

# Tuesday General Info

**Get your badge** - starting at 7 am at the Event Office in the upper level of the Convention Center

**Beverage Services** - water stations will be available outside the meeting rooms. Complimentary coffee and tea and other beverages will be available daily from 8 am - 5 pm in the WCC upper atrium. Official Coffee breaks from 10-10:30 am and 3-3:30 pm.

**Networking Space** - Networking space sponsored by Baylor University can be found in the WCC upper atrium.

## FOOD and Drink

### In the Convention Center

Upper Atrium  
Daily 11 am - 2 pm

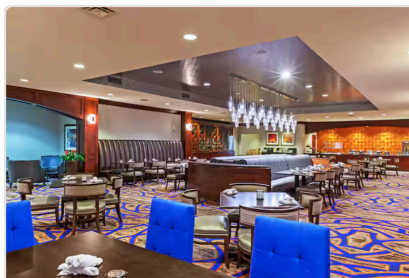
#### **Brown Bag Special**

Pulled Pork Sandwiches  
Brisket Sandwiches  
Sausage Sandwiches  
Chips  
Sodas/water  
BBQ Frito pie  
BBQ Nachos



### In the Hilton

Breakfast, lunch, and dinner daily



#### **Brazos Grille**

Brazos Grille at the Hilton Waco hotel offers a variety of regional Italian inspired dishes to meet everyone's tastes at an affordable price. Offering a casual, yet festive atmosphere with a wide variety of menu selections, it provides the perfect place to enjoy the panoramic views of Indian Hills Park & the Brazos River. Brazos Grille is open daily for breakfast, lunch and dinner serving fresh indigenous local products.

### Across the Street



WiFi Network Name: ccpublic Password: wacocc17

# Tuesday Events

**Senior Chemists Breakfast** - (7-8 am) meet Pat Farmer in the Hilton Brazos Grille (Patrick\_Farmer@baylor.edu)

**Merck Recruiting Breakfast** - students and postdocs (and disgruntled faculty?) can join Merck reps for a informational recruiting breakfast. 7:30-9 am Chisolm Hall (WCC Upper level)

**Bruker Coffee Break** Goodies courtesy of Bruker; 10-10:30 am, Brazos Ballroom

**ACS Governance Reception** 3-4 pm Brazos Ballroom

**EXPO** 3-5 pm Brazos Ballroom - A great chance to catch up with the vendors in a less hectic environment

**Gooch-Stephens Lecture** - Professor Andrew Ellington will present the Gooch-Stephens lecture, beginning at 5:45 pm. The lecture (open to the public) will be in McLennan Hall (WCC upper level).

*“Is a blind watchmaker the same  
as a blind neural net?”*

**Reception/Poster Session3** A reception (with awesome food from Georges and a cash/ticket bar) will be held concurrently with Poster Session 3, Brazos Ballroom.

WiFi Network Name: ccpublic Password: wacocc17

# Tuesday Morning Technical Program

## ***Chemical Biology***

A. T. Wright, *Presiding* Texas 117

## ***Computational and Theoretical Chemistry***

K. L. Shuford, *Organizer, Presiding* Texas 116

## ***Electrocatalysis: Molecular and Material Approaches to Electrified Chemical Processes***

D. Boucher, *Organizer, Presiding* Lone Star 104

## ***F-elements: Structure and Applications Part 1***

A. E. Gorden, *Organizer*, J. Ducilon, *Presiding* Texas 113

## ***Materials and Interfaces***

Z. Zhang, *Organizer, Presiding* Texas 118

## ***Metalloenzyme Design***

I. V. Korendovych, *Organizer, Presiding* Texas 114

## ***Novel Approaches to Drug Delivery***

R. R. Kane, *Organizer*; J. J. Gassensmith, *Organizer, Presiding*  
Texas 115

## ***Polymers and Sustainability Challenges 1***

R. Foudazi, *Organizer, Presiding* Ranger 106/107

## ***Assessments for Learning and Engaging with Students***

A. Sra, M. Stover, *Organizers, Presiding* Ranger 110

## ***Atmospheric Chemistry***

Y. Li, R. J. Sheesley, *Organizers, Presiding* Lone Star 103

# Tuesday Afternoon Technical Program

## *Atmospheric Chemistry*

Y. Li, R. J. Sheesley, *Organizers, Presiding* Lone Star 103

## *Battery Materials, Chemistries, and Strategies*

J. Larson, *Organizer, Presiding* Texas 116

## *Chemical Biology*

A. T. Wright, *Presiding* Texas 117

## *Engineering of Biochemistry for Enhanced or Novel Activity*

J. Clinger, I. V. Korendovych, *Presiding* Texas 115

## *F-elements: Structure and Applications*

A. E. Gorden, *Organizer*, J. Ducilon, *Presiding* Texas 113

## *Materials and Interfaces*

Z. Zhang, *Organizer, Presiding* Texas 118

## *Opportunities at the Interface of Academia and Industry*

D. Anderson, *Organizer, Presiding* Ranger 109

## *Organic Chemistry (General)*

N. Matsumoto, *Organizer, Presiding*. Texas 114

## *Polymers and Sustainability Challenges 2*

R. Foudazi, *Organizer, Presiding* Ranger 106/107

## *Assessments for Learning and Engaging with Students*

A. Sra, M. Stover, *Organizers, Presiding* Ranger 110

# Tuesday Evening Plenary Lecture

## *Gooch-Stephens Award Lecture*

J. Clinger, *Organizer, Presiding*    McLennan Hall    5:45 pm

## **Is a blind watchmaker the same as a blind neural net?**

Professor Andrew Ellington

The University of Texas at Austin

## Tuesday Evening: Reception and Posters

Brazos Ballroom    7-9 pm

### *Analytical Chemistry Poster Session*

E. S. Gallagher, *Organizer*

### *Inorganic Chemistry Poster Session*

M. AKRAM, *Organizer*

### *Physical Chemistry Poster Session*

K. L. Shuford, *Organizer*

WiFi Network Name: ccpublic    Password: wacocc17

## TUESDAY MORNING

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### *Chemical Biology*

A. T. Wright, *Presiding*

Texas 117

**8:00 467.** Lighting up cellular chloride transport. **J. Tutol**, W. Ong, H.C. Kam, S. Phelps, W. Peng, H. Goenawan, S. Dodani

**8:30 468.** Development of a fluorescent lateral flow test for the detection of the obesity biomarker leptin. **M. Ortiz**, K. Kourentzi, R.C. Willson, M. Rito-Palomares, M. González-González

**9:00 469.** Digital light processing (DLP) fluorescence microscopy for 3D microprinting and single cell photoactivation. **A.R. Lippert**

**9:30 470.** Unraveling the molecular interactions of trehalose glycolipids with bioorthogonal chemical approaches. **J.A. Buonomo**

**10:00** Coffee Break.

**10:30 471.** Leveraging catalytically promiscuous enzymes to probe the basis for enzyme specificity and epistasis. D. Truong, A.W. McMillan, D. Odokonyero, R. Dharmatti, D. Suriadinata, R. Skouby, J. Huddleston, S. Fults, C. Davila, R. Bayana, M. Zhu, K. Hull, D. Romo, F.M. Raushel, **M. Glasner**

**11:00 472.** Biomolecular condensates promote cancer signaling. **J. Guan**

**11:30 473.** Responsive protein switches to probe cell and tissue behavior. **B. Belardi**

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### *Computational and Theoretical Chemistry*

K. L. Shuford, *Organizer*

U. De Alwis, *Presiding*

Texas 116

**8:00 474.** Enhancing material development through multiscale molecular modeling: case studies in viscosity prediction and polymer optimization with Simcenter Cugli. J. Lopez, T. Sweere, **R. Aglave, C. Tourani**

**8:20 475.** Simulations of core-hole induced attosecond electron dynamics. **L. Kurkowski**, T. Hua, K. Lopata

**8:40 476.** Hybrid and mixed basis set strategies for XPS calculations of small water clusters. **A. Delgado**, D. Matthews

**9:00 477.** Simulating fluorescence for mesoscale molecular aggregates. **T. Gera**, A.J. Hartzell, D. Raccah

**9:20 478.** LModeA Extension to Periodic System: The gateway for a quantitative characterization of normal modes in neutron scattering and terahertz spectroscopy. **F. Bodo**, A. Erba, E. Kraka

**9:40 479.** Computer-aided design of 2D transition metal-based alloy compounds for sustainable energy applications. **U. De Alwis**, V. Choutipalli, K.L. Shuford

**10:00** Coffee Break.

**10:20 480.** Mechanistic insights into S-depalmitoylase activity of Cln5 protein linked to neurodegeneration and Batten disease: A QM/MM study. **Y. DANGAT**

**10:40 481.** *Withdrawn*

11:00 482. Signatures of hydrogen bonding in soft X-ray spectroscopy. **A. Yousaf**

11:20 483. Predicting halogen bond properties through machine learning. **D. Devore**, K.L. Shuford

11:40 484. Noncovalent interactions in apo-myoglobin proteins revealed through local vibrational mode theory. **J. Antonio**, E. Kraka

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## ***Electrocatalysis: Molecular and Material Approaches to Electrified Chemical Processes***

D. Boucher, *Organizer, Presiding*

Lone Star 104

8:00 485. Quantum-mechanical molecular dynamics simulations and analysis of graphene-catalyzed oxygen reduction reactions. **R.A. Grove**, C.F. Negre, M.E. Wall, I. Matanovic, J.D. Finkelstein, A.M. Niklasson

8:30 486. Metal-free C–H amination via bidirectional proton-coupled electron transfer (PCET) at anodically generated iodanyl radical intermediates. **P. Thai**, B.L. Frey, L.H. Patel, R. Lalis, Z. Song, R. Carmieli, O. Gutierrez, D. Powers

9:00 487. Symmetry driven silicon-molecule interfacial design for photoelectrochemical hydrogen generation. **C.D. Hallock**, J. Brinker, M.J. Rose

9:30 488. Interfacing high-throughput electrosynthesis and mass spectrometric analysis of azines. **E.A. Hirtzel**, K.M. Kulesa, X. Yan, L.A. Baker

10:00 Coffee Break.

10:30 489. Deciphering the Role of Aromatic Cations in Electrochemical CO<sub>2</sub> Reduction: Interfacial Ion Assembly Governs Reaction Pathways. **W. Guo**, B. Liu, S.R. Anderson, S.G. Johnstone, M.A. Gebbie

11:00 490. Confocal Raman microscopy in the study of electrode-supported catalyst and thin films. **C.L. Korzeniewski**

11:30 491. Mapping the local electrocatalytic activity and selectivity via hybrid SECM-SECCM. **C. Ryu**, **H. Ren**

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## ***F-elements: Structure and Applications Part 1***

A. E. Gorden, *Organizer*

J. Ducilon, *Presiding*

Texas 113

8:00 Introductory Remarks.

8:10 492. Discovery and strategic synthesis of *f*-element quantum intermetallics. **J. Chan**

8:40 493. Fostering new aspects of organolanthanide pincer chemistry: Applications for lanthanide luminescent complexes. **S. Chowdhury**, A.B. Altman, A.R. Fout

9:00 494. Synthesis and characterization of *d-f* heterometallic clusters. **B.G. Barnes**, A. Briseño, C. Windorff

9:20 495. Engendering orbital specific control in lanthanide complexes. **A.B. Altman**, S. Chowdhury, P. Reuel, H. Jemison, R. O'Shea

9:50 Coffee.

**10:30 496.** Unexpected products from lanthanide coordination reactions: Consequences and solutions. **E. Fatila**

**11:00 497.** Pursuit of organouranium nitride clusters and preparation of a transuranium facility. **C.J. Windorff**

**11:30 498.** F- element complexes with functionalized salophen-type mixed donor ligands. **A.E. Gorden**

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## ***Materials and Interfaces***

Z. Zhang, *Organizer, Presiding*

Texas 118

**8:00 499.** Examining technologically relevant materials via interface engineering. **A. Yost**

**8:30 500.** Digital atomically precise lithography for direct write and nanoImprint mask writing. **J.N. Randall,** J.H. Owen, J.B. Ballard, U. Fuchs

**9:00 501.** Enhanced operational stability of perovskite light-emitting devices through differential ion motion. **J. Slinker**

**9:30 502.** Element-sensitive characterization of high-entropy oxide perovskite thin films. **A. Farhan**

**10:00** Coffee break.

**10:30 503.** Fundamental investigation of the interfacial properties of CoCrFeNi high entropy alloy. F.A. McKay, A.N. Okafor, D.P. Young, P. Sprunger, **Y. Xu**

**11:00 504.** Advanced surface engineering coating technologies for industry applications. **J. Lin,** V. Zorbas Poenitzsch

**11:30 505.** Phase transition and melting of oxide via plasmonic heating. **Z. Zhang**

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## ***Metalloenzyme Design***

I. V. Korendovych, *Organizer, Presiding*

Texas 114

**8:00 506.** Hybrid metalloproteins for photocatalytic CO<sub>2</sub> and proton reduction. **G. Ghirlanda,** A. Banerjee, M. Rahman

**8:40 507.** Copper-catalyzed cross coupling approaches to selective PTM modifications. **Z.T. Ball**

**9:20 508.** Achieving catalytic hydroxylation of methane through manipulation of P450BM3 biotransformations with decoy molecules. **O. Shoji**

**10:00** Coffee break.

**10:30 509.** Spectroscopic evaluation of the stability of the New Delhi metallo- $\beta$ -lactamase (NDM-1).. **S. Pennock,** **G.A. Caputo**

**11:00 510.** Designing catalytic amyloids to function as highly efficient metalloenzymes. **L.R. Marshall,** I.V. Korendovych

**11:30 511.** How does modulation of the primary, secondary, and outer-sphere interactions in de novo-designed artificial Cu proteins (ArCuPs) affect their electron transfer and C-H peroxidation functionality?. **S. Chakraborty,** D. Prakash, S. Mitra, S. Sony

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## ***Novel Approaches to Drug Delivery***

R. R. Kane, *Organizer*

J. J. Gassensmith, *Organizer, Presiding*

Texas 115

**8:00 512.** Guns, germs, and MOFs (and COFs!). **J.J. Gassensmith**

**8:30 513.** Developing drug delivery systems for chronic infectious diseases. **h. Smyth**

**9:00 514.** Image-guided drug delivery using radiation therapy: Strategic trade-offs in chemical design. **M. Miller**

**9:30 515.** Engineering cell based drug delivery with chemically self-assembled nanorings. **C.R. Wagner**

**10:00** Coffee Break.

**10:30 516.** Biomaterial for *in situ* manufacturing and delivery of CAR t-cells. **Y. Brudno**

**11:00 517.** Bioengineering cell-based therapeutics. **O. Veiseh**

**11:30 518.** Amphiphilic polycaprolactone diblock copolymers for drug delivery of anticancer drugs. H. Polara, M.C. Biewer, **M. Stefan**

**12:00 519.** Lectin drug conjugates targeting high mannose N-glycans. S. Kurhade, **M.P. Farrell**

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## ***Polymers and Sustainability Challenges 1***

R. Foudazi, *Organizer, Presiding*

Ranger 106/107

**8:00** Introductory Remarks.

**8:05 520.** Stochastic model regression and analysis of repeat unit sequencing of Poly(lactide-co-glycolide). **N.A. Lynd**

**8:30 521.** Sugars as a platform for functional materials. **S.L. Kristufek**

**8:55 522.** Self-contained cost effective plastic recycling facilities:. **R.K. Vaidyanathan**, S.P. Chaudhari, C. Switzer, A. Maheshwari, F.D. Blum

**9:20 523.** Dynamic covalent polymer networks: Stereochemically controlled shape morphing. **S.A. Sukhishvili**

**9:45** Intermission.

**10:15 524.** Sustainability through microarchitecture. **W. Voit**

**10:40 525.** Engineering and chemistry considerations to enable a circular economy of polymers. **D.S. Germack**

**11:05 526.** Valorization of cottonseed byproducts for bioplastic (biocomposite, biofilm) applications. **Z. He**, S. Nam, H.N. Cheng, A. Biswas

**11:30 527.** Carpets and bottle parts: A match made in the lab. **F.D. Blum**, R.Y. Azarfam, A. Maheshwari, L.A. Kamran, A.S. Nayar, S.P. Chaudhari, C. Switzer, J.C. Hanan, R.K. Vaidyanathan

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## ***Assessments for Learning and Engaging with Students***

A. Sra, M. Stover, *Organizers, Presiding*

Ranger 110

**8:30** Welcome and Brief Introduction.

**8:35 528.** Assessments: Time for a change. **A. Sra**

**9:05 529.** Using particulate representations to assess students in introductory chemistry courses. **S.G. Prilliman**

**9:30 530.** Microcredentials in the co-curricular undergraduate experience. **R.T. Macaluso**

**10:00** Coffee Break.

**10:30 531.** Contextualized Chemistry Learning Materials and the Impacts on General Chemistry Students' Learning Outcomes. **I. Sristy**, Y. Vasquez, J. Mutambuki

**10:55 532.** Introducing activities to enhance literature reading skills in biochemistry. **M. Kopecki-Fjetland**

**11:25 533.** Examining analytical chemistry student interpretation of IR spectra. **M. Atkinson**

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## ***Atmospheric Chemistry***

Y. Li, R. J. Sheesley, *Organizers, Presiding*

Lone Star 103

**10:30 534.** Modeling atmospheric decamethylcyclopentasiloxane (D5) concentrations in Houston using the community multiscale air quality model. **H. Yim**, A. Dodero, Y. Zhang, Q. Ying

**10:45 535.** Atmospheric oxidation capacity and air quality trends in Texas due to long-term climate and anthropogenic emission scenarios. **A. Gonzalez**, Q. Ying

**11:00 536.** Comparison of mobile and stationary measurement of formaldehyde by Picarro's G2307 and Aero-Laser's AL4021. **P. Sharma**, S.L. Alvarez, S. Yoon, J.H. Flynn, S. Usenko, R.J. Sheesley

**11:15 537.** Quantification of atmospheric alkanes and polycyclic aromatic hydrocarbons (PAHS) in the arctic region. **P.K. Verma**, T. Matthews, R.J. Sheesley

**11:30 538.** Role of Aerosol Chemical and Physical Properties in Cloud Formation. **S.D. Brooks**, Z. Lei, T. Pena, S.A. Thompson, B. Chen, B.H. Matthews, A. Rapp, C.J. Nowotarski

**11:45 539.** Identification and quantification of Per- and Polyfluoroalkyl Substances (PFAS) using Vocus 2R Chemical Ionization Mass Spectrometer (CIMS) with NO<sup>+</sup> Reagent Ion. **S. Gagan**, M. Olin, S. Niu, A. Dodero, M.J. Davern, G.V. West, B.J. Turpin, J. Surratt, Y. Zhang

## **TUESDAY AFTERNOON**

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### ***Atmospheric Chemistry***

Y. Li, R. J. Sheesley, *Organizers, Presiding*

Lone Star 103

**1:00 540.** Spectroscopy and Photochemistry of Wildfire Brown Carbon. **A.W. Harrison**

**1:15 541.** Identification of biomass burning smoke influence using aerosol optical properties and hydrogen cyanide in Fort Worth, Texas. **J. Poudel**, L. Senkbeil, M. Mehra, S. Yoon, J.H. Flynn, T.I. Yacovitch, C. Daube, E. Fortner, S. Usenko, R.J. Sheesley

**1:30 542.** Identification and characterization of biomass burning smoke in Houston, TX: Insights from the BC2 Aerosol Optical Network. **M.T. Ramirez**, L. Senkbeil, M. Mehra, S. Shrestha, J. Flynn, R.J. Sheesley, S. Usenko

**1:45 543.** Assessing air quality benefits of better managing natural and working lands in California. **S.M. Lindsey**, Y. Li

**2:00 544.** Investigating climate impacts of reducing methane emissions from U.S. landfills. **A. Folorunsho**, Y. Li

**2:15 545.** Estimating surface methane concentrations across the U.S. using Artificial Neural Network (ANN) and their application for tracking landfill emissions. **M. Bade**

**2:30** Discussion.

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### ***Battery Materials, Chemistries, and Strategies***

Cosponsored by ENFL

J. Larson, *Organizer, Presiding*

Texas 116

**1:00 546.** Unravelling the fundamental issues for improving lithium metal anodes based on three-dimensional nanostructured carbon hosts. **J. Li**, S. Rajendran, a. sekar

**1:28 547.** Structural, Electronic, and Chemical Evolution at Interfaces: Impact on Meso- and Macroscopic Properties. **P. Balbuena**, S.P. Beltran, D. Kuai, F. Ospina-Acevedo

**1:56 548.** Materials design strategies for elastic ceramic-based solid state electrolytes in advancing performance in lithium metal batteries. S. Bashir, **J.L. Liu**

**2:24** Coffee Break.

**2:54 549.** Rapid synthesis and surface engineering of oxide solid electrolytes for lithium-metal batteries. **H. Khani**

**3:18 550.** Analysis and simulation of lithium-metal anodes of rechargeable batteries for vehicular transport. **J.M. Seminario**

**3:42 551.** Chemical and physical activation methods to develop highly porous materials for Li-S Batteries. **N. Siraj**, A. Oyeade, I. Denmark

**4:06 552.** Biomaterials for lithium-ion batteries. **H. Ardebili**, **N. Khiabani**, Q. Fu, M. Yuan, S. Adaryan, J. Fan, K. Bourland, M. Kammoun, D.F. Rodrigues

**4:30 553.** Regulating crystallization at dynamic electrochemical interfaces in battery electrodes. **K.J. Zheng**

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## ***Chemical Biology***

A. T. Wright, *Presiding*

Texas 117

**1:00 554.** DNA-based tools for chemical and biological sensing. **D. Samanta**

**1:30 555.** Ubiquitin azapeptide esters as next-generation activity-based probes for mapping cysteine enzyme activities in the ubiquitin-proteasome pathway. **W. Liu**

**2:00 556.** Broadening the ligandable proteome using tyrosine-reactive electrophiles. D.M. Leace, H.M. Budaraju, N. Reddy, **K. Hsu**

**2:30 557.** Aza-enediynes: From DNA cleavage agents to covalent probes for protein kinases. **S.M. Kerwin**

**3:00** Coffee Break.

**3:30 558.** Using chemical biology tools to study amino-acid based (proton-coupled) electron transfer. **C. Tommos**

**4:00 559.** Crosslinking technologies for studying viral and allergenic protein complexes. **S.M. Chowdhury**, A. Talukder, S. Cornelius

**4:30 560.** Photocrosslinking sugars for glycoconjugate interaction discovery. A. Ghorashi, R. Konada, **J.J. Kohler**

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## ***Engineering of Biochemistry for Enhanced or Novel Activity***

J. Clinger, I. V. Korendovych, *Presiding*

Texas 115

**1:00 561.** Incorporation of synthetic metal complexes into heme acquisition protein HasA for selective photosterilisation of *Pseudomonas aeruginosa*. **O. Shoji**

**1:40 562.** Protein engineering to combat pathogens. **B. Berger**

**2:20 563.** Ancestral proteins as scaffolds for enzyme engineering and evolution. **J. Sanchez-Ruiz**

**3:00** coffee break.

**3:30 564.** Stimuli-responsive materials for wound healing and drug delivery. **O. Makhlynets**

**4:00 565.** NMR-guided directed evolution. **I.V. Korendovych**

**4:30 566.** Development of biologically equivalent simulant for forensic applications. **J.L. Liu**, E. Rancourt, M. Sandoval, S. Bashir

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## ***F-elements: Structure and Applications***

A. E. Gordon, *Organizer*

J. Ducilon, *Presiding*

Texas 113

**1:00** Introduction and Discussion.

**1:10 567.** Design Principles for Insertion Electrodes and Solid Electrolytes of Anion Batteries. **S. Banerjee**

- 1:40 568.** Tuning the  $\text{Ru}_3\text{Sn}_7$  structure type with samarium. **K. Brown**, B. Schundelmier, K. Wei, G. McCandless, J. Chan
- 2:00 569.** Promoting covalent bonding in lanthanides: Reduced lanthanide-aluminum heterobimetallic complexes. **P. Reuel**, A.B. Altman
- 2:20 570.** New developments in actinide organometallic chemistry. **J.L. Kiplinger**
- 2:50** Coffee.
- 3:30 571.** Predicting structure type and properties in the  $\text{Ln}_2\text{M}_3\text{X}_5$  family. **M. Plata**, S. Smith, J. Chan
- 3:50 572.** Enabling wide-gamut human-centric display lighting. **S. Hariyani**, X. Xing, M. Amachraa, J. Bao, S. Ong, J. Brgoch
- 4:20 573.** Coordination network of trivalent plutonium with bromoterephthalate and glutarate entities. **R.A. Zehnder**
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## ***Materials and Interfaces***

J. Larson, Z. Zhang, *Organizers, Presiding*

Texas 118

- 1:00 574.** Theory-guided design of "golden triangle metal-inorganic frameworks" (GT-MIFs) with chemisorption-active macrometallo-cyclic inorganic linkers. **M.A. Omary**, R. Yasmeen, N.G. Rabah, S.M. Islam, C.M. Williams
- 1:30 575.** Data-driven Analysis and Atomistic Simulations of Electrical Conductivity in Two-dimensional Metal-organic Frameworks. **Y. Shi**, F.A. Shakib
- 1:45 576.** Layer-by-layer assembly and structured color of  $\text{Ti}_3\text{C}_2\text{Tz}$  MXene/polyelectrolyte heterostructures. **N. Neal**, P. Stevenson, M. Radovic, M. Green, J. Lutkenhaus
- 2:00 577.** Freeform additive manufacturing of carbon fiber reinforced composites using dielectric barrier discharge-assisted Joule heating. **S. Dasari**, M. Green
- 2:15 578.** High-throughput screening, crystal structure prediction, and carrier mobility calculations of organic molecular semiconductors as hole transport layer materials in perovskite solar cells.. **M. Faruque**, S. Akter, D. Limbu, K.V. Kilway, Z. Peng, M. Momenitaheri
- 2:30 579.** Synthesis and characterization of the novel Zintl Phase  $\text{Eu}_{14}\text{InAs}_{11}$ . **O. Pokhvata**
- 2:45 580.** Impact of selected ionic liquids on the properties of metal halide perovskites. **M. Grubbs**, S. Dzyuba, J. coffer
- 3:00** Coffee Break.
- 3:30 581.** From chemical expertise to AI precision: Progress in forensic fingerprint agent development and analysis. **J.L. Liu**, A. Enz, Z. Wang, S. Bashir
- 3:45 582.** Upconverted Hot electrons in Mn-doped quantum dots can drive efficient solvated-electron mediated chemical transformation. **C. Orrison**, D. Son
- 4:00 583.** Novel synthesis of modified ceria nanomaterials. **C.C. Watkins**
- 4:15 584.** Sustainable Geopolymer Composite Reinforced with Natural Fibre: Preparation and Characterization. **Z. MOUJOD**, A. El Bouari, O. Tanane
- 4:30 585.** Crystal and electronic structure characterization of  $\text{Ba}_3\text{As}_2\text{O}$  and  $\text{Ba}_{32}\text{As}_{23}\text{O}_2$ , two new ternary barium oxyarsenide Zintl phases. **S. Watts**, L. Wingate, S. Baranets

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## ***Opportunities at the Interface of Academia and Industry***

D. Anderson, *Organizer, Presiding*

Ranger 109

**1:00 586.** *Withdrawn*

**1:30 587.** Promote industry careers through academia and water sector collaborations. **H. Adams**, C. Fulton, M. Southard, J. Price, S. Reeder, C.A. Hansen, E. Appleton, J. Shao, D. Nix, K. Mahmud, B. Colvin

**2:00 588.** Bridging the Gap: AI-driven innovations in academic and industrial drug discovery. **D. Anderson**

**2:30** Networking Break.

**3:00 589.** Translating research into innovations with impactful applications. **S. Anderson**

**3:30 590.** Closing the gap through entrepreneurial education. **S.M. Kerwin**

**4:00 591.** What now? Next steps for tech transfer and startup development. **L.E. Martinez**

**4:30** Panel Discussion and Q&A.

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## ***Organic Chemistry (General)***

N. Matsumoto, *Organizer, Presiding*

Texas 114

**1:00 592.** Stilbenes: Source plants, chemistry, biosynthesis, pharmacology, application, and problems related to their clinical application: A comprehensive review. **T.T. Teklehaimanot**

**1:20 593.** Synthesis, biological assessment and molecular docking studies of new pyrazolone compounds as potential anticancer agents against non-small cell lung cancer. **P. Anim Addo**, S. Murru, S. Dahal

**1:40 594.** Non-toxic polysaccharide-based anti-cancer drug delivery system utilizing Osajin and polymerized fenugreek seeds. **E. Soward**

**2:00 595.** *Withdrawn*

**2:20 596.** Development and synthesis of methylene spacer functionalized prodrugs of TLR4-signaling inhibitor TAK-242 (Resatorvid) for controlled delivery. **C.A. Sells**, R. Gaykar, J.H. Kostyo, R.R. Kane

**2:40 597.** Photocatalyzed strain-release retro-Diels-Alder reaction. P. Das, **S. Kharbanda**, J.D. Weaver

**3:00** Coffee Break.

**3:30 598.** New strategies for the synthesis of heterocyclic organotellurium compounds. K.M. Gaborit, A.K. Turner, S.R. Ponzo, F.R. Fronczek, **T. Junk**

**3:50 599.** *Withdrawn*

**4:10 600.** Synthesis, Structure, and Optical Properties of 8-Anilino BODIPYs. **K.H. Pannell**, A. Metta-Magana

**4:30 601.** *Withdrawn*

**4:50 602.** Synthesis and crystal structures of 18-crown-6 stabilized potassium salts of dioxalatodiphenylstannate and oxalatotriphenylstannate. **J. Sun**, **M. Rahman**, Y. Torres, T. Greaves, X. Song

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## ***Polymers and Sustainability Challenges 2***

R. Foudazi, *Organizer, Presiding*

Ranger 106/107

**1:30 603.** Improving photovoltaic module lifetimes via creation of novel, low coefficient of thermal expansion backsheet polymers. **E.M. Redline**, E.M. Nagel, A.O. Scarlett, C.L. Staiger

**1:55 604.** Efficient photobase generators towards sustainable 3D printing. **Z.A. Page**

**2:20 605.** Spirocyclic inter-crosslinked polymer membranes: a materials platform to implement sustainable separations in gas and liquid phase. L.C. Condes, **M. Galizia**

**2:45 606.** Polymer films for sustainable solid-state capacitive energy storage and separation membranes. **A. Karim**

**3:10** Intermission.

**3:30 607.** Polyelectrolyte solutions and brushes. **A. Marciel**

**3:55 608.** Ion-mediated reprocessable polymer thermoset. **S. Xie**

**4:20 609.** *Withdrawn*

**4:45 610.** High surface area crosslinked CNT-Microgel or CNT-CNT networks for sustainable agricultural and environmental applications. **Y. Gao**

**5:10** Concluding Remarks.

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## ***Assessments for Learning and Engaging with Students***

A. Sra, M. Stover, *Organizers, Presiding*

Ranger 110

**1:35** Welcome and Brief Introduction.

**1:40 611.** In-state vs. out-of-state readiness for general chemistry. **D.S. Mason**, B. Mamiya

**2:10 612.** How word choice and phrasing can affect student performance in multiple choice assessments. **G.R. Dieckmann**, **S.M. Taylor**, B. Hefley, C.S. Tucker King, R. Davis, M. Islam

**2:35 613.** Using competency based assessment and a novel outcome framework to improve engagement in general chemistry. **J.A. Hebda**

**3:00** Coffee Break.

**3:30 614.** Teamwork in the chemistry lab: instruction, practice and assessment. **E. Trufan**, E. Bouhoutsos-Brown

**3:55 615.** A novel way of teaching and assessing Organic II labs. **E.A. Nalley**

## TUESDAY EVENING

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### *Gooch-Stephens Award Lecture*

J. Clinger, *Organizer, Presiding*

McLennan Hall

5:45 Introductory Comments.

6:00 **616.** Is a blind watchmaker the same as a blind neural net? **A.D. Ellington**

6:55 Gooch-Stephens Award.

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### *POSTER SESSIONS and RECEPTION*

Brazos Ballroom

7:00 - 9:00 pm

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### *Analytical Chemistry Poster Session*

E. S. Gallagher, *Organizer*

**617.** From lab bench to career: Developing essential skills in chemistry labs. **E. Trufan**, E. Bouhoutsos-Brown

**618.** Analytical research & development at Merck: Leveraging diverse expertise to be partners in problem solving. **E.L. Schwalm**

**619.** Fiber-optic studies of the kinetics of myoglobin oxidation. **N.U. Dickson**, S. Mojeeb, D.E. Thompson

**620.** Optimizing tissue mimicking phantoms for gold nanorod photoacoustic imaging. **B.C. Fallon**, N. Mathuria, A. Martino, R. Bouchard, C.S. Filgueira

**621.** Nonlinear laser wave-mixing spectroscopy coupled with capillary electrophoresis and microchips for sensitive detection of SARS-CoV-2 biomarkers. **N. Shatirishvili**

**622.** Deep Ultraviolet Laser Ablation Electrospray of Proteins with Ion Mobility Mass Spectrometry. **K.B. Hines**, N. Feizi, T. Solouki, K.K. Murray

**623.** Comparing the ionization response factors of single-stranded DNA binding protein (SSB) oligomers bound to ssDNA using native mass spectrometry. **A.J. Blue**, M.G. Bannon, E.S. Gallagher, M.A. Trakselis

**624.** Molecular dynamics simulations of native-protein charging in electrosprayed droplets with experimentally relevant composition. **M.S. Cordes**, M.G. Bannon, E.S. Gallagher

**625.** Zn(II) affinity of a Zinc Finger Motif peptide model from competitive threshold collision-induced dissociation. **R.A. Adomako**, M.B. Owusu, K.N. Senyah, P. Asare, L.A. Angel

**626.** Comparing mice cardiac proteins extracted with different buffers using SP3 and SP4 clean-up methods. **S. Senarathne**, M.L. Law, E.S. Gallagher

**627.** Comparison of Byonic vs. GlycanFinder for identification and quantification of glycopeptides in biological samples. **V. Sandilya**, Y. Mechref

**628.** Chronic glyphosate exposure alters serum *N*-glycan profiles in rats. **M. Adeniyi**, C.D. Gutierrez-Reyes, J. Chávez-Reyes, B.A. Marichal-Cancino, J. Solomon, M. Fowowe, S. Onigbinde, J.A. Flores-Rodriguez, M. Al Amin Bhuiyan, Y. Mechref

629. Comparing solvents used for separation of carbohydrates in positive- and negative-ion mode mass spectrometry to improve ionization efficiency. **L.A. Garber**, A.N. Thurman, E.S. Gallagher
630. Characterizing carbohydrate isomers of varying size with in-ESI HDX-MS. **A.V. Quintero**, E.S. Gallagher
631. Utilizing  $\text{Co}^{2+}$  and electron-transfer higher-energy collisional dissociation to distinguish isomeric, sialylated human-milk oligosaccharides. **H.T. Wilson**, D.T. Gass, E.S. Gallagher
632. Identifying dysregulated lipids in human brain of Alzheimer's disease and their effects on biological pathways. **A. Sanni**, A.I. Bennett, M. Adeniyi, Y. Mechref
633. Lipid analysis of milk varieties using liquid chromatography-mass spectrometry. **S.W. Raja Hewage**, B. Williams, H. Fernando
634. Does Texas wildflower honey smell of Texas wildflowers? A GC-MS/O analysis. **M.J. Maguire**, T. Holland, K. Oyler
635. Metal removal and fractionation of asphaltene samples for multimodal characterization via derivatization for Kendrick Mass deficiency manipulation. **T. Thilakarathna**, B.A. Nyaaba, S. Makhani, T. Solouki, P.J. Farmer
636. Time-resolved extraction and quantitative detection of metals present in asphaltene samples: Using EPR, ICP MS, IM-MS, NMR, Synchronous Fluorescence, and UV-Absorption for asphaltene characterization. **B.A. Nyaaba**, T. Thilakarathna, S. Makhani, P.J. Farmer, T. Solouki
637. Direct lithium extraction from complex waste-streams based on electrochemical ion insertion in a 1D tunnel-structured positive electrode. **C.A. Larriuz**, J.L. Carrillo, A. Ezazi, H. Kohl, S. Banerjee
638. Lithium recovery from discarded lithium-ion batteries by electrodialysis. **K. Dumre**, C.P. Shelor
639. Unveiling synergistic dopants in copper, selenium manganese co-doped nickel sulfide metal organic framework electrocatalysts for superior urea electrooxidation and efficient hydrogen liberation. **y. sana**
640. Preparation of copper oxide/(Cu-S)<sub>n</sub> metal-organic framework/reduced graphene oxide hierarchical structure for electrochemical quercetin sensing. S. Velmurugan, M. Tse, X. Lin, Y. Yu, **S. Cheng**, K. Lu
641. Analytical challenges and considerations for Iodine detection in Urine. **J. Girme**
642. Electrocatalytic properties of human liver subcellular fractions: Comparison of S9 fractions and human liver microsomes. **E. Alwarsh**, D. Medina, C.T. Walgama
643. Forbidden ion transport through cation exchange membranes. **C. Chaudhary**
644. Functionalization of high-density polyethylene capillaries for open tubular ion chromatograph. **E. Yousef**
645. Zirconia: A fluoride selective stationary phase for anion chromatography. **C. Warren**, P.K. Dasgupta, C.P. Shelor
646. Simple evaporative concentration method for the measurement of per- and polyfluoroalkyl substances in water matrices. **C.V. Odinaka**, C.P. Shelor
647. Probing the surface assembly of tetraphenyl porphyrin molecules linked with tin tetrachloride using atomic force microscopy. **Q. Do**, J.C. Garno

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## ***Inorganic Chemistry Poster Session***

**M. AKRAM**, *Organizer*

648. Exploration of s-block coordination chemistry via aggregation manipulation. **K. Martinez-Fair**, S. Yruegas
649. Accessing phenoxyimine calcium complexes via manipulation of the Schlenk equilibrium. **K. Birkhoff**, I. Lin, S. Yruegas
650. Isolation and reactivity of multidentate s-block carbene complexes. **D.N. Rodriguez**, S. Yruegas

651. Use of *para*-hydrogen to elucidate first-row reaction mechanisms. **B.M. Vaught**, A. Fout
652. Carboxylate-rich iron(III) complexes as phosphoesterase mimics in aqueous media. **E.T. Iqbal**, M.M. Mamori, H. Arman, G.T. Musie
653. Probing the influence of phenanthroline-based ligands on group 11 metal-ethylene complexes: discoveries and catalytic prospects. **D. Karade**, R. Dias
654. Photophysical studies of the three coordinate Cu(I)  $\beta$ -diketiminato triphenylphosphine complexes. **A. Kumar**
655. Synthesis and primary characterization of Histidine-Salicylaldehyde metal complexes using microwave assisted technique. **D. Toole**, G. Chiarella, J. Ndongou
656. Ligand-to-ligand charge transfer (LLCT) transitions in square-planar metal-bipyridyl complexes of heteroatom-substituted maltol derivatives. **M. Usman**
657. Synthesis of antimony compounds with phosphorus and nitrogen based ligands. **L.D. Hale**, F.P. Gabbai
658. New fused-pincer ligand allowing the creation of novel bimetallic complexes. **J. Daum**
659. Using a Lewis basic bis-thiourea ligand to stabilize copper(I) complexes and explore oxygen activation. **S. Gupta**, A.R. Fout
660. Exploring the coordination chemistry of transition metal cobalt with pyrazole-based tripodal ligands. **J. Smith**, G. Lyubartseva
661. Complexation of a quinoline-based ambiphilic ligand platform to rhodium. **S. Bedajna**, F.P. Gabbai
662. Copper(II) phenanthroline complexes with polyphenols: Therapeutic agents for the treatment of hypertension and cardiovascular diseases. **V. Torres**, H. Arman, R.A. Adrian
663. **Withdrawn**
664. Novel cobalt(II) and copper(II) imidazole and phenanthroline complexes: Relationship between structure and antifungal efficacy. **O. Towers**, C.G. Pierce, H. Arman, R.A. Adrian
665. Synthesis and Characterization of Light-Triggered Metal Complexes for Cancer Treatment. **D. Lucas**, A. Talgatov, G. Shi, G. Kaur, A. Vali, C. Cameron, S.A. McFarland
666. **Withdrawn**
667. Investigation of the DSF/Cu reaction using LC HD MS. **j. lyons**
668. Approaches for optimization of the photodynamic therapy (PDT) efficiency with metallodrug photosensitizers in cancer treatment. **G. Shi**, A. Talgatov, A. Vali, D. Lucas, C. Cameron, S.A. McFarland
669. Synthesis and characterization of novel neodymium(III) bipyridine complexes: Structural analysis and theoretical correlation. **G.Y. Berrocal**, H. Arman, R.A. Adrian
670. Metal-Metal interactions in uranyl salophen-type complexes with the addition of early transition metals. **J. Ducilon**, J. Gorden, A.E. Gorden
671. Samarium(III) complexes with substituted 1,10-phenanthroline derivatives: Synthesis, characterization and crystal structures. **M. Cartwright**, H. Arman, R.A. Adrian
672. Lanthanide open networks incorporating derivatives of terephthalic acid. **D. Rios**, **E. Brandon**, **W. Best**, R.A. Zehnder
673. Lanthanide coordination polymers as surrogates to create isomorphous actinide counterparts. **T. Hodge**, **J. Turner**, R.A. Zehnder
674. Stabilizing ion pairs to access carbene-pyridine gallium complexes. **K.J. Francis**, S. Yruegas
675. Incorporating Lewis Acids into heterogeneous supports. **S. Ranasinghe**, C. Martin
676. Carborane-arene hybrid boron doped PAHs. **Y. Li**, M. Tamizmani, M. AKRAM, C. Martin
677. Improved solubility and the chlorination of the 1-*Closo*-Carborane Anion. **J. Raker**

678. Synthesis of azaborapyrenes from fused boroles. **A. Begum**, H. Zacharias, J. Han, T. Bartholome, T.B. Marder, C. Martin
679. Hydroboration of alkenes utilizing boronic acid catalysts. S. Mummadi, **R.L. Perry**
680. Exploring the reactivity of electrophilic boron compounds. **R. Thornton**, C. Martin
681. Polyborylated Lewis acids in Frustrated Lewis Pair (FLP) catalysis. **E. Sarkissian**, C. Krempner
682. Frustrated Lewis Pair Reactivity of Tris(*ortho*-carboranyl) Borane. **K. Vashisth**, S. Dutta, M. AKRAM, C. Martin
683. Stimuli-responsive donor-acceptor systems containing carbenium ions. **C. Lee**, F.P. Gabbai
684. Alloyed metal nanoclusters for triplet sensitizers. **K. Binkley**, S. Maiti, U. Ariyaratna, M. Kenari, A. Das
685. Enhancing PVDF triboelectric nanogenerators with CuFeO<sub>2</sub>, CuCoO<sub>2</sub>, CuMnO<sub>2</sub>, and CuGaO<sub>2</sub> delafossites. A. James, **E. Varughese**, D. Phillips, F. Viesca, S. Mohan, M.J. Uddin
686. Impact of synthesis route on Ti<sub>3</sub>C<sub>2</sub> MXene properties and applications. **S. Pas**, K. Arole, J.L. Lutkenhaus, M. Radovic, M. Green
687. Alloying-induced expansion in a metastable tunnel-structured cathode. **Y. Chiang**, P. Schofield, J. Ponis, S. Chakraborty, G. Agbaworvi, J.L. Carrillo, J. Ayala, B.J. Schultz, L. Gobbato, S. Banerjee
688. Redox-active Metalloligands as hosts for Cerium-based Photocatalysts. **Y. Shandilya**, S. Arnold, S. Phillips, K. Figueroa-Baez, O. Nachtigall
689. Advancing heteroanionicity in Zintl phases: Crystal structures, thermoelectric and magnetic properties of two quaternary semiconducting arsenide oxides, Eu<sub>8</sub>Zn<sub>2</sub>As<sub>6</sub>O and Eu<sub>14</sub>Zn<sub>5</sub>As<sub>12</sub>O. **M. ISHTIYAK**
690. Leveraging lone pairs in search of fluoride-ion battery insertion anodes. **A. Pakhira**
691. Leveraging optically transparent porous salt thin films as a platform for solid-state organometallic chemistry and photochemistry. **S. Sarkar**
692. Disorder of Mn in Ce<sub>2</sub>MnGe<sub>6</sub> and its effect on physical properties. **M. Raines**, B. Schundelmier, G. McCandless, K. Wei, J. Chan
693. Probing the limits of the Remeika tolerance factor. **R. Meduri**, A. Dominguez-Montero, J. Chan
694. Laser induced synthesis of cobalt oxide oxygen evolution catalysts. **A. Garza**
695. Synthesis, characterization, and photothermal effect of transition metal cobaltate nanoparticles deposited on nanographene oxide and nanographene.. **C.U. Ogbonna**, G. Neelgund
696. Synthesis and characterization of thiocyanate-capped copper ferrite nanoparticles. **D. Kumarage**, A. Picon, M. Escochea, S. Neugent, L. Marder, T.M. Trad
697. Controlling chemical and physical properties of tellurate inorganic pigments to achieve desirable colors and optical properties. **B. Amiri**
698. Developing eco-friendly coinage metal complexes using greener synthetic methods and natural materials as ligands for diverse applications. **H. Kouadio**, W. Ekhatior, S. Banna, A. Tantish, D. Lene, Z. Taimuri, M. Rawashdeh-Omary
699. Investigation of Cu(II)-exchange reactions with a calcium tantalate. **M. Mongkhonratanachai**, **P.A. Maggard**, **S. Jana**
700. From insertion to interphases: Exploring the competition between fluoride-ion insertion and interphase formation in 1D tunnel-structured transition metal antimonites. **A. Giem**, W. Zaheer, S. Banerjee
701. Synthesis and characterization of dodecyl xanthate-capped magnetite nanoparticles and their bactericidal efficacy against *Xanthomonas* pathogens. **A. Picon**, L. Marder, D. Kumarage, S. Neugent, M. Escochea, T.M. Trad
702. Manganese doped Zinc Germanate (Mn:Zn<sub>2</sub>GeO<sub>4</sub>): Exploring a novel synthesis and its potential application in bioimaging. **D.A. Philips**, S.U. Shohag, B. Srivastava, S. Mohan, M.J. Uddin

**703.** Chemical vapor deposition synthesis of  $\beta$ -Gallium Oxide Nanostructures: Reaction Parameters' Effect on Morphology and Photoluminescence. **M. Jaekel**, L. Marder, T.M. Trad

**704.** Innovative approaches in low temperature material synthesis: Exploring crystal and electronic structures of novel metal cluster compounds composed of Ru, Os, and Bi. **G. Samarakoon Mudiyansele**, S. Baranets

**705.** Novel Cis-Platin Alternatives with a Double-Headed Monster Action Against Cancer. **G.R. Calderon**, B. Adeyemi, M. Mehta, E. Skellam, M.A. Omary

**706.** Investigation of photoactive metallodrugs as antimicrobials. **G. Kaur**, A. Talgatov, G. Shi, A. Vali, C. Cameron, S.A. McFarland

**707.** Development of a web application for characterizing molecular vibrations for inorganic chemistry students. **O.M. Ayeni**, D. Omary, I. Migliaro, M.A. Omary, M. Atkinson

**708.** Redox cooperativity analysis with computational chemistry: Interplay between energy matching and geometric arrangement in redox non-innocent systems. **H. Watts**, J.B. Gary

**709.** Superhydrophobicity and Superhydrophobication Ability of Methylated Metal-Organic Frameworks (MeMOFs) and Hybrids Thereof as PFAS Alternatives for a Broad Spectrum of Apps. **O.M. Ayeni**, N.P. Davange, J. Fripp, M.A. Omary

**710.** Use of versatile luminescent complexes of Ruthenium(II) for moisture sensing. **B. Adeyemi**, J. Adebajo, R. Perera, P. DiCarmine, M.A. Omary

**711.** Iridium- and rare earth-free amber/white/monochrome (O)LED solutions for video display/street or room lighting/traffic light apps. **D. Lene**, S. Li, Z. Lu, M.A. Omary

**712.** Beauty Beyond Jewelry: Glowing Gold Triangles as Genuine Metallointercalators. **N.G. Rabah**, A. Momeni, O. Valsson, M.A. Omary

**P010.** Highly emissive zero-dimensional hybrid antimony chlorides  $A_2SbCl_5$  featuring long-chain cations. H. Majumder, **A.A. Miranda**, K. Thanabalasingam, K. McCall

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## ***Physical Chemistry Poster Session***

K. L. Shuford, *Organizer*

**713.** Analysis of microwave spectrum of Cyclopentanecarboxylic acid. **F. Jimenez**

**714.** Investigation of acetaldehyde photodissociation at 308 nm: Stereodynamics in competitive roaming. **D. Krongauz**, S.W. North

**715.** *Withdrawn*

**716.** Red Light Stress on *Chaetoceros* Diatoms. **K.C. Salaz**, J. Glenn-Millhouse, C.L. Waldie, A. Slover, S.C. Massey

**717.** Utilizing sum frequency generation spectroscopy to determine the ice nucleating mechanism of perfluorooctanoic acid. **L. Towers**, O. Curtin, J.D. Cyran

**718.** Red light and prolonged red light stress on *Phaeodactylum tricornutum*. **A. Slover**, **C.L. Waldie**, M.M. Nittala, M.Y. Buhari, K.C. Salaz, J. Glenn-Millhouse, S.C. Massey

**719.** Towards VENOM laser diagnostic technique to characterize multicomponent turbulent boundary layers. **T.B. Best**, S.W. North

**720.** Investigating the effects of low magnesium on *Phaeodactylum tricornutum* F710 fluorescence. **J. Glenn-Millhouse**, K.C. Salaz, A.K. Slover, C.L. Waldie, S.C. Massey

**721.** Characterization of hydrochar derived from *Chlorella pyrenoidosa* contaminated with copper and cadmium ion. **N. Smith**, K. Lasiter, C. Mitchell, B. Jang

**722.** Bacterial growth inhibition driven by surface phenomena of Microcrystalline  $Ga_2O_3$  and  $GaO(OH)$ . **D. Johnson**, P. Ahluwalia, P. Jodhka, A. Blom, J. Brannon, Y. Strzhemechny

723. Analysis of biosorption of heavy metal contaminated wastewater using kinetic and isotherm modeling for *Chlorella pyrenoidosa*. **K. Lasiter**, N. Smith, C. Mitchell, B. Jang
724. Experimental and computational studies of crystal violet removal from aqueous solution using sulfonated graphene oxide. **O. Oluwasina**, A. Adelodun, O. Oluwasina, H. Daurte, S. Olusegun
725. Formation of a silicon-carbon hybrid material from reacting silicon nanoparticles with acetylene. **G.J. Smith**, L. Canlom
726. Analysis of dispersed functionalized and non-functionalized single-walled carbon nanotubes. **D. Woodring**, **M. Schwickert**, B. Robinson, J.D. Beatty, N. Mirsaleh-Kohan
727. Surface tension measurements of charged microdroplets containing surfactants. **M. Johnston**, M. Jacobs
728. Molecular dynamics study of organochlorine ligand interaction with human serum albumin. **A. Mishra**, R. Yadav, D.S. Sanford
729. Impact of the SARS CoV2 viral fragment FI10 on amyloid  $\beta$ -42 aggregation. **M. Premathilaka**, A.D. Chesney, U. Hansmann
730. Identifying novel D-retro-inverso peptide inhibitors for mouse Serum Amyloid A 3 aggregation. **A.D. Chesney**, U. Hansmann
731. Analysis of SARS-COV-2 protein fragments on alpha-synuclein monomer conformations. **L. Coleman**, A.D. Chesney, U. Hansmann
732. Computational investigation of  $\alpha$ CGRP monomers and interactions with SARS-CoV-2 spike protein fragment. **V.K. Anand**
733. Intrinsic energetics of proton transfer in concentrated binary  $(\text{HCl})_m(\text{H}_2\text{O})_n$  clusters. **M. Tucker**, G.S. Tschumper
734. Revisiting the hydrogen halide dimers to probe the effects of sub-valence electron correlation. **Y. Xue**, G.S. Tschumper
735. Assigning the electronic absorption spectra of highly conjugated macromolecules. **H.A. Moran**, S. Kempel, Q. Michaudel, D.P. Tabor
736. Molecular insight on the hydration process of al-bearing species using density functional theory. **T. Fisher**, M.I. Malek, M.L. Pantoya, A. Aquino
737. An energy storage system that uses chemical bonds. **D. Medina**, S.A. Alexander
738. Vibrational polaritons revealed from infrared spectra by cavity quantum electrodynamical density functional theory within Gaussian atomic basis. **Z. Pei**, Y. Shao
739. Moving basis tensor implementation of Hierarchy of Pure states (HOPS). **B. Citty**
740. Spatially resolved fluorescence simulations of heterogeneous molecular semiconductors. **A. Hartzell**, T. Gera, D. Raccah
741. Ammonium perchlorate decomposition in the presence of  $\text{TiO}_2$  anatase surface: a theoretical investigation.. **J. Zamora**, A. De Rezende, M.L. Pantoya, A. Aquino
742. Exploring the potential of Alloyed XMenes (aXMenes) for advanced energy applications: A computational study on stability and electronic properties. **P. Rijal**, U. De Alwis, K.L. Shuford
743. Finding molecules with large hyperpolarizabilities. D. Mashak, **S.A. Alexander**
744. Multireference calculations on bond dissociation and biradical polycyclic aromatic hydrocarbons as guidance for fractional occupation number weighted density analysis in DFT calculations. **J. Carvalho**, R. Nieman, M. Kertesz, A. Aquino, A. Hansen, H. Lischka
745. Quantum mechanical MP2 study of the electronic effect of nonplanarity on the carbon pyramidalization of fullerene C60. **Y. Liu**, Y. Gao, D. Liu
746. Modeling the chemiluminescence mechanism of ADLumin-5. **C. Wickizer**, C. Lander, Y. Shao, C. Ran

**747.** Charge transfer mechanism in excited states of boron/nitrogen doped polycyclic aromatic hydrocarbons.

**L. Fonseca dos Santos**, F. Machado, A. Aquino, H. Lischka

**748.** Computational investigation of the thermal and photochemical mechanisms for the conversion of  $(TTP)Mo(\eta^2-O_2)_2$  to  $(TTP)MoO_2$ . **C. Lander**, Y. Shao, K.M. Nicholas

**P002.** Targeted Inhibition of SARS-CoV-2 Main Protease (Mpro) Using Proteolysis Targeting Chimeras (PROTACs). **K. Chidambaranathan**, G. Sharma