanthanum cuprate (La_2CuO_4) aerogel based composite for hybrid supercapacitor application. **Presented by: S M ANYET ULLAH SHOHAG**

8:00 PM [SW462] Exploring multimetal coordination in salophene-based complexes. **Presented by: Tanzim Ahsan**

8:00 PM [SW463] Frustrated Lewis pair-functionalized PCN-333(Cr) for enhanced hydrogen binding and storage at ambient temperature. **Presented by: Roknuzzaman Roknuzzaman**

8:00 PM [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. **Presented by: Kyle McCall**

8:00 PM [SW465] Isomorphous series of lanthanide pimelate 2-bromoterephthalate coordination polymers, $Ln_2(pim)_2(TPBr)(H_2O)_2$. **Presented by: Chanvisal Tith**, **Evan Hernandez**, **Stephen Hale**

8:00 PM [SW466] Synthesis, crystal structure and optical properties of $(CH_3)_2(C_6H_5)_2PCu_2I_3$. **Presented by: SHAK ABIR HOSSAIN**

8:00 PM [SW467] Synthesis, structural diversity, and optical properties of a series of hybrid organic-inorganic copper(I) bromides. **Presented by: Tamanna Akhter Pinky**

8:00 PM [SW468] Withdrawn

8:00 PM [SW469] Exploring the structural and functional properties of a novel category of hybrid double metal halide perovskites. **Presented by: Kanika Parashar**

8:00 PM [SW470] Degradation and fouling of anion-exchange membranes in a semi-pilot MEC treating fermented food waste. **Presented by: Minsu Noh**

8:00 PM [SW471] Effects of a NiO coating on FTO|WO_3-$BiVO_4$ photoanodes for TEMPO mediated conversion of HMF to DFF. **Presented by: Md Lutfor Rahman**

8:00 PM [SW472] Layered Na-ion cathodes in minutes: Microwave synthesis as a platform for phase and composition control. **Presented by: Matthew Wright**

8:00 PM [SW473] Engineering thermal transport in multifunctional liquid crystal elastomers via sequential infiltration synthesis. **Presented by: Akhila Joy**

8:00 PM [SW474] Effects of Fe-doping on surface polarity, morphology, and antibacterial action in microscale ZnO. **Presented by: John Hunter Brannon**

8:00 PM [SW475] Polyphosphazene based solid state electrolyte for Li-ion batteries. **Presented by: Mayank Tiwari**

New Instrumentation and Methods of Analysis

Session Type: Poster

Time: 8:00 PM - 10:00 PM

Location: Crystal C/D

Invited and open call for new and emerging analytical instrumentation, automated sample processing, and data analysis including artificial intelligence that solve critical problems in environmental, industrial, and health related applications. Advances in spectroscopic, electrochemical, and mass spectrometric detection and and separation technologies are encouraged. The application of computational tools such as

machine learning and artificial intelligence for analyte detection, deconvolution, sample preparation and separations optimization, etc. are welcome.

Organizer(s): Charles Phillip Shelor

Presentations:

8:00 PM [SW476] Electrochemistry in air: Coupled electron and phase transfer at three-phase interfaces enabled by electric-field spillover. **Presented by: Kenta Kawashima**

8:00 PM [SW477] Occurrence and quantitation of perfluoroalkyl substances (PFAS) in wastewater samples from an activated wastewater treatment plant in Deep East Texas (USA). **Presented by: Kefa K Onchoke**

8:00 PM [SW478] Withdrawn

8:00 PM [SW479] Abraham solvation parameter model: Experiment based solute descriptor values for potential medicinal candidates, dietary healthcare supplements and pharmaceutical formulation ingredients. **Presented by: Chelsi Wilson**

8:00 PM [SW480] Hydrophilic interaction chromatography coupled with evaporative light scattering detection for inorganic cations and anions. **Presented by: Reza Salehi**

8:00 PM [SW481] Simple salt assisted liquid-liquid extraction method for analysis of poly- and perfluoroalkyl substances in meconium. **Presented by: Chimauchem Valentine Odinaka**

8:00 PM [SW482] Flow-through fluorescence detection of fluoride using the zirconium–calcein blue system. **Presented by: Pranta Acharjee**

8:00 PM [SW483] Simultaneous deep-UV fluorescence and high-dynamic-range absorbance detection in a liquid-core waveguide flow cell. **Presented by: Charles Phillip Shelor**

8:00 PM [SW484] Exploring the spectrochemical behavior of derivatized amino acids for HPLC-fluorescence detection. **Presented by: Sakil Islam**

8:00 PM [SW485] Identifying and eliminating systematic errors in laboratory gas permeability and non-Darcy flow measurements. **Presented by: Deborah Oluwatosin Rufus**, **Mashhad Fahes**

8:00 PM [SW486] Withdrawn

8:00 PM [SW487] Micro solid phase extraction-liquid chromatography tandem mass spectrometry strategy for evaluating subcutaneous enzyme replacement therapy in Fabry disease. **Presented by: Sabrina Islam**

8:00 PM [SW488] Evaluating column selectivity for forensic applications: A comparison of diphenyl, C18/AR, and C12 phases using liquid chromatography-mass spectrometry. **Presented by: Kei Osawa**

8:00 PM [SW489] PFAS screening by real-time tandem mass spectrometry. **Presented by: Raghvendra Sengar**

8:00 PM [SW490] Novel triple quad approaches for sensitive quantification of 1000 compounds in single runs. **Presented by: Raghvendra Sengar**, **Artem Filipenko**

Polymers and Sustainability Challenges

Session Type: Poster

Time: 8:00 PM - 10:00 PM

Location: Crystal C/D

The goal of "Polymer and Sustainability Challenges" symposium is to emphasize the pivotal role of polymers in confronting sustainability challenges and to explore methods of engineering and design that enable these materials to effectively tackle such issues. This symposium will cover the spectrum of research on bio-

based polymers, biodegradability, and polymers aimed at mitigating the carbon footprint across various processes and industrial applications.

Organizer(s): Reza Foudazi

Presentations:

8:00 PM [SW491] Selective oxidation of ethylene–vinyl alcohol facilitates multilayer plastic film recycling. **Presented by: Mohammad Reza Razzaghi**

8:00 PM [SW492] Lyotropic liquid crystal templated ultrafiltration membranes for virus removal in mAb purification. **Presented by: Mostafa Tabatabaei**

8:00 PM [SW493] Polymerization of Frank-Kasper A15 phase formed by Pluronic P105-diacrylate and ethylammonium nitrate mixtures. **Presented by: Shirin Tahazadeh**

8:00 PM [SW494] Study of the segmental dynamics in PEO-based polymer electrolytes using quasi-elastic neutron scattering. **Presented by: Pattuwe AALD Pattuwearachchi**

Supramolecular Chemistry and Functional Molecular Materials

Session Type: Poster

Time: 8:00 PM - 10:00 PM

Location: Crystal C/D

This symposium will bring together researchers developing supramolecular systems that enable new functions through molecular recognition, self-assembly, and noncovalent interactions. Presentations will span macrocyclic chemistry, host□guest systems, supramolecular polymers, crystal engineering, charge-transfer materials, molecular machines, biomolecular assemblies, and functional organic materials for applications in energy, sustainability, catalysis, sensing, and biomedicine. The symposium seeks to promote interactions across traditionally separate research areas while highlighting emerging directions in functional supramolecular materials.

Organizer(s): Yuanning Feng

Presentations:

8:00 PM [SW495] Minimalist peptide assemblies as metal-free catalysts for esterase activity. **Presented by: Shams Aaghaz**

8:00 PM [SW496] Polydiacetylene-based colorimetric detection of PFAS. **Presented by: Nicholas Payne**

8:00 PM [SW497] Deep ultraviolet fluorescence detection using liquid core waveguide flow cells. **Presented by: ANIKA HAIDER**

8:00 PM [SW498] Symmetric azobenzene photoswitches in multiple solvents. **Presented by: Nicole Litvak**

8:00 PM [SW499] 1,2-dioxetane probe for imaging of select reactive oxygen species. **Presented by: Caleb Griffin**

8:00 PM [SW500] Cucurbit[6]uril-β-cyclodextrin PEG-based polyrotaxanes and interlocked slide-ring materials. **Presented by: Aunindya Jyoti**

8:00 PM [SW501] Programming multidomain peptides with molecular frustration into biomolecular condensates. **Presented by: Debdatta Das**

8:00 PM [SW502] pH-sensitive peptide nanofibers and: Innovations in self-assembling peptides with ionizable non-coacervatesn-natural amino acids. **Presented by: Jenny Nguyen**

8:00 PM [SW503] Optimizing DNA-barcoded peptides for the detection of disease-relevant proteases. **Presented by: Gabriel Pohlman**

8:00 PM [SW504] Mechanochemical synthesis and co-former-controlled assembly of azobenzene polycarboxylate organic salts: From framework node to passive guest in HOF-like architectures. **Presented by: JYOTISHKA NATH**

8:00 PM [SW505] Synthesis and characterization of mixed-ratio bis-urea organogelator systems. **Presented by: Andrew J Carr**

8:00 PM [SW506] Synthesis and characterization of 2,5-dihydroxytereohthaldehyde derived organogelators. **Presented by: Andrew J Carr**

8:00 PM [SW507] Synthesis and characterization of quinoline-based ligands for metalorganic gelators. **Presented by: Andrew J Carr**

Wednesday, November 18, 2026

Registration

Session Type: Registration

Time: 7:00 AM - 7:00 PM

Location: Promenade

Badge pick-up and onsite registration.

Biotechnology Innovations at the Chemistry-Biology Interface

Session Type: Oral

Time: 8:00 AM - 10:35 AM

Location: Continental

The proposed symposium is expected to cover the recent development of biotechnologies with chemical biology emphasis, covering new approaches in diagnostics and therapeutics.

Organizer(s): Ziwen Jiang

Presider(s): Ziwen Jiang

Presentations:

8:00 AM [SW508] Structure-based design of alpha-helix mimetics for inhibiting protein-protein interactions and treating cancers. **Presented by: Jung-Mo Ahn**

8:20 AM [SW509] Phagophore-associated protein-inspired antibody-fusion degraders for targeted clearance of intracellular protein aggregates. **Presented by: Tianqi Wang**

8:32 AM [SW510] SuFEx-enabled tyrosine specific bioconjugation of near-infrared fluorophores. **Presented by: Syed Usama**

8:52 AM [SW511] Withdrawn

9:04 AM Intermission.

9:19 AM [SW512] Killing time: Rapid kinetic profiling for antiparasitic drug discovery. **Presented by: Brad Anthony Haubrich**

9:39 AM [SW513] Light-triggered decoding of hydrophobic interactions in living systems. **Presented by: Peng Ji**

9:51 AM [SW514] Quantitative evaluation of bacterial binding affinity of self-bacterial panning-derived silver nanoparticles using Kd analysis. **Presented by: James Cho**

10:11 AM [SW515] Pulsed blue light as a potential approach for modulating *Lactobacillus* survival and bacterial-host interactions. **Presented by: Violet Bumah**

Computational Chemistry In Action

Session Type: Oral

Time: 8:00 AM - 11:15 AM

Location: Citizens B

Real-world chemical applications of molecular simulation, AI, machine learning, and related computational tools. The symposium welcomes work from experimental groups incorporating computation and computational groups developing tools for nonspecialists.

Organizer(s): Donatus Atsu Atsu Agbaglo, Muhammad Hammad Ali, Benjamin G Janesko

Presider(s): Donatus Atsu Atsu Agbaglo, Muhammad Hammad Ali, Benjamin G Janesko

Presentations:

8:00 AM [SW516] Probing alternative reaction pathways in complex condensed-phase systems via first-principles machine-learning force fields. **Presented by: Deepa Ranabhat**

8:25 AM [SW518] Computational prediction of solvent-dependent NMR chemical shifts in flexible macrocycles. **Presented by: Kien Tran**

8:50 AM [SW519] GauOpen: An interfacing toolkit. **Presented by: Edward N Brothers**

9:15 AM Intermission.

9:35 AM [SW520] Accurate and time-efficient condensed-phase free energy simulations with reaction-specific delta-machine learning potentials in CHARMM. **Presented by: Saroj Kumar Panda**

10:00 AM [SW521] Discovery of a novel KEAP1 inhibitor screened via a virtual screening workflow and validated biologically. **Presented by: Nitish Kumar**

10:25 AM [SW522] Exploring chameleonicity of PROTACs via atomistic simulation. **Presented by: Kabita Sharma**

10:50 AM [SW523] Design and insight into the photophysics of photochromic dyes: A DFT and ML study. **Presented by: Juganta Kumar Roy**

Emerging Trends in Synthetic Inorganic Chemistry

Session Type: Oral

Time: 8:00 AM - 12:00 PM

Location: Texas A

Contributions covering transition-metal, main-group, coordination, organometallic compounds, and cluster chemistry along with interdisciplinary research at the interface of inorganic chemistry and related fields, are welcome. This symposium will showcase recent progress in the preparation and study of molecular and materials-based inorganic systems with relevance to catalysis, electronic materials, energy conversion, environmental chemistry, and chemical transformations.

Organizer(s): MANJUR OYASIM AKRAM, Anindita Das

Presider(s): MANJUR OYASIM AKRAM, Anindita Das

Presentations:

8:00 AM [SW524] Pyridinium-derived carbene ligands in nickel-catalyzed carbon–heteroatom coupling. **Presented by: William George Whitehurst**

8:20 AM [SW525] Highly Lewis acidic main group cations partnered with carborane anions as catalysts for hydrodefluorination of PFAS. **Presented by: Oleg Ozerov**

8:40 AM [SW526] Exploring ligand noninnocence towards s-block-mediated hydrofunctionalization. **Presented by: Samantha Yruegas**

9:00 AM [SW527] Fascinating chemistry of coinage metal ions supported by fluorinated *N*-heterocycles. **Presented by: Rasika Dias**

9:20 AM [SW528] Design and synthesis of multifunctional tetra-aza macrocycles for antioxidant and redox applications. **Presented by: Kayla N Green**

9:40 AM Intermission.

10:00 AM [SW529] Carborane substituted boron compounds. **Presented by: Caleb Martin**

10:20 AM [SW530] Withdrawn

10:40 AM [SW531] Alkyl/aryl phosphido ligands as tunable bridging ligands for controlling dipolar coupling interactions in Ln-cluster single-molecule magnets. **Presented by: Trevor Latendresse**

11:00 AM [SW532] Photochemical reactivity trends of early transition metal oxos for sustainable oxidation catalysis. **Presented by: Matthew Burke Chambers**

11:20 AM [SW533] Molecular design for uranyl coordination and reactivity. **Presented by: Anne Elizabeth Vivian Gorden**

11:40 AM [SW534] Diarylselenides potentiated by carbenium functionalities: Synthesis, reactivity and catalytic studies. **Presented by: Arkamitra Roy**

General Organic Chemistry

Session Type: Oral

Time: 8:00 AM - 11:30 AM

Location: Crystal B

This symposium will provide a general platform for researchers working across all areas of organic chemistry to present their latest advances. Topics may include, but are not limited to, synthetic methodology, catalysis, physical organic chemistry, mechanistic studies, chemical biology, organometallic chemistry, and natural product synthesis. The symposium aims to highlight innovative approaches, emerging technologies, and interdisciplinary applications that are shaping the future of organic chemistry.

Organizer(s): Jeremiah J Gassensmith

Presider(s): Jeremiah J Gassensmith

Presentations:

8:00 AM [SW535] Withdrawn

8:25 AM [SW536] Withdrawn

8:39 AM [SW537] Synthesis and evaluation of a carbapenem C8 diastereomer with standalone activity against KPC-producing Enterobacterales. **Presented by: Md Mahbub Kabir Khan**

8:53 AM [SW538] Dual catalytic and convergent approach to δ- and γ-lactones via photo- and lutidinium-catalysis. **Presented by: Parul Sharma**

9:07 AM [SW539] Enantioselective *N*-heteroaryl C–H functionalization for piperidine–azine conjugation via dearomative addition–hydrogen auto-transfer. **Presented by: Seoyoung Lee**

9:21 AM [SW540] Photophysical investigation of BODIPY molecular systems promoting aggregation-induced emission. **Presented by: Snigdha Dutta**

9:35 AM [SW541] Investigation of cobalt complexes for visible-light-driven radical reactions: Insights from axial and square planar ligand variation. **Presented by: Subrata Pal**

9:49 AM [SW542] Radical and photochemical amination of polymers and small molecules. **Presented by: Robert Comito**

10:14 AM [SW543] Highly stereoselective olefin cyclopropanation via enzyme-catalyzed reductive activation of *gem*-dibromoalkanes. **Presented by: Aakash Pal**

10:28 AM [SW544] Withdrawn

10:42 AM [SW545] Synthesis of fluorosulfonyl aziridines and β-lactams from alkenes as multifunctional hubs. **Presented by: Varun Prabhakar**

10:56 AM [SW546] Withdrawn

11:10 AM [SW547] Cooperative non-covalent rigidification for enantioselective and regioselective C–H hydroarylation via chiral transient directing groups. **Presented by: Weinan Tan**

Make It Make Sense: Innovative Teaching Practices

Session Type: Oral

Time: 8:00 AM - 11:00 AM

Location: Texas C

This symposium explores a range of pedagogical innovations including active learning, integration of digital tools, laboratory redesigns, and assessment strategies that support student success. The use of learning assistants and peer-led team learning programs that improve performance, increase retention, and foster belongingness will also be highlighted. This session specifically focuses on actionable ideas and practical instructional experience in the classroom.

Organizer(s): Amandeep Sra, Michele Stover

Presider(s): Amandeep Sra, Michele Stover

Presentations:

8:00 AM [SW548] Academic celebrations and digital portfolios: Alternative assessment strategies for scientific literacy in inorganic chemistry. **Presented by: Julia Chan**

8:20 AM [SW549] Bridging the gap between chemical education research and classroom practice. **Presented by: Stephen Gerald Prilliman**

8:40 AM [SW550] Focus on successful students in general chemistry. **Presented by: Diana Sue Mason**

9:00 AM [SW551] Using language mindfully to effectively assess students' learning. **Presented by: Stephanie M Taylor**

9:20 AM Intermission.

9:40 AM [SW552] Teaching organic chemical nomenclature through an educational game. **Presented by: Celyna Rackov**

10:00 AM [SW553] Teaching thermodynamics; a journey of pedagogical partnership. **Presented by: Mashhad Fahes**

10:20 AM [SW554] Memes, molecules, and mechanisms: Making organic chemistry click. **Presented by: Roxane Jourdain**

10:40 AM [SW555] Flesh-eating flies, fake tequila, radioactive rhinoceri, and conflict-affected critical minerals: Exploring new topics and ways to teach 21st century chemistry. **Presented by: Scott Joseph Donnelly**

Materials Chemistry: Emerging Contaminant Remediation in Impacted Environments

Session Type: Oral

Time: 8:00 AM - 12:00 PM

Location: Texas D

Invited and open call for oral and poster presentations highlighting recent advances in materials chemistry focused on the discovery, design, and characterization of materials for the remediation of emerging contaminants in impacted environments.

Organizer(s): Shengqian Ma, Mario Wriedt

Presider(s): Shengqian Ma, Mario Wriedt

Presentations:

8:00 AM Opening Remarks.

8:05 AM [SW556] Cobalt tritolycarboxyl porphyrin-carbon black composite as a bifunctional electrocatalyst for NO_3RR and CO_2RR. **Presented by: Kamal Dhakal**

8:35 AM [SW557] Selective ammonia synthesis via electrocatalytic nitrate reduction reaction using chalcogenide vacancy engineered transition metal dichalcogenides. **Presented by: Piumi Kularathne**

9:05 AM [SW558] Withdrawn

9:35 AM [SW559] Computational study of pesticide capture by metal-organic frameworks. **Presented by: Lauryn Guzman**

10:05 AM Networking Break.

10:25 AM [SW560] Fluorescent carbon dots sensing for PFAS and PFOS detection and removal through integrated membrane filtration. **Presented by: SUNITH BABU MADDURI**

10:55 AM [SW561] Anaerobic digestion–assisted hybrid ceramic membrane filtration for microplastic and nanoplastic removal. **Presented by: PRASHAN RODRIGO**

11:25 AM [SW562] Fluorescent NU-1000 metal–organic framework for sensitive PFAS detection and environmental water monitoring. **Presented by: Nafees Iqbal**

11:55 AM Closing Remarks.

Supramolecular Chemistry and Functional Molecular Materials

Session Type: Oral

Time: 8:00 AM - 12:00 PM

Location: Texas B

This symposium will bring together researchers developing supramolecular systems that enable new functions through molecular recognition, self-assembly, and noncovalent interactions. Presentations will span macrocyclic chemistry, host□guest systems, supramolecular polymers, crystal engineering, charge-transfer materials, molecular machines, biomolecular assemblies, and functional organic materials for applications in energy, sustainability, catalysis, sensing, and biomedicine. The symposium seeks to promote interactions across traditionally separate research areas while highlighting emerging directions in functional supramolecular materials.

Organizer(s): Yuanning Feng

Presider(s): Yuanning Feng

Presentations:

8:00 AM [SW563] Augmenting DNA nanotechnology using synthetic macrocycles. **Presented by: Janarthanan Jayawickramarajah**

8:20 AM [SW564] Single-molecule DNA–peptide nanostructures for protease activity detection. **Presented by: Imon Kanta Phukan**

8:40 AM [SW565] Sequence encoded molecular interactions in peptide biomolecular condensates revealed by NMR, Raman and FT-IR spectroscopy. **Presented by: Navneet Sahoo**

9:00 AM [SW566] Withdrawn

9:20 AM [SW567] Withdrawn

9:40 AM [SW568] Non-covalent interactions in chemosensor design for molecular recognition. **Presented by: Rashid Mia**

10:00 AM Coffee Break.

10:20 AM [SW569] Design and application of porous porphyrin-derivative frameworks. **Presented by: Shengqian Ma**

10:40 AM [SW570] Can porous structures be constructed without interactions between building blocks. **Presented by: Ognjen Miljanic**

11:00 AM [SW571] Directed hydrogen bonding for stabilizing mesoporous covalent organic frameworks. **Presented by: Ronald Smaldone**

11:20 AM [SW572] Coordinative-inclusion of pyridine molecules within hydrogen-bonded metal-organic frameworks (HBMOFs). **Presented by: Greg A. Hogan**

11:40 AM [SW573] Intrinsic chirality in organic-inorganic hybrid materials. **Presented by: Daniel B. Straus**

SWRM Wellness Room

Session Type: Wellness

Time: 8:00 AM - 6:00 PM

Location: Keystone Room

Exposition

Session Type: Expo

Time: 9:00 AM - 5:00 PM

Location: Crystal C/D

Wednesday Morning Coffee Break

Session Type: Coffee Break

Time: 9:30 AM - 10:30 AM

Location: Crystal C/D

ACS Career Workshop – Acing the Interview: Setting Yourself Up for Success in an Interview

Session Type: Workshop

Time: 10:00 AM - 12:00 PM

Location: Citizens C

Biotechnology Innovations at the Chemistry-Biology Interface

Session Type: Poster

Time: 12:00 PM - 2:00 PM

Location: Crystal C/D

The proposed symposium is expected to cover the recent development of biotechnologies with chemical biology emphasis, covering new approaches in diagnostics and therapeutics.

Organizer(s): Ziwen Jiang

Presentations:

12:00 PM [SW574] MYC activation induces selective snRNP imbalance and coordinated splicing-polyadenylation remodeling. **Presented by: Ayesha Khan**

12:00 PM [SW575] Establishing cellular models of cancer-associated mutations of U1 snRNA to investigate snRNP biogenesis. **Presented by: Arunprasath Duraisamy**

12:00 PM [SW576] Protein engineering for precise control over organelle-organelle interaction. **Presented by: Ura Kang**

12:00 PM [SW577] Autophagy receptor-inspired antibody-fusion proteins for targeted intracellular degradation. **Presented by: Tianqi Wang**

12:00 PM [SW578] Investigating thymine DNA glycosylase-RNA interactions in the chromatin. **Presented by: Laura Ruemmele**

12:00 PM [SW579] Investigating the impact of CXCR4 S338X mutation on receptor internalization, signaling, and dimerization. **Presented by: MOJEED AYOOLA ASHIRU**

12:00 PM [SW580] Mechanisms of synergistic cellular toxicity between α-synuclein and zinc probed by systematic mutagenesis. **Presented by: Meghana Mani Nittala**

12:00 PM [SW581] Identifying protein targets of sulfated glycosaminoglycan mimetics using photoaffinity labeling. **Presented by: Shakila Madhuhansi Silva**

12:00 PM [SW582] Identification of zoliflodacin as a potent inhibitor against tuberculosis DnaE1 polymerase through high throughput docking and scaffold hopping. **Presented by: Ragavishagan Rajasekar**

12:00 PM [SW583] Withdrawn

12:00 PM [SW584] Biochemical blockade of the SARS-CoV-2 RBD-ACE2 interface by a mutation-tolerant DNA aptamer. **Presented by: Arnav Peram**

12:00 PM [SW585] Multiplex RNA sensor for accurate infectious disease biomarker detection. **Presented by: Sathya Samaraweera**

12:00 PM [SW586] Withdrawn

12:00 PM [SW587] Bioengineered virus like particles: A delivery platform for central nervous system. **Presented by: Neelima Koti**

12:00 PM [SW588] Withdrawn

12:00 PM [SW589] Filter-resolved *in vivo* NIR-II imaging of the biodistribution and pharmacokinetics of CoMoCAT single-walled carbon nanotubes. **Presented by: Pramita Sharma**

12:00 PM [SW590] Improved *in vivo* transient tissue transparency. **Presented by: Zoya U Chaudhry**

12:00 PM [SW591] Polymer mediated precipitate suppression to increase stability in optical clearing agents. **Presented by: Kelsey Isabella Arze**

12:00 PM [SW592] Miniaturized spectrophotometer for monitoring fluidic performance in a portable microsampling backpack. **Presented by: Esther Kalejaye**

12:00 PM [SW593] Programmable transport gating converts the apparent Michaelis-Menten constant into a design metric in a microneedle biosensor: The case of glucose oxidase. **Presented by: Rahul Pandit Kumarchinchole**

12:00 PM [SW594] Tuning pore microenvironments in covalent-organic frameworks for controlled enzyme loading and release. **Presented by: Wenlu Fan**

12:00 PM [SW595] Relating nanoscale film characteristics to electrochemical performance in cytochrome P450 membrane enzyme films. **Presented by: Silan Bhandari**

12:00 PM [SW596] Species-dependent myoglobin redox behavior: Linking electrochemical signatures to protein structural features in beef, pork, and chicken. **Presented by: Sachinthani Ayabadda Devage**

12:00 PM [SW597] Toward the three-dimensional structure of AprL: Crystallization and computational insights into a PLP-dependent sugar aminotransferase. **Presented by: Oluwaseun Olanike Ajayi**

12:00 PM [SW598] Integrating enzyme kinetics and NMR spectroscopy to elucidate the catalytic mechanism of an F_{420}-dependent sugar-6-phosphate dehydrogenase from *Nocardioidaceae brasiliensis*. **Presented by: Md Sabid Ahamed**

12:00 PM [SW599] Kinetic characterization of AncD1, an ancestral F_{420}-dependent dehydrogenase. **Presented by: Ana Ledesma**

12:00 PM [SW600] Withdrawn

12:00 PM [SW601] Biocatalytic, enantioselective oxa-Pictet-Spengler reactions for the asymmetric synthesis of tetrahydropyranoindoles. **Presented by: William Jones**

12:00 PM [SW602] Biocatalytic asymmetric oxa-Pictet Spengler cyclization for the synthesis of pyranopyrazole derivatives. **Presented by: Yashodha Aluth Gedara**, **Mackenzie Armstrong**, **David C. Miller**

12:00 PM [SW603] Backbone nitrogen substitution to control the conformation and interactions of glycine residues in peptides. **Presented by: Diana Thomas**

12:00 PM [SW605] Experimental framework for assigning quenching mechanism in the dimethyl trisulfide–albumin system. **Presented by: Md Sohanur Rahman**

12:00 PM [SW606] Mass spectrometry-guided discovery of a novel anabaenopeptin from benthic cyanobacterium *Floridanema evergladense* BLCC-F167. **Presented by: Mir Maaz Ali**

12:00 PM [SW607] Comparative chemical characterization and bioactive properties of *Calotropis gigantea* and *Calotropis procera* latex. **Presented by: Saakshi Kumar**

12:00 PM [SW608] Antimicrobial effects of pulsed blue light on probiotic lactic acid bacteria. **Presented by: Ashley Renee Chandler**

12:00 PM [SW609] Wavelength and growth phase-dependent susceptibility of *Lactobacillus* co-cultures to pulsed blue light. **Presented by: Ezequiel Mora**

Computational Chemistry In Action

Session Type: Poster

Time: 12:00 PM - 2:00 PM

Location: Crystal C/D

Real-world chemical applications of molecular simulation, AI, machine learning, and related computational tools. The symposium welcomes work from experimental groups incorporating computation and computational groups developing tools for nonspecialists.

Organizer(s): Donatus Atsu Atsu Agbaglo, Muhammad Hammad Ali, Benjamin G Janesko

Presentations:

12:00 PM [SW610] Asymmetric radical sulfinylation via stereoablative sulfinyl radical generation. **Presented by: Jacob Sanchez**

12:00 PM [SW611] Withdrawn

12:00 PM [SW612] Investigation of the stability of amyloid-β (Aβ) fibrils upon interaction with SARS-CoV-2 protein fragment FI10: A molecular dynamics study. **Presented by: Al Amin**

12:00 PM [SW613] Thermodynamic and mechanical stability of hydrogen-bonded organic frameworks: Insights from density functional theory. **Presented by: Muthukumar Devarasu**

12:00 PM [SW614] Computational characterization of mesothelin-navenibody complexes using AI-driven structural prediction and molecular docking for targeted small cell lung cancer therapy. **Presented by: Geetash Muddara**

12:00 PM [SW615] Many-body second order Green's function theory for *ab initio* molecular quantum electrodynamics. **Presented by: Amir Amini**

12:00 PM [SW616] Early steps of virus-induced TTR amyloid formation. **Presented by: Malinda Bimsara Premathilaka**

12:00 PM [SW617] Ligand-dependent inter-site coupling in human glutathione synthetase. **Presented by: Matthew Stankus**

12:00 PM [SW618] Tilted material in an optical cavity: Light-matter moiré effect and coherent frequency conversion. **Presented by: Arshath Manjalingal**

12:00 PM [SW619] ProPrep: Making biomolecular simulations accessible to experimental biochemists. **Presented by: Matthew J. Guberman-Pfeffer**

12:00 PM [SW620] Electronic structure insights into composition-dependent magnetism in alloyed two-dimensional transition-metal compounds. **Presented by: Puja Rijal**

12:00 PM [SW621] Transient magnesium is an essential cofactor for phosphoryl transfer in CDK2. **Presented by: Muhammed Shameem**

12:00 PM [SW622] Quantifying the strength of acid/base functional groups in metal-organic frameworks. **Presented by: Alitza Gracia**

12:00 PM [SW623] Mapping neutral and autocatalytic mechanisms in polyester hydrolysis using bis(2-hydroxyethyl) terephthalate. **Presented by: Amir Olatunbosun Egberongbe**

12:00 PM [SW624] Optoelectronic properties and charge transfer mechanisms of naphthopyrone-based dyes on TiO_2 and ZnO. **Presented by: Thatcher Bentley**

12:00 PM [SW625] AI-accelerated *ab initio* bottom-up polymer structure prediction (AI2-BPSP) framework via hybrid DFT-based machine-learning force fields. **Presented by: Bharatha Kaushalya Gunawardana**

12:00 PM [SW626] Comparison of computational modelling techniques for structure prediction of c-type cytochromes from *Yersinia enterocolitica*. **Presented by: Newton Hilliard**

12:00 PM [SW627] Enabling high-throughput training of machine-learning force fields with long-range electrostatic interactions with robust orbital localization methods. **Presented by: Teresa Shah**

12:00 PM [SW628] Robust parameter estimation of microkinetic models for heterogeneous catalysis. **Presented by: M M Faruque Hasan**

12:00 PM [SW629] AI-accelerated *ab initio* bottom-up polymer structure prediction of amorphous polyethylenimine. **Presented by: Priya Narayan Limbu**

12:00 PM [SW630] Benchmarking force fields and water models for MDM2–p53 unbinding kinetics. **Presented by: Aloka Patabendi Mudiyanselage**

12:00 PM [SW631] Infrequent metadynamics study of SH3-peptide dissociation kinetics: Effects of terminal capping. **Presented by: Jaya Pathak**

12:00 PM [SW632] Conformational equilibrium of geldanamycin and its reduced hydroquinone form in aqueous solution: A DFT and MD study. **Presented by: Yubo Fan**

12:00 PM [SW633] Unraveling mutation-driven changes in barnase-barstar dissociation kinetics through full atomistic simulations. **Presented by: Dipesh Shrestha**

12:00 PM [SW634] Unusual deep tunneling properties promoted by the Ni^+ cation in the dissociative rearrangement reaction of CH_3COOH and its deuterium labeled isomers. **Presented by: Darrin J Bellert**

12:00 PM [SW635] From lipid composition to reactivity: Molecular simulation of olefin accessibility in wastewater-grown *Yarrowia lipolytica*. **Presented by: Esau Obuong**

12:00 PM [SW636] First-principles investigation of surface functionalization in MXenes. **Presented by: Michelle Becerra**

12:00 PM [SW637] Diagnosing and remediating failure modes of machine-learned interatomic potentials in reactive nitromethane decomposition. **Presented by: Cary Darwin**

12:00 PM [SW638] How well do classical water models capture orientation-dependent hydrogen bonding? A HEALPix benchmark against quantum mechanics. **Presented by: Laxmi Pandey**

12:00 PM [SW639] Molecular docking and dynamic simulation analysis of NADH binding to bovine myoglobin at pH 5.6. **Presented by: Greeshma Sreejesh**

12:00 PM [SW640] Molecular drivers of asphaltene aggregation: Evaluating the role of persistent radicals and molecular architecture through computed dimerization energies. **Presented by: Gretel Ann Stokes**

12:00 PM [SW641] Electronic stopping power and nonlinear lattice response in Sr-doped halide perovskites. **Presented by: Mario Borunda**

General Inorganic Chemistry

Session Type: Poster

Time: 12:00 PM - 2:00 PM

Location: Crystal C/D

This symposium will provide a broad platform for researchers working across all areas of inorganic chemistry to present their latest research. Topics may include organometallic chemistry, coordination chemistry, main-group chemistry, catalysis, solid-state chemistry, materials chemistry, bioinorganic chemistry, energy-related inorganic chemistry, computational inorganic chemistry, and interdisciplinary applications. The objective of the symposium is to foster scientific discussion, collaboration, and networking among graduate students, postdoctoral researchers, faculty members, and industry scientists within the inorganic chemistry community.

Organizer(s): MANJUR OYASIM AKRAM, Anindita Das

Presentations:

12:00 PM [SW642] Expanding the synthetic scope of AEI zeolite by rational control of organic-inorganic structure directing agents. **Presented by: Ivan Garcia**

12:00 PM [SW643] Quasi-reversible sodium insertion into a copper benzenehexathiol framework. **Presented by: Ovie Soman**

12:00 PM [SW644] Microcanonical kinetics reveal competing reaction pathways and hydrogen tunneling in cobalt mediated activation of acetic acid. **Presented by: Simon Okafor**

12:00 PM [SW645] Rational molecular engineering of mixed alkynyl-phosphine interfaces in atomically precise Au and Au-Cu nanoclusters. **Presented by: Ayomide Oladele**

12:00 PM [SW646]*In-crystallo* and matrix-isolated spectroscopic observations of catalytically relevant Co(III) porphyrin-nitrene intermediates. **Presented by: Subham Sarkar**

12:00 PM [SW647] Site-selective Cu doping of Au nanoclusters: Tunable optical properties and mechanistic insights into Au-Cu catalysis. **Presented by: Nagaraju Vodnala**

12:00 PM [SW648] Synthesis of gold-copper alloy nanocluster frameworks. **Presented by: Joshua Taylor Plank**

12:00 PM [SW649] Pyridyl and naphthylpyrasal lanthanide(III) complexes and their upconversion. **Presented by: Pooja Dogra**

12:00 PM [SW650] Synthesis and spectroscopic characterization of mono-ruthenium complexes with chiral thione ligands. **Presented by: Carla Hyppolite**, **Vivian Tran**, **Phaith Harris**, **Bukuo Ni**, **Tuan Phan**

12:00 PM [SW651] Design and synthesis of symmetric β-oxo-δ-diimine (BODDI) ligands with tunable steric and electronic properties for aluminum and zinc catalysts. **Presented by: Bhawana Khatri**

12:00 PM [SW652] Beyond the primary coordination sphere: Tellurium–metal interactions in Cu(I) and Au(I) complexes. **Presented by: Nishita Deb**

12:00 PM [SW653] Separation of molybdenum from other fission fragments by using a phase transfer agent. **Presented by: Ashirafu "Ash" Tuyishime**

12:00 PM [SW654] Ligand-to-ligand charge transfer (LL'CT) transitions in square-planar metal-bipyridyl complexes of heteroatom-substituted maltol derivatives. **Presented by: Muhammad Ahsan Usman**

12:00 PM [SW655] Accessing rare Cu(I)–Bi bonding with tris(pyrazolyl)borate scorpionates. **Presented by: Khadijatul Kobra Meem**

12:00 PM [SW656] Stabilization of classical coinage metal carbonyl complexes using a sterically encumbered tris(pyridyl)borate ligand. **Presented by: Achala Rajathunga**

12:00 PM [SW657] Chemical non-innocence of porphyrin ligands in Mn-catalyzed nitrene transfer chemistry. **Presented by: Arka Sinha**

12:00 PM [SW658] Synthesis and characterization of (^{Dipp}CCC)Mn-carbonyl complexes. **Presented by: Aishee De**

12:00 PM [SW659] Metallodithiolates as ligands to various transition metal ions: Coordination geometries and magnetic properties. **Presented by: Dakota Jones**

12:00 PM [SW660] Synthesis and characterization of Cu(I) complexes bearing 2-picolyl-substituted mono-NHC ligands: Effect of NHC wingtips on coordination geometry. **Presented by: Janet Sanwo-Olu**

12:00 PM [SW661] Metal–ligand cooperation in lutidine-linked bis-NHC Cu(I)–CNC complexes for the tandem carboxylation–esterification of terminal alkynes. **Presented by: Nick Back**

12:00 PM [SW662] Thermodynamic and electrocatalytic studies of M(triphosphine)(monophosphine) complexes containing group 10 metals and a bifunctional monophosphine ligand containing an organic hydride donor. **Presented by: Clifford Alewine**

12:00 PM [SW663] Covalent modification of glassy carbon electrodes with transition metal complexes for hydrogen production. **Presented by: Olbelina A Ulloa**

12:00 PM [SW664] Fluorinated B-phenylated scorpionates as tunable platforms for stabilizing silver(I)–ethylene complexes. **Presented by: Vo Quang Huy Phan**

12:00 PM [SW665] Selective binding and oxidation of cannabinoids mediated by copper complexes. **Presented by: Brianna Kathryn Neilan**

12:00 PM [SW666] Müller versus Gutmann–Beckett for assessing the Lewis acidity of boranes. **Presented by: Sameera Ranasinghe**

12:00 PM [SW667] Withdrawn

12:00 PM [SW668] Calcium phenoxyimine complexes for application towards C-H activation. **Presented by: Carolyn Brown**

12:00 PM [SW669] Synthesis and preparation of germanium amides as precursors to germanium telluride dimers. **Presented by: Patrick Kitzel**

12:00 PM [SW670] Divergent outcomes from the reactions of borole with Michler's ketone and thioketone. **Presented by: Dinithi Alwis**

12:00 PM [SW671] Investigating sequential quantum yield steps of LMCT photocatalysts via cyclic voltammetry. **Presented by: Nya E Black**

12:00 PM [SW672] Directing selective photocatalytic C-H activation with electrochemistry. **Presented by: Nalinda Chathuranga Senevirathna Mudiyanselage**

12:00 PM [SW673] [5+2] Cycloaddition reactions of oxidopyrylium, oxidopyridinium, oxidothiopyrylium ylides derived from hetero-substituted maltol derivatives. **Presented by: Thanuja Thilakarathna**

12:00 PM [SW674] Highly robust Zr-MOF platform featuring aromatic rich cores for efficient paraffin/olefin separation. **Presented by: Gaurav Verma**

12:00 PM [SW675] Synthesis of MOF-based composites. **Presented by: Marianna Espeleta**

12:00 PM [SW676] Synthesis and characterization of anion receptors featuring hydrogen and chalcogen bonding. **Presented by: Andres Perez Gomez**

12:00 PM [SW677] Beyond hydrogen bonding: Multidentate anion receptors integrating chalcogen bonding. **Presented by: Francisca Gonzalez Ortiz**

12:00 PM [SW678] From oxygen-atom transfer to electronic frustration in antimony–borane Lewis pairs. **Presented by: Thien Nguyen**

12:00 PM [SW866] Iron-catalyzed ethylene dimerization in the absence of a cocatalyst. **Presented by: Nir Kadosh**

12:00 PM [SW867] EPA-based method for the quantification of primary inorganic chemical contaminants of drinking water along the Gulf Coast in South Texas. **Presented by: Ayesha Khalid**

Undergraduate Luncheon

Session Type: Networking Event

Time: 12:00 PM - 1:30 PM

Location: Crystal A

Biotechnology Innovations at the Chemistry-Biology Interface

Session Type: Oral

Time: 2:00 PM - 4:20 PM

Location: Continental

The proposed symposium is expected to cover the recent development of biotechnologies with chemical biology emphasis, covering new approaches in diagnostics and therapeutics.

Organizer(s): Ziwen Jiang

Presider(s): Tianqi Wang

Presentations:

2:00 PM [SW679] Selective inhibition of HAT1 using AB oligomers: A tunable platform for targeting enzymes. **Presented by: Ismail Lalami**

2:10 PM [SW680] Edman sequencing evolved: Precise native peptide *C*-terminal ligation. **Presented by: Aisosa Omere**

2:20 PM [SW681] Reprogrammed autophagy for targeted organelle degradation using engineered protein therapeutics. **Presented by: Ura Kang**

2:30 PM [SW682] Assesment of *in vitro* nano-cytotoxicity with fluorescence microscopy through convolutional neural network-based live/dead cell classification. **Presented by: Ugur C Topkiran**

2:40 PM [SW683] Improving the stability of food-dye-based optical clearing agents with polymer additives. **Presented by: Rohit Kajla**

2:50 PM [SW684] Accelerating transient *in vivo* tissue optical clearing. **Presented by: David Asante-Asare**

3:00 PM Intermission.

3:15 PM [SW685] Spectroscopic investigation of bifunctional naphthalimide salt interactions with calf thymus DNA. **Presented by: Perla M. Tovar**

3:25 PM [SW686] Improving leukocyte-mediated cell-based disease diagnostics across diverse biomatrices via a novel MP-AES cytometry assay. **Presented by: McKenna McKay**

3:35 PM [SW687] Targeting intracellular uropathogenic *Escherichia coli* with a small-molecule antibacterial agent. **Presented by: Miguel Gaspar**

3:45 PM [SW688] Dual-function molecular probe for fluorescent detection and photothermal treatment of intracellular urinary tract infections. **Presented by: Emily Osborn**

3:55 PM [SW689] Strain-dependent interactions between lactic acid bacteria and *Bacillus thuringiensis* in mixed-species cultures. **Presented by: Cephus Bess-Grunewald**

4:05 PM [SW690] β-carotene production from CO_2-fed microbial electrosynthesis using adaptively evolved and metabolically engineered *Rhodobacter sphaeroides*. **Presented by: Yuri Kim**

4:15 PM Closing Remarks.

Computational Chemistry In Action

Session Type: Oral

Time: 2:00 PM - 5:40 PM

Location: Citizens B

Real-world chemical applications of molecular simulation, AI, machine learning, and related computational tools. The symposium welcomes work from experimental groups incorporating computation and computational groups developing tools for nonspecialists.

Organizer(s): Donatus Atsu Atsu Agbaglo, Muhammad Hammad Ali, Benjamin G Janesko

Presider(s): Donatus Atsu Atsu Agbaglo, Muhammad Hammad Ali, Benjamin G Janesko

Presentations:

2:00 PM [SW691] Confidence as an oracle for orthogonal protein design: Boltz-2 and ESMFold2 lead the way for designed proteins. **Presented by: Colter Isaiah Buffford**

2:25 PM [SW692] Unravelling the impact of linker architecture on PROTAC conformations via atomistic simulation. **Presented by: Shikshya Bhusal**

2:50 PM [SW693] Closing the experiment–model–decision loop in chemical science: Chemistry and physics-informed scientific machine learning tools. **Presented by: M M Faruque Hasan**

3:15 PM [SW694] Learning slow collective variables via spectral autoencoder maps and iterative metadynamics. **Presented by: sara alinejad**

3:40 PM Intermission.

4:00 PM [SW695] AI-accelerated *ab-initio* bottom-up polymer structure prediction of amorphous polyethylene glycol. **Presented by: Kriti Alam**

4:25 PM [SW696] Computational study of Zr/Hf-MOF-808 catalyzed sulfoxide oxidation. **Presented by: Lauryn Guzman**

4:50 PM [SW697] Structural plasticity and functional dynamics of pigeon cryptochrome 4 as avian magnetoreceptor. **Presented by: CHUANYE XIONG**

5:15 PM [SW698] Understanding hydrogen evolution reaction on CoCrFeNi(111) high-entropy alloy surface. **Presented by: Ye Xu**

Emerging Trends in Synthetic Inorganic Chemistry

Session Type: Oral

Time: 2:00 PM - 6:00 PM

Location: Texas A

Contributions covering transition-metal, main-group, coordination, organometallic compounds, and cluster chemistry along with interdisciplinary research at the interface of inorganic chemistry and related fields, are welcome. This symposium will showcase recent progress in the preparation and study of molecular and materials-based inorganic systems with relevance to catalysis, electronic materials, energy conversion, environmental chemistry, and chemical transformations.

Organizer(s): MANJUR OYASIM AKRAM, Anindita Das

Presider(s): MANJUR OYASIM AKRAM, Anindita Das

Presentations:

2:00 PM [SW699] Task-specific design of metal-organic frameworks for selective gas adsorption. **Presented by: Shengqian Ma**

2:20 PM [SW700] Taming molecular boron nitride. **Presented by: Todd W Hudnall**

2:40 PM [SW701] Intramolecular cooperativity of polytopic Lewis acids in frustrated Lewis pair catalyzed hydrogenations. **Presented by: Clemens Krempner**

3:00 PM [SW702] Harnessing tetrel bonding in donor–acceptor molecular design. **Presented by: Gyeongjin Park**

3:20 PM [SW703] Bimetallic catalysis for polymer synthesis and degradation. **Presented by: Robert Comito**

3:40 PM Intermission.

4:00 PM [SW704] Intraligand secondary interactions as a design principle for organometallic catalysts. **Presented by: LeGrande Marcel Slaughter**

4:20 PM [SW705] Exploring the synthesis, characterization, and reactivity of various home- and heteroleptic mono-N-heterocyclic carbene Cu(I) complexes. **Presented by: Laleh Tahsini**

4:40 PM [SW706] Construction and reactions of bidentate bis-chalcogenium Lewis acids. **Presented by: Brendan Murphy**

5:00 PM [SW707] Trapping gold(I) nitrenes with crystalline matrix isolation. **Presented by: Debasmita Dutta**

5:20 PM [SW708] Stabilizing boravinylidenes through interrupted 1,1-hydroboration and 1,1-carboboration reactions. **Presented by: MANJUR OYASIM AKRAM**

General Organic Chemistry

Session Type: Oral

Time: 2:00 PM - 5:50 PM

Location: Crystal B

This symposium will provide a general platform for researchers working across all areas of organic chemistry to present their latest advances. Topics may include, but are not limited to, synthetic methodology, catalysis, physical organic chemistry, mechanistic studies, chemical biology, organometallic chemistry, and natural product synthesis. The symposium aims to highlight innovative approaches, emerging technologies, and interdisciplinary applications that are shaping the future of organic chemistry.

Organizer(s): Jeremiah J Gassensmith

Presider(s): Jeremiah J Gassensmith

Presentations:

2:00 PM [SW709] Carbon nucleophile-mediated pyridine ring-opening enables polymethine-functionalized cyanine 9. **Presented by: Syed Usama**

2:25 PM [SW710] Withdrawn

2:35 PM [SW711] Biocatalytic, asymmetric oxa-Pictet-Spengler reaction for the synthesis of oxazinoindole derivatives. **Presented by: Pratap Rijal**

2:49 PM [SW712] 5-Methylene 1-azaspiro[2.3]hexanes: Gateway to high Fsp^3 amine chemical space. **Presented by: Uddalak Sengupta**

3:03 PM [SW713] Carbenium-enhanced halogen bonding and applications to catalysis. **Presented by: Dylan Zhong**

3:13 PM [SW714] Base-free C–N cross-electrophile coupling. **Presented by: Lauv Patel**

3:27 PM [SW715] Concise synthesis of kopsiyunnanine E and synthetic efforts toward arboflorine. **Presented by: Tarak Nayak**

3:41 PM [SW716] Anti-amyloidogenic behaviour of 1,3,6-trisubstituted 4-cinnolinols. **Presented by: SIDDHARTHA MAJI**

3:55 PM [SW717] Withdrawn

4:09 PM [SW718] Nickel-catalyzed deaminative C–C cross-coupling via photosensitized 1,2-dialkyldiazene intermediates. **Presented by: Mark Jeffrey Diaz**

4:23 PM [SW719] Rapid mechanochemical synthesis of biologically important enamino carbonyl compounds via ball milling. **Presented by: Maqhawe Ndlovu**

4:37 PM [SW720] Proton relaying in carbenium-based oxygen reduction. **Presented by: Sean Rooney**

4:47 PM [SW721] Carbenium ions enabled by proximal phosphine oxides: Redox chemistry, radical formation and hydrogen evolution catalysis. **Presented by: Xinyue Tan**

5:07 PM [SW722] Leaving group controlled skeletal editing of pyrroles. **Presented by: UPASANA CHATTERJEE**

5:21 PM [SW723] Withdrawn

5:35 PM [SW724] Stereochemically defined cyclohexylamide scaffolds as chiral peptidomimetics for mimicking α-helical surfaces. **Presented by: Henry Neal**

Make It Make Sense: Innovative Teaching Practices

Session Type: Oral

Time: 2:00 PM - 4:40 PM

Location: Texas C

This symposium explores a range of pedagogical innovations including active learning, integration of digital tools, laboratory redesigns, and assessment strategies that support student success. The use of learning assistants and peer-led team learning programs that improve performance, increase retention, and foster belongingness will also be highlighted. This session specifically focuses on actionable ideas and practical instructional experience in the classroom.

Organizer(s): Amandeep Sra, Michele Stover

Presider(s): Amandeep Sra, Michele Stover

Presentations:

2:00 PM [SW725] Atom Animator: An open-source plugin for generating animated mechanisms from Chemical Markup Language files. **Presented by: Timothy Bonzon**

2:20 PM [SW726] Practical strategies for integrating programming into existing chemistry courses: Lessons from the ACT-CMS community. **Presented by: Prajay Patel**

2:40 PM [SW727] From generative AI to VASR: Integrating AI into advanced chemistry education. **Presented by: Peng Tao**

3:00 PM [SW728] From classroom to research: Engaging undergraduate chemists in wine metabolomics through the Freshman Research Initiative and the UT Wine Initiative. **Presented by: Diana Zamora-Olivares**

3:20 PM Intermission.

3:40 PM [SW729] Building-in student success in general chemistry. **Presented by: David L. Catlett**, **Ellen Steinmiller**

4:00 PM [SW730] Making laboratory skill assessment make sense. **Presented by: Eszter Trufan**

4:20 PM [SW731] From following procedures to scientific reasoning: Redesigning the general chemistry I laboratory. **Presented by: Jordan Rector**, **Pamela Auburn**

Materials Chemistry: Emerging Contaminant Remediation in Impacted Environments

Session Type: Oral

Time: 2:00 PM - 6:00 PM

Location: Texas D

Invited and open call for oral and poster presentations highlighting recent advances in materials chemistry focused on the discovery, design, and characterization of materials for the remediation of emerging contaminants in impacted environments.

Organizer(s): Shengqian Ma, Mario Wriedt

Presider(s): Shengqian Ma, Mario Wriedt

Presentations:

2:00 PM Opening Remarks.

2:05 PM [SW734] Simultaneous electro-oxidation and electrocoagulation of contaminated water using modified carbon electrodes under pulse and steady current. **Presented by: riju s robin**

2:35 PM [SW735] Runways to waterways: Fate of PFAS and tire-derived organic pollutants in Louisiana's airports. **Presented by: Md Firoz Al Mamun**

3:05 PM [SW736] Statewide wastewater monitoring of psychostimulants and synthetic opioids in Louisiana. **Presented by: Ramesh Sapkota**

3:35 PM [SW737] MgFe layered double hydroxide for excess NO_3^- and PO_4^{3-} nutrient remediation. **Presented by: aaron caesar**

4:05 PM Networking Break.

4:25 PM [SW738] Bypassing the spatial limits of acoustic remediation: From interfacial partitioning to anaerobic solid-state nanozymes. **Presented by: Yunxiang Gao**

4:55 PM [SW739] Removal of per- and polyfluoroalkyl substances from contaminated water using scalable metal-organic frameworks. **Presented by: Arefeh Mirsharifian**

5:25 PM [SW740] Semiconducting copper(II) oxide sulfate: Synthesis, solid-state chemistry, and electronic structure. **Presented by: Katheryn R Cruz**

5:55 PM Closing Remarks.

Wednesday Afternoon Coffee Break

Session Type: Coffee Break

Time: 3:30 PM - 4:30 PM

Location: Crystal C/D

ACS Resume Reviews

Session Type: Workshop

Time: 4:00 PM - 5:00 PM

Location: Citizens C

SWRM Awards Dinner

Session Type: Special Event

Time: 6:00 PM - 8:00 PM

Location: Crystal A

General Organic Chemistry

Session Type: Poster

Time: 8:00 PM - 10:00 PM

Location: Crystal C/D

This symposium will provide a general platform for researchers working across all areas of organic chemistry to present their latest advances. Topics may include, but are not limited to, synthetic methodology, catalysis, physical organic chemistry, mechanistic studies, chemical biology, organometallic chemistry, and natural product synthesis. The symposium aims to highlight innovative approaches, emerging technologies, and interdisciplinary applications that are shaping the future of organic chemistry.

Organizer(s): Jeremiah J Gassensmith

Presentations:

8:00 PM [SW741] Advances toward the Ewing sarcoma cytotoxin altertoxin II. **Presented by: Max Balderas**

8:00 PM [SW742] Synthesis and evaluation of 6-chloro-N-hydroxy-1H-indole-4-carboxamide as a potential HDAC1 inhibitor. **Presented by: Inioluwa Adetiloye**

8:00 PM [SW743] Design and synthesis of self-assembling peptides for the formation of coacervates. **Presented by: Raniyah Ali**

8:00 PM [SW744] Application of pharmacophore-directed retrosynthesis to the dichapetalin family: Synthetic studies toward the C8 side chain and cyclopropane. **Presented by: Alyssa Nicole Garcia**

8:00 PM [SW745] Expanding the fluorinated natural product space: Synthesis of novel phytocannabinoid derivatives. **Presented by: Jessica Carol May Thompson**

8:00 PM [SW746] Asymmetric Ir-catalyzed migratory alkene hydrosilylation: Chirality transfer from chiral *N,O*-silyl acetals. **Presented by: Linda Lallawmsangi**

8:00 PM [SW747] Synthesis of highly substituted electron-rich [*n*]-dendralenes via one-pot electrocyclic ring-opening and enolate protection. **Presented by: Dinorah Ponce**

8:00 PM [SW748]*N*–phenothiaziniums as *N*–centered radical precursors. **Presented by: Melissa Ojeda**

8:00 PM [SW749] Enantioselective Michael addition of malonate to 3-methyl-4-nitro-5-alkenyl-isoxazoles using chiral Ni(II)-diamine catalysts. **Presented by: Bukuo Ni**

8:00 PM [SW750] Asymmetric Michael-aldol cascade reactions of 1,2-diones with 3-methyl-4-nitro-5-alkenyl-isoxazoles catalyzed by Ni(II)-diamine complex. **Presented by: Bukuo Ni**

8:00 PM [SW751] Pd- and Cu-cocatalyzed anaerobic olefin aminoboration. **Presented by: Clay West**

8:00 PM [SW752] Dearomative C2-borylation of indoles. **Presented by: Ayesha Begum**

8:00 PM [SW753] Olefin borylation with electrophilic palladium. **Presented by: Elizabeth G Milem**

8:00 PM [SW754] Pd- and Cu-cocatalyzed anaerobic aminoboration of unactivated alkenes. **Presented by: Saurabh Sandip Satpute**

8:00 PM [SW755] Green synthesis: Selective cleavage of isatin in peroxide free conditions. **Presented by: Erika Rochelle**

8:00 PM [SW756] Synthesis and separation of hexose-6-phosphate utilizing ion exchange techniques. **Presented by: Ashton Drake**

8:00 PM [SW757] Reductive transformations of carbonyl compounds mediated by 1,4-dihydropyridine anions and visible light irradiation. **Presented by: Viraj Miyuranga Miyuranga**

8:00 PM [SW758] Enantioselective Stork-Danheiser transposition enabled by a computationally designed chiral phosphoric acid catalyst. **Presented by: Jordan Michael Martinez**

8:00 PM [SW759] Copper-containing N/O-donor macrocycles for benzylic and allylic oxidation catalysis. **Presented by: Amreet Kaur**

8:00 PM [SW760] Synthesis of achiral squaramide catalysts for use in organocatalyzed reactions. **Presented by: Francis Klenam Kekessie**

8:00 PM [SW761] Synthesis of β-diketone scaffolds for the selective formation of α-acyloxy ketone motifs. **Presented by: Claire Martinez**

8:00 PM [SW762] Substituent effects on hydration equilibria of biomass-burning-relevant aromatic aldehydes by variable-temperature H NMR spectroscopy. **Presented by: madiha mazhar**

8:00 PM [SW763] Developing prototype Raman-active drugs for real-time *in situ* drug delivery. **Presented by: Christian Morkeh**

8:00 PM [SW764] Withdrawn

8:00 PM [SW765] Withdrawn

8:00 PM [SW766] Synthesis and characterization of *β*-functionalized porphyrins as building blocks for covalent organic frameworks. **Presented by: Rajendra Adhikari**

8:00 PM [SW767] Thermodynamic characterization and optimization of imidazolium based ionic liquid modified reversed phase HPLC system. **Presented by: Ayan Paul**

8:00 PM [SW768] Speciation of silver complexes and their effect on palladium-catalyzed C–H functionalization. **Presented by: Sophia de Aquino Veras**

8:00 PM [SW769] Light-activated natural products as deployable antimicrobials. **Presented by: Brayden Stackhouse**

8:00 PM [SW770] Nature meets light: Investigating natural product for antimicrobial photodynamic therapy. **Presented by: Kim Luu**

8:00 PM [SW771] Development of a synthetic route to highly substituted quinazolines via isatoic anhydride and phthalimide intermediates. **Presented by: Mediha Noor Siddiqui**

8:00 PM [SW772] Synthetic approach toward sulfonamide-substituted quinazolines from isatin sulfonic acid derivatives. **Presented by: Mediha Noor Siddiqui**

8:00 PM [SW773] Programmable C-H functionalization of N-heterocycles. **Presented by: Buddhadeb Pal**

8:00 PM [SW774] Harnessing hypervalent silicon: In sustainable organic synthesis. **Presented by: Neetesh Yadav**

8:00 PM [SW775] Oxidant-efficient benzylic and allylic C–H oxidation using a water-soluble Cu(II) Schiff base/TEMPO system. **Presented by: Xander Duke**

8:00 PM [SW776] Synthesis of benzoborole-based macrocycles utilizing dialkoxy phenylene linkers. **Presented by: Kylie Victoria Bartusek**

8:00 PM [SW777] Stereoselective functionalization of carbon-hydrogen bond with collaborative enantiomeric control. **Presented by: Weinan Tan**

8:00 PM [SW778] Cell organelle-targeted Schaap's dioxetane for sub-cellular imaging. **Presented by: Gen Chen**

8:00 PM [SW779] Concentration-dependent photochemical evolution of primary brown carbon under irradiation. **Presented by: Sithumi M Liyanage**

8:00 PM [SW780] Synthesis and characterization of water-soluble prodrugs of a Toll-like receptor 4 (TLR-4) inhibitor, TAK-242. **Presented by: Jacquelin LaBerteaux**

Make It Make Sense: Innovative Teaching Practices

Session Type: Poster

Time: 8:00 PM - 10:00 PM

Location: Crystal C/D

This symposium explores a range of pedagogical innovations including active learning, integration of digital tools, laboratory redesigns, and assessment strategies that support student success. The use of learning assistants and peer-led team learning programs that improve performance, increase retention, and foster belongingness will also be highlighted. This session specifically focuses on actionable ideas and practical instructional experience in the classroom.

Organizer(s): Amandeep Sra, Michele Stover

Presentations:

8:00 PM [SW732] Start data collection, organization, and analysis in general chemistry lab week one: Why wait. **Presented by: Scott Joseph Donnelly**

8:00 PM [SW733] GC-MS, ^{13}C NMR, polarimetery, and thermography: Advancing the teaching of general chemistry with modern instrumentation. **Presented by: Scott Joseph Donnelly**

8:00 PM [SW781] Speed of sound in a circular acoustic resonator. **Presented by: Adam Mansell**

8:00 PM [SW782] Reviving the Finkelstein reaction: Supramolecular chemistry in the undergraduate teaching laboratory. **Presented by: Xuxian He**

8:00 PM [SW783] Power of alumni: Bringing real-world experiences and career pathways to students in STEM deserts. **Presented by: Candice Fulton**

8:00 PM [SW784] Withdrawn

Materials Chemistry: Emerging Contaminant Remediation in Impacted Environments

Session Type: Poster

Time: 8:00 PM - 10:00 PM

Location: Crystal C/D

Invited and open call for oral and poster presentations highlighting recent advances in materials chemistry focused on the discovery, design, and characterization of materials for the remediation of emerging contaminants in impacted environments.

Organizer(s): Shengqian Ma, Mario Wriedt

Presentations:

8:00 PM [SW785] Comparison of β-Mo2C thin film and nanoparticles as a catalyst for selective C=O bond scission: Addressing pressure and material gaps. **Presented by: Abdullah Ali Maruf**

8:00 PM [SW786] Tuning the coordination sphere of metal-integrated two-dimensional covalent organic frameworks for selective toxic gas capture. **Presented by: SAYAN MAITI**

8:00 PM [SW787] Removal of uranium from water using a water-insoluble urea polymer. **Presented by: Gifty Dudzilah**

8:00 PM [SW788] Removal of fluoride from groundwater using inexpensive biocompatible materials. **Presented by: DennAsia Cordova**

8:00 PM [SW789] Identification of microplastic concentrations in Matagorda Bay sediments. **Presented by: Joseph Dulaney**

8:00 PM [SW790] Tailored crystallization for extremely stable wide-band gap perovskite solar cell. **Presented by: Nilanjana Nandi**

8:00 PM [SW791] Fluorescent sensing of per- and polyfluoroalkyl substances in water using functionalized metal–organic framework. **Presented by: Danidu M Jayasuriya**

8:00 PM [SW792] Mesoporous tin oxide-based electrochemical flow sensor for per and polyfluorinated alkyl substances (PFAS). **Presented by: Andrea Razo**

8:00 PM [SW793] Toward PFAS destruction: Metal–organic frameworks for adsorption and photocatalytic degradation. **Presented by: Najeeb Ullah**

8:00 PM [SW794] Photodegradation of PFAS in water by silver-based MOF–persulfate systems. **Presented by: Prapti Shende**

8:00 PM [SW795] Urea-functionalized cerium metal–organic framework for fluorescent detection of PFBA and TFA. **Presented by: Maryam Piroozzadeh**

8:00 PM [SW796] Predicting contaminant transport and environmental persistence through sustainable solvation modeling. **Presented by: Anika Varadharajan**

8:00 PM [SW797] Validation of iron-based oxide nanoparticles as arsenic sequestering agents for commercial fertilizers. **Presented by: Leandro Hildeberto Obama**

8:00 PM [SW798] Label-free impedimetric detection of perfluorooctanoic acid using silane-functionalized FTO electrodes. **Presented by: QAMAR HAYAT KHAN**

8:00 PM [SW799] Deep eutectic solvent-assisted synthesis of ferrocene-derived Fe-functionalized activated carbon for adsorption-assisted heterogeneous Fenton oxidation in complex dye matrices. **Presented by: Sungjik Oh**

8:00 PM [SW800] Arsenic removal from aqueous solutions using green synthesized Fe-Ti mixed nanoparticles. **Presented by: Harshica Fernando**

Thursday, November 19, 2026

Registration

Session Type: Registration

Time: 7:00 AM - 1:00 PM

Location: Promenade

Badge pick-up and onsite registration.

SWRM Executive Board Meeting (Invite Only)

Session Type: Board Meeting

Time: 7:00 AM - 12:00 PM

Location: Citizens C

Immune-Active Materials and Protein Delivery

Session Type: Oral

Time: 8:00 AM - 12:00 PM

Location: Texas A

Invited and open call for chemistry-driven approaches for integrating materials with immune function and biologic delivery, including immune-active biomaterials, protein and adjuvant delivery, vaccine platforms, antigen carriers, and materials that modulate innate and adaptive immunity. The session will bring together researchers in chemistry, materials science, immunology, and bioengineering focused on molecular and materials design for immune activation and therapeutic efficacy.

Organizer(s): Jeremiah J Gassensmith

Presider(s): Jeremiah J Gassensmith

Presentations:

8:00 AM [SW811] Using virus-like particles to develop vaccines for infectious and chronic diseases. **Presented by: Bryce Chackerian**

8:35 AM [SW812] MOXI-214: A fully manganese-based metal-organic framework for antigen delivery and immune activation. **Presented by: Ziqi Wang**

9:00 AM [SW813] Linker strategies for local delivery of small-molecule immunomodulators in transplantation. **Presented by: Robert Ronald Kane**

9:35 AM Coffee Break.

9:50 AM [SW814] Unlock the subdominant B cell repertoire with polymeric nanoparticle adjuvant for the next-generation vaccine development. **Presented by: Qian Yin**

10:25 AM [SW815] Injectable multidomain peptide (MDP) hydrogel for controlled drug delivery in the immunotherapy of oral cancer. **Presented by: Arghadip Dey**

10:50 AM [SW816] Turning focused ultrasound histotripsy into an *in situ* cancer vaccine for systemic antitumor immunity. **Presented by: Ashish Ranjan**

11:25 AM [SW817] Injectable biomaterial scaffolds to prevent orthopaedic device infection. **Presented by: Alexander M Tatara**

Macrocycles

Session Type: Oral

Time: 8:00 AM - 9:20 AM

Location: Texas B

The design, synthesis, characterization and applications of macrocycles are the focus of this symposium with special emphasis on the use of these molecules for therapeutic/diagnostic/theranostic applications.

Organizer(s): Eric Simanek

Presider(s): Eric Simanek

Presentations:

8:00 AM [SW818] Ready access to 24-atom macrocycles: Conformation, computation and application. **Presented by: Eric Simanek**

8:20 AM [SW819] Aromatic heterobicycle-fused porphyrins: Synthesis, characterization and study of impact on aromaticity and excited state electron transfer leading to long-lived charge separation. **Presented by: Joshua Alexander Martinez**

8:40 AM [SW820] Triazine macrocycles: From library synthesis to unexpected membrane permeability. **Presented by: Gretel Ann Stokes**

9:00 AM [SW821] When hydrogen bonds compete: Primary amine auxiliaries reveal new conformational isomers in 24-atom triazine macrocycles. **Presented by: Harsha Vardhan Reddy Kasireddy**

SWRM Wellness Room

Session Type: Wellness

Time: 8:00 AM - 1:00 PM

Location: Keystone Room

The Sweet Chemistry of Life: The Chemistry and Biology of Carbohydrates

Session Type: Oral

Time: 8:00 AM - 11:20 AM

Location: Texas D

A symposium that describes the synthesis, biology, and material properties of carbohydrates ranging from monosaccharides to polymeric materials. Abstracts discussing probe synthesis, novel carbohydrate materials, and applications of carbohydrate probes of fundamental and translatable biological function will be welcome. Ideally, all oral presentations relate to the biological function of carbohydrates present in primary and secondary metabolism, as signaling modalities, and as parts of biomacromolecules including glycolipids, glycoproteins, and glycans.

Organizer(s): Joseph Anthony Buonomo

Presider(s): Md Tareque Hassan Mukut, Aisosa Omere

Presentations:

8:00 AM [SW822] LC–MS/MS glycomics reveals high-fat diet–modulates hemisphere-specific *N*-glycan remodeling in the thalamus following traumatic brain injury. **Presented by: Abiodun Adewolu**

8:30 AM [SW823] Serum *N*-glycan fucosylation reveals distinct remodeling patterns across mild cognitive impairment and Alzheimer's disease. **Presented by: Abdulrahman Abdulmumin**

9:00 AM [SW824] Serum N-glycome profiling identifies candidate biomarkers for genotype discrimination and severity stratification in sickle cell disease. **Presented by: Abderrahmane Koraich**

9:30 AM Intermission.

9:50 AM [SW825] Earth-abundant metal-carbene/nitrene-mediated stereoselective glycosylation. **Presented by: Umesh Chaudhary**

10:20 AM [SW826] Chemoselective monosubstitution of mono- and disaccharides. **Presented by: Desiree R Czapski**

10:50 AM [SW827]*O*-Glycosylation through the photochemistry of electron-donor-acceptor complexes. **Presented by: Justin Robert Ragains**

Transformative Research at Primarily Undergraduate Institutions

Session Type: Oral

Time: 8:00 AM - 11:40 AM

Location: Texas C

Symposium focused on how programs at PUI's are creating undergraduate research opportunities despite limited infrastructure and heavy teaching loads. Contributions can include (1) Course-based undergraduate research experiences (CUREs) (2) Research mentoring at teaching-focused institutions (3) Supporting first-generation and commuter students (4) Building instrumentation capacity at smaller institutions and (5) Partnerships between PUIs and R1 universities

Organizer(s): Scott Alan Grimes, Muhammed Yousufuddin

Presider(s): Scott Alan Grimes

Presentations:

8:00 AM [SW828] Strategies for establishing a research program at a primarily undergraduate institution. **Presented by: Muhammed Yousufuddin**

8:20 AM [SW829] Undergraduate research into predicting pK_a using machine learning, quantum mechanical workflows with explicit solvation. **Presented by: Prajay Patel**

8:40 AM [SW830] Withdrawn

9:00 AM [SW831] Withdrawn

9:20 AM [SW832] From growing environment to geographic origin: HPLC-based phenolic profiling of Sri Lankan and global teas. **Presented by: Felicity Gomez**

9:40 AM [SW833] Cell-mediated delivery of liposomal nanoparticles for tumor-targeted therapy. **Presented by: Mina Poursharifi**

10:00 AM Intermission.

10:20 AM [SW834] Introduction to chemical research: Guidelines for success. **Presented by: Ruth Ann Murphy**

10:40 AM [SW835] Abraham solvation parameter model: Experiment based solute descriptor values for potential medicinal candidates, dietary healthcare supplements and pharmaceutical formulation ingredient. **Presented by: Andrew Evans**

11:00 AM [SW836] Multi-generational inheritance of plastic degradation traits in superworms and mealworms. **Presented by: Sophia Flores-Arguello**

11:20 AM [SW837] Proposed synthetic strategy for a thioether-linked bis-quaternary ammonium compound: An undergraduate research collaboration between a PUI and research-intensive institution. **Presented by: Gustavo Gomez**

Women in Energy and Sustainability

Session Type: Oral

Time: 8:00 AM - 11:55 AM

Location: Citizens B

A blended symposium with faculty from organic or inorganic chemistry or catalysis doing research that supports new advances in energy or sustainable chemistry

Organizer(s): Anne Elizabeth Vivian Gorden

Presider(s): Anne Elizabeth Vivian Gorden

Presentations:

8:00 AM Opening Remarks.

8:10 AM [SW838] Sustainable olefin functionalization reactions. **Presented by: Kami Hull**

8:35 AM [SW839] Biocatalysts for selective functionalization: A sustainable approach to small molecule oxidation. **Presented by: Meagan E Hinze**

9:00 AM [SW840] Designing molecular copper catalysts for sustainable chemistry: Oxidation and C–N bond formation. **Presented by: Anne Elizabeth Vivian Gorden**

9:25 AM Intermission.

9:45 AM [SW841] Direct carboxylation and esterification of terminal alkynes by Cu-CNC complexes: The role of metal ligand cooperativity. **Presented by: Laleh Tahsini**

10:10 AM [SW842] Withdrawn

10:35 AM [SW843] Advancing water and energy catalysis by controlling electrochemical properties through confinement. **Presented by: Noemie Elgrishi**

11:00 AM [SW844] Leveraging computational tools to reduce experimental burden in the optimization of organic transformations. **Presented by: Jacquelyne Read**

11:25 AM Discussion.

Thursday Morning Coffee Break

Session Type: Coffee Break

Time: 9:30 AM - 10:30 AM

Location: Crystal C/D

Macrocycles

Session Type: Poster

Time: 12:00 PM - 2:00 PM

Location: Crystal C/D

The design, synthesis, characterization and applications of macrocycles are the focus of this symposium with special emphasis on the use of these molecules for therapeutic/diagnostic/theranostic applications.

Organizer(s): Eric Simanek

Presentations:

12:00 PM [SW855] Synthesis and characterization of carbazole-based porphyrinoid-metal complexes. **Presented by: Biswash Guragain**

12:00 PM [SW856] Synthesis and study of optical properties of aromatic heterocycle π-extended porphyrin. **Presented by: Prabha Sharma**

12:00 PM [SW857] Enhancing π-conjugation in perimidine-fused porphyrins: Exploring their distinct optical and electronic properties. **Presented by: Thi Nguyen**

12:00 PM [SW858] Metal-free ligand-centered radical scavenging in pyridine-modified tetraaza macrocycles. **Presented by: Hannah Kathleen Pyle**

12:00 PM [SW859] Creating libraries of macrocycles with engineerable conformations. **Presented by: Andrea E Rangel**

12:00 PM [SW860] Utilization of rings to increase blood-brain barrier permeability. **Presented by: Nathaniel McKinney**

12:00 PM [SW861] Using nucleophilic catalysis to probe stability and exchange in 24 atom triazine macrocycles comprising bishydrazones. **Presented by: THIRUPATHI REDDY**

Immune-Active Materials and Protein Delivery

Session Type: Oral

Time: 1:00 PM - 3:00 PM

Location: Texas A

Invited and open call for chemistry-driven approaches for integrating materials with immune function and biologic delivery, including immune-active biomaterials, protein and adjuvant delivery, vaccine platforms, antigen carriers, and materials that modulate innate and adaptive immunity. The session will bring together researchers in chemistry, materials science, immunology, and bioengineering focused on molecular and materials design for immune activation and therapeutic efficacy.

Organizer(s): Jeremiah J Gassensmith

Presider(s): Jeremiah J Gassensmith

Presentations:

1:00 PM [SW862] Intranasal delivery of NanoSTING confers broad protection against seasonal and highly pathogenic influenza strains. **Presented by: Ankita Leekha**

1:35 PM [SW863] Ready, aim, MOF: A metal–organic framework gun for needle-free delivery. **Presented by: Nithish Agamendran**

2:00 PM [SW864] Withdrawn

2:25 PM [SW865] Adjuvants affect the quality and quantity of neutralizing antibodies stimulated in response to *Alphavirus* protein antigens. **Presented by: Catherine H Schein**