

SERMACS 2021 Technical Program

For Workshops, Expo, Graduate Fair, Social Events and Meal events see the SERMACS 2021 Event Program

Maps are at the end of the technical program

WEDNESDAY AFTERNOON

Birmingham Jefferson Convention Center
East Exhibit Hall 1

Biochemistry

Poster Session

J. Zhang, *Organizer*

1:00 - 3:00

2. Investigation of Protein Complexes Involved in the Activation of Methyl-coenzyme m Reductase. **S. Yavari**
3. Thermodynamics of the Competition Between Netropsin and AT-hook Peptides for AT-rich sites. **T. Townsend**, M. Fuenmayor Llanos, K.L. Buchmueller
4. Screening of EndoV variants as a tool for mapping A-to-I editing. **A. Scott**, S. Knutson, **A. Quillin**, J.M. Heemstra
5. Partial Formation of a Protein-based Cofactor in *M. tuberculosis* KatG and Its Impact on Catalysis. **T. Aziz**, **D.C. Goodwin**
6. Investigating the Interactions Between DNA Oligomers and Gemini Surfactants. **E. Boatwright**, A. Ginegaw, H. Nembaware, R.D. Sheardy
7. Probing Conformational Dynamics of GQ Formation in Varying Na⁺/K⁺ Ratios. **A. Lacen**, H. Lee

8. Expression, Purification, and Crystallization of a Putative Monooxygenase Key to Global Sulfur Cycling. **H.C. Frohock**, M. Culpepper, S. Bober
9. Testing the Methylation Ability of Mmp10, a New Radical SAM Methyltransferase. **K. Clohan**, N. Shao, W.B. Whitman, E.C. Duin
10. Allosteric Regulation of Human Epithelial 15-lipoxygenase-2. **A. Ohler**, E. Patel, A.R. Offenbacher
11. Role of Intrinsically Disordered Electronegative Clusters in RNA-binding Proteins. **S.M. Zaharias**, T. Fargason, Z. Zhang, T.M. Paul, J. Zhang
12. Ionic Liquid Loaded Nanoparticles to Deliver drug Candidates to Mammary Carcinomas. **G.S. Dasanayake**
13. Active Pharmaceutical Ingredient-Ionic Liquid (API-IL) Drug Loaded Polymer Nanoparticles for Targeted Drug Delivery Applications.. **G. Singh**, E.E. Tanner
14. Characterization Initiation of Alternative Splicing: The Interaction of SR Proteins and the U1 Spliceosomal Complex. **T.M. Paul**, T. Fargason, s. jamal, Z. Zhang, J. Zhang
15. Biophysical Studies of Genomic West Nile virus RNA G-quadruplexes. **T. Le**, A. Paul, W. Wilson, M.W. Germann
16. Determining the Mechanistic Role of the A12.2 Subunit in the Kinetics of Multi-nucleotide Addition Catalyzed by RNA Polymerase I. **K. Fuller**, D. Schneider, A.L. Lucius
17. Using X-ray Structures to Probe the Molecular Properties of the Specific Binding of Heterocyclic Diamidines in AT-Rich DNA Sequences. **E. Ogbonna**, A. Paul, A. Kumar, a. Farahat, D.W. Boykin, W. Wilson
18. Determining the Role of Metal Ions in Inhibiting Topoisomerase II α . K.R. Lyons, W. Medawala, **E.C. Lisic**, X. Jiang
19. Mechanistic insights into photochemical processes of a de novo designed artificial metallopeptide hydrogenase. **S. Maliyam Parambath**, A.E. Williams, L.A. Hunt, D. Selvan, N. Hammer, S. Chakraborty
20. Characterization of the substrate binding site for the poly(aspartic acid) hydrolase PahZ2 from *Sphingomonas* Sp. KT-1. **A. Jansch**, M. Weiland

21. Development of Spectroelectrochemical Techniques for Redox-Active Neurotransmitter Detection. **P.A. Evans**, B. Sharma
22. Synthesis and Cytotoxic Evaluation of 15-deoxy-Prostamide J₂ and Related Derivatives. **D. Halatek**, R. Van Dross, C. Burns
23. Crystallographic Examination of Inhibition by Diamidine Minor Groove Binders on the Transcription Factor PU.1. **J. Terrell**, A. Paul, G. Poon, W. Wilson
24. Observations and Conformational Changes of Zinc Dependent AdcR by Structurally Inspired Inhibitors. **A. Cutright**, J. Emerson
25. Role of Outer-Sphere H-bond Donation on the 3-Mercaptopropionic Acid Dioxygenase (3MDO) Transition State. **A. Schmittou**, N. York, M. Lockart, B.S. Pierce
26. Analysis of Microbial Colonization Patterns of Forensically Important Flies. **C. Huhn**, S. Bucheli
27. Analysis of Green Fluorescent Protein using Polarized Resonance Synchronous Spectroscopy. **K.R. Carter**, S. Stokes, D. Zhang, J. Emerson
28. Insights into the Local Structural Impact of Neighboring Nucleotides in Duplex DNA. **S.T. Brenden**, M.W. Germann
29. Investigating the Production and Biosynthesis of Coenzyme F₄₃₀ Variants in Methanogenic Archaea. **K. Boswinkle**, K. Allen
30. A suicide diiron oxygenase in *p*-aminobenzoate biosynthesis in *Chlamydia trachomatis*. **R.S. Wooldridge**, K. Allen
31. *Ribonucleotide damage near a replication fork. Enzymatic and structural consequences.* **S.T. Brenden**, R.M. Brosh, M.W. Germann
32. Stimuli-responsive Nucleic acid Activation via Catalyzed Glyoxal Decaging. **D. Karloff**, A. Sanford, S. Knutson, J.M. Heemstra
33. Elucidation of the Structural Mechanism for RNA Recognition of SR Proteins. **N.U. De Silva**, T. Fargason, Z. Zhang, J. Zhang
34. Interactions of RRM Motifs of SRSF1 Proteins. **E. King**, J. Zhang, T. Fargason

- 35.** Characterization of the Interaction Between U2AF35 and SRSF1 in RNA Splicing. **Z. Zhang**, J. Zhang
- 36.** NIR Donor Acceptor Fluorophores: Stability, DNA Interactions, and DNA Photocleavage. **C.P. Seudieu**, G.E. Ozmen, D.T. Brewer, E.O. Ahoulou, M. Henary, K.B. Grant
- 37.** Synthesis and Antiviral Evaluation of 6-Azauridine Prodrugs. **S.D. Karyakarte**, L.D. Bratton, O. Moukha-Chafiq, J.L. Smith, K. Keith, N. Haese, F. Ahmad, Y. Martinez-Gzregorzewska, L. Rasmussen, B. Ying, M. Diamond, H. Xia, P. Shi, B. Tekwani, R. Bostwick, D. Streblow, A.J. Hirsch, C.E. Augelli-Szafran, A.K. Pathak
- 38.** Hepatic Genomic Assessment of Dietary Ingestion of 2-Aminoanthracene in Sprague Dawley Rats. **A.M. Cisse**, W.E. Gato, J. Erber
- 39.** 4-Substituted-2-Thiazole Amides as Viral Replication Inhibitors of Alphaviruses and Flaviviruses. **A. Garzan**, S. Ahmed, N. Haese, S. Zhang, N. Tower, F. Ahmad, L. Rasmussen, V. DeFilippis, A.J. Hirsch, J.L. Smith, B. Tekwani, R. Bostwick, C.E. Augelli-Szafran, M.J. Suto, T. Morrison, M. Heise, D. Streblow, A. Pathak
- 40.** Analysis of the Optical Properties and DNA Photocleaving Abilities of NIR Carbocyanine Dyes Containing a Triphenyl Phosphonium Moiety. **D. Brewer**, E.O. Ahoulou, K. Ilina, M. Henary, K.B. Grant
- 41.** Characterization of the Flavin-dependent Tryptophan 7-halogenase (PrnA) from *Burkholderia ambifaria*. **M. Akter**, M.R. Uddin, J. Emerson
- 42.** Enhanced Structural Characterization of Multi-stranded Nucleic Acid Nanoparticles. **L.A. Rolband**, M. Chandler, C. West, D. Beasock, I. Danai, J. Krueger, K. Afonin
- 43.** Environment Matters: Lipid Composition and Stability of Staphylococcal Membrane Preparations from Supplemented Growth Media. **A. Pokorny Almeida**, D. Raskovic, G. Alvarado, K. Hines, C. Gatto, L. Xu, B. Wilkinson
- 44.** Redox Inactive Chloride Salts can Enhance the Ability of Methylamine Polycyclic Aromatic Hydrocarbons to Photosensitize ROS Production. **A.M. Ugboya**, K.B. Grant, M. Safiarian
- 45.** Computational Studies Evaluate Experimentally Observed Binding of Novel glycopeptide Antibiotics to Bacterial Cell Wall Analogs. **K.L. McWhorter**, V.T. Chioti, M.R. Seyedsayamdost, K.M. Davis

- 46.** Thermodynamic, Dynamic Light Scattering, and Hydrogen-Deuterium Exchange Investigation of Fatty Acid Regulation of Soybean Lipoxygenase Reveals Dynamically Driven Allostery. **D. Roberts**, A. Benton, S. Lindsay, Y. Li, A.M. Spuches, A.R. Offenbacher
- 47.** Experimental Validation of Computationally Generated Structure-Based Pharmacophores. **M. Guerrero**, G. Szwabowski, K. Ruddick, A.L. Parrill-Baker, D.L. Baker
- 48.** Surface energy profiling of adhesin proteins. **P. Ayres Galhardo**, M. Phan, A. Brown
- 49.** Synthesis and Evaluation of Novel, Small Molecule Inhibitors of Spermine Oxidase as Neuroprotective Agents. **A. Furbish**, P.M. Woster
- 50.** Exploring Microsphere Suspensions for High throughput detection of label-free RNA. **M.C. Adams**, V.T. Milam
- 51.** Quantum Dot Tracking Illuminates the Role of Membrane Microdomains in Serotonin Transporter Function and Cell Surface Dynamics. **L. Bellocchio**, O. Kovtun, I.D. Tomlinson, S. Rosenthal
- 52.** Synthesis and Evaluation of KDM4B inhibitors for the Treatment of Inflammation in Periodontal Disease. **K. Garrabrant**, J. Gerasco, C. Novince, P.M. Woster
- 53.** Controlled Disorder: Phosphorylation tunes Intramolecular Interactions of the Protein SRSF1. **T. Fargason**, E. King, Y. Thompson, I.U. De Silva, Z. Zhang, T.M. Paul, S. Zaharias, J. Zhang
- 54.** Quantum Dot Tracking Uncovers D2 Dopamine Autoreceptor-dependent Dynamic Rescue of Bipolar Disorder-associated Dopamine Transporter Mutant. **R. Torres**, O. Kovtun, I.D. Tomlinson, S. Rosenthal
- 55.** Kinetic Mechanism of Translocation of ClpB, an Hsp100 Protein, on Protein Substrates. **J. Banwait**, A.L. Lucius
- 56.** Evaluation the Efficacy of Various Hydrophobic Degrons for PROTAC-Mediated Degradation of the Androgen Receptor. **J. Crowe**
- 57.** Comparison of sequence and Structural Features of Fish and Mammalian Protamine using Multiple Trajectory MD Simulation to Understand their Role in DNA Condensation. **H. Shadman**, C. Gallops, J. Ziebarth, Y. Wang

58. Withdrawn. Tracking Individual Endogenous Dopamine Transporters using Antagonist-conjugated Quantum Dots. **B. DeMarco**, R. Torres, O. Kovtun, I.D. Tomlinson, S. Rosenthal

59. Uncovering the Unique Biochemical Properties of RNA Polymerases I, II, and III. **R.Q. Jacobs**, Z.M. Ingram, A.L. Lucius, D. Schneider

60. Structures Of Repressor: DNA Complexes From Different Mycobacteriophage Subclusters Reveal The Molecular Details Of Heteroimmunity Phenotypes. R. McKinney, M.D. Gainey, **J. Wallen**

61. Identifying the tolerance of CRISPR-Cas10 to mismatches in the crRNA-target duplex. **S. Khweis**

62. Engineering Reversibly Thermo-Responsive Gold Nanoparticles for Photothermal Therapy. **D. Amarasekara**, C. Kariyawasam, M. Hejny, N.C. Fitzkee

63. Withdrawn. SWiCAM (Sliding Window Comparative Alignment Metrics): An open-source program for visualizing differential amino acid enrichments in subsets of homologous protein families. **A. Schoeffler**, E. Hill, **A. Hill**

64. Secondary Amine Selective Pectin Bioconjugation. **O. Nwajiobi**, M. Raj

65. Synthesis of Hibiscone C. **M. Turnipseed**

66. Interactions Between Emerging Per and Poly-fluoroalkyl Substance (PFAS) with Human Serum Albumin (HSA). **D. Perera**, K.E. O'Shea, J. Miksovská

67. Development of Molecular Probes for Imaging of CD206 Positive Macrophages in Cancer. **C. Parker**, A. Bin Salam, C. Yates, S.E. Lapi

68. Characterization of Radical SAM Aminomutases Involved in Compatible Solute Biosynthesis in Methanogenic Archaea. **T. Tunckanat**, A. Gendron, K. Allen

69. Growth Outcomes of *Pseudomonas aeruginosa* after Knockout and Restoration of the Inhibitor of Vertebrate Lysozyme in Conditions Mimicking the Cystic Fibrosis Lung. **A. Gaddy**, T. Leeper

70. Recombinant Expression of Methyl-coenzyme M Reductase Reveals the Importance of Accessory Proteins for Proper Assembly. **A. Gendron**, K. Allen

Birmingham Jefferson Convention Center
East Meeting Room F

Bioinorganic Chemistry

B. S. Pierce, *Presiding*

1:00 Introductory Remarks.

1:05 71. Iron-sulfur (Fe-S) Cluster Biogenesis: Studies of the Suf Pathway in *E. coli*.
F. Outten, C.E. Fisher, T.D. Carter

1:25 72. Site-Directed NiS₃ type Model of the Proximal Ni of the A Cluster of Acetyl Coenzyme Synthase / ACS using a De Novo Designed Trimer Peptide. **D. Selvan**, S. Chakraborty

1:45 73. Investigating the Biosynthesis of N-Nitroglycine. **G. Padilla**, R. Lake, D.E. Graham, J.D. Caranto

2:05 74. Biomimetic Polyimidazole Chelates Investigating Mn²⁺ Affinity in Immune Protein Calprotectin. **R.B. Gaynor**, S. Creutz

2:25 75. Platinum Indazole Complexes with Potential Anti-cancer Activity: Synthesis, Characterization, and Reactivity. **R.E. Bachman**, K. Wills, K. Barwick, G. Ferrence, K.A. Wheeler

2:45 Intermission.

3:15 76.

Connecting Conformational Entropy Changes to Zinc(II) and Copper(II) Binding in Human Carbonic Anhydrase II. **J. Emerson**

3:35 77. Manganese Complex with a Redox-active Ligand acts as an Efficient Superoxide Dismutase Mimic. **S. Karbalaei**, D.D. Schwartz, I. Ivanović-Burmazović, C. Goldsmith

3:55 78. Ferric-superoxo Intermediate of the TxtE Nitration Pathway Resists Reduction, facilitating its Reaction with Nitric Oxide. **C.P. Martin**, M. Chen, M. Martinez, Y. Ding, J.D. Caranto

4:15 79. H₂ Evolution by Rationally Designed Biomolecular Catalysts: Insights into Electron and Proton Transfer Processes. **S. Chakraborty**, S. Malayam Parambath, D. Selvan, P. Prasad

4:35 80. Two Nickel Binding De Novo Designed Tetramer as an Artificial Hydrogenase: The Role of Cooperative Bimetallic Active Sites in Increasing Hydrogen Production. **P. Prasad**, S. Chakraborty

4:55 Concluding Remarks.

Birmingham Jefferson Convention Center
East Meeting Room A

Biophysics of Macromolecular Machines

A. L. Lucius, *Presiding*

1:00 Introductory Remarks.

1:05 81. Structural Analysis of the *Legionella pneumophila* Dot/Icm type IV Secretion System. **C. Durie**, M. Sheedlo, M. Swanson, D.B. Lacy, M. Ohi

1:30 82. Elucidating the Role of Zinc in Salmon Sperm Nuclear DNA Packaging. **M. Dinar**, A. Drake, S. Rankin, J.E. Derouchey

2:20 Intermission.

2:40 83. Defining and Exploiting Unique Properties of Eukaryotic RNA Polymerases. R.Q. Jacobs, Z.M. Ingram, K. Fuller, S. Cooper, A.L. Lucius, **D.A. Schneider**

3:05 84. Falling off: ClpB and Hsp104 Operate as Non-Processive Translocases. **A.L. Lucius**

Birmingham Jefferson Convention Center
East Meeting Room D

Chemical and Biochemical Approaches to the Investigation of Lipid Membranes

Financially supported by Avanti Polar Lipids, T&T Scientific
M. Best, *Presiding*

1:00 Introductory Remarks.

1:05 85. Stimuli-Responsive Liposomes via Engineering of Membrane Properties. **M. Best**, J. Lou, R. Sagar, M.L. Qualls, J. Schuster, F. Barrera

1:30 86. Natural Products as Selective Glucocorticoid Signaling Modulators. **F. Rivas**

1:55 87. Toward Applications of Synthetically Evolved, Membrane-permeabilizing Peptides That Form Macromolecule-sized Pores. L. Sun, E. Wu, K.A. Hristova, **W.C. Wimley**

2:20 88. Delivery of Recombinant SARS-CoV-2 Envelope Protein into Human Cells. **C.R. Sanders**, J. Hutchison, R. Capone, D. Luu, W.D. Van Horn

2:45 Intermission.

3:00 89. A picture Worth a Thousand Words: Optimizing cryo-EM for Membrane Structural Studies. **F.A. Heberle**, D.A. Welsch, E. Chaisson, E. Crumley, M. Doktorova, N. Waxham

3:25 90. New Approaches to Uncover how Membrane Rafts and Caveolae Form and Function. **A. Kenworthy**

3:50 91. Coupling between Protein Condensates and Membrane Domains Regulates T Cell Membrane Structure and Protein Organization. **I. Levental**

4:15 92. A General Approach to Understand Lipid Interactions in Membranes. **P.F. Almeida**

4:40 Concluding Remarks.

Birmingham Jefferson Convention Center
East Meeting Room J

Discovery of Therapeutic Agents for Emerging Viruses

Corinne E. Augelli-Szafran, *Presiding*

1:00 Introductory Remarks

1:05 93. Small Peptide Inhibitors of SARS-CoV-2 3-chymotrypsin-like Protease. **J. Stewart**, M. Halim

1:35 94. Design and Synthesis of Potential Drug Candidates for SARS-CoV-2 using Molecular Hybridization Approach. **S.S. Panda**

2:05 95. Vinyl Sulfone-based Inhibitors of Non-structural Protein 2 Block the Replication of Venezuelan Equine Encephalitis Virus. **I.V. Ogungbe**, H. Zhang, M. Harmon

2:35 96. Discovery and Optimization of BCX 5191 a Novel Nucleotide RNA Dependent RNA Polymerase Inhibitor of Hepatitis C virus. **P.L. Kotian**, M. Wu, S.K. Vadlakonda, Y. El-Kattan, X. cheng, X. Chen, S. Bantia, T. Lin, P. Chand, Y.S. Babu

3:05 Intermission

3:25 97. Structural Analyses Reveal the Mechanism of Inhibition of Influenza virus NS1 by two Antiviral Compounds. **C. Petit**

3:55 98. Pyrimidone inhibitors targeting Chikungunya Virus nsP3 macrodomain by fragment-based drug design. **M. Wu**, S. Zhang, A. Garzan, N. Haese, R. Bostwick, Y. Martinez-Gzregorowska, L. Rasmussen, M.I. Sosa, D. Streblow, M. Heise, A.K. Pathak, C.E. Augelli-Szafran

4:25 99. Computer-Aided Drug Discovery of Anti-Alphavirus and Anti-Coronavirus Agents. **S. Zhang**, A. Garzan, N. Haese, R. Bostwick, Y. Martinez-Gzregorowska, L. Rasmussen, M.I. Sosa, D. Streblow, M. Heise, A. Pathak, C.E. Augelli-Szafran, M. Wu

4:55 Concluding Remarks.

Birmingham Jefferson Convention Center
East Meeting Room L

General Session - Energy and Fuels

S. Pan, *Organizer*

1:00 Introductions.

1:10 100. Improvement of Weibull Breakdown Strength in Single-Phase Multiferroic Films with High Dielectric Constant for Supercapacitors. **R. Harry**, S. Zainuddin, S. Jeelani

1:30 101. Ethanol Upgrading to Olefins Over Metal-containing Beta Zeolites: Characterization and Catalysis. **N. Samad**, J. Zhang, E.C. Wegener, S. Purdy, K.A. Unocic, D. Liu, Z. Li, J.W. Harris

1:50 102. Pyrolysis of Butyl Acetate Isomers Inside a Shock Tube. F. Arafin, **S. Vasu**

2:10 103. Computational Studies of the Substituent Effect on Fe(II) Arylisocyanide Complexes. **M. Deegbey**, E. Jakubikova

2:30 Intermission.

3:00 104. Main Group, Alkali, and Alkaline Earth Metal Amine Borane-based Chemical Hydrogen Storage Molecular Systems. **M.P. Confer**, D.A. Outlaw, D.A. Dixon

3:20 105. “The Use of Lithium ion Conducting Sulfonate MOFs as Anode Materials for Li-S Batteries.”. **D.K. Panda**

3:40 106. The Prediction of Diesel Fuel Economy and Emissions Using Python Machine Learning Tools.. **D.T. Daly**

4:00 107. Asymmetric glycerol derivatives: Synthesis, properties, and application in CO₂ absorption. **S. Qian**, J.E. Bara

4:20 108. Free-base Porphyrin Polymer for Bifunctional Electrochemical Water Splitting. **Y. Ge**, D. Villagran

4:40 Concluding Remarks.

Birmingham Jefferson Convention Center
East Meeting Room E

General Session - Environmental Chemistry

Financially supported by Nashville Local Section of the ACS

R. C. Wingfield, *Presiding*

1:00 Introduction .

1:05 109. Community based Participatory Research in Monitoring of Criteria and Toxic Air Pollutants in Environmental justice Communities and Vulnerable Populations. **D. Padgett**

1:25 110. Silica Fiber-based Visible Colorimetric Method for On-site Polycyclic Aromatic Hydrocarbons Detection. C. Duprey, H. Rouhi, Y. Lu, M. Elliott, **E.K. Wujcik**

1:45 111. Synthesis and Studies on Photophysical Properties of Rhodamine dyes and their Metal Complexes for Application in Dye Sensitized Solar Cell. **O. Oloyede**, F. Abebe, W. Gahnn, J. Uddin

2:05 112. Spectroscopic Studies (Raman, FTIR) of Boron in Aqueous Solutions. **J. Mierzwa**, R. Avedananda, R. Mumbi, S. Rakshit

2:25 113. In-situ Synthesis Nanoscale Zero-valent Iron-decorated Biochar for Water Remediation. **X. Zhang**, J. Zhang

2:45 114. Effect of Ultrasonicated Sustainable Biochar Reinforcement on Mechanical and Thermal Properties of Polypropylene Biocomposite.. **Z. Mohammed**, S. Jeelani, V. Rangari

3:05 Intermission.

3:20 115. Preparing Vulnerable Populations for the Impacts of Climate Change Amid a Global Pandemic: The Path Forward to Building Sustainable and Resilient Communities. **R.C. Wingfield**, N. Lake, A. Scarce, B. Holmes, A. Lee

3:40 116. CO₂ Reduction in Acetonitrile Enhanced by Electrolyte-assisted Mass Transport of Water. **A.J. Wilson**

4:00 117. Simultaneous Sorption of Multioxyanions (arsenate, phosphate, selenate, and chromate) using Magnetic Douglas Fir Biochar. **P.M. Rodrigo**, C. Navarathna, T. Mlsna

4:20 118. Immobilization of Lead in Simulated Polluted Soil by Douglas Fir Biochar-supported Phosphate. **B. Arwenyo**, J. Varco, A. Dygert, F. Afstar, S. Sabrina, R. Thirumalai, C.U. Pittman, T. Mlsna

4:40 119. Withdrawn. Effective Removal of Anionic Dyes (Remzol Brilliant blue and Remzol Reactive black) from Aqueous Solution by Novel Ozone Oxidized Hydrochar Treated with Polyethyleneimine.. **S. Madduri**, I. Elsayed, E.M. Hassan

Birmingham Jefferson Convention Center
East Ballroom B

High Performance Computing Applications in Chemistry 1

T. P. Straatsma, *Presiding*

1:00 Introduction .

1:00 120. High Performance Computing for Rapid Generation of Benchmark-quality Quantum Chemistry Data. **C.D. Sherrill**

1:35 121. Multilayer Linear-scaling Coupled Cluster Methods. **D. Bykov**, A. Barnes, D. Lyakh, T. Straatsma

2:10 122. Fast Coulomb matrix Construction via a Hierarchical Block Low-rank Representation of the ERI Tensor. **E. Chow**, X. Xing, H. Huang

2:45 Intermission.

3:05 123. ACE2 Glycans Preferentially Interact with SARS-CoV-2 spike Protein Over SARS-CoV. **A. Acharya**, D.L. Lynch, A. Pavlova, Y. Pang, J.C. Gumbart

3:40 124. Mechanistic Investigations into Benzylic Amine-Directed C-H Borylation with Iridium. **N. Le**, N. Chuang, C. Oliver, A. Samoshin, K.B. Morris, S. Hyland, H. Guan, T.B. Clark, C.E. Webster

4:15 125. Exploiting Graphical Processing Units (GPUs) to Enable Large-scale Quantum Chemistry of Molecules in Realistic Environments. **F. Liu**

Birmingham Jefferson Convention Center
East Meeting Room C

N-Heterocyclic Carbenes in Synthesis, Catalysis and Material Science

K. Marichev, *Presiding*

1:00 Introductory Remarks.

1:10 126. Tweaking NHC Ligand Design for Gold Nanoparticle and Surface Applications. I.M. Jensen, J.F. DeJesus, S.L. Strausser, R.K. Borsari, L.M. Sherman, N.L. Dominique, J.P. Camden, **D.M. Jenkins**

1:45 127. Merging Single-electron Processes with Carbene Catalysis. **A.V. Bay**, K.P. Fitzpatrick, G.A. Gonzalez-Montiel, A.O. Farah, P.H. Cheong, K. Scheidt

2:05 128. N-Heterocyclic Carbenes as a Surface-Functionalization Platform for Molecular Sensing. **J.P. Camden**

2:40 129. Experimental and Theoretical Investigations of a Copper(II) Bipyridyl-*N*-Heterocyclic Carbene Macrocycle. **S. Sahil**, K.M. McCardle, P. Magueres, J. Panetier, J.W. Jurss

3:00 Intermission.

3:20 130. Organometallic Polymers Comprising Janus bis(*N*-heterocyclic carbenes) Linkers and Metal-sulfur Cubane-type Clusters. **C. Bejger**, J. Gillen, M. Vuong

3:55 131. Metal Carbenes in Synthesis of Chiral Carboxylic Acid Derivatives and Natural Products using Strain Release Methodology. **K. Marichev**

4:30 132. Study of Effect of Polyethylene Glycol Chain Lengths in the Synthesis of Water-Soluble Metal phthalocyanines, and Incorporation into Hierarchically Porous Carbon Monolith Catalysts. **A. Shrestha**

4:50 Concluding Remarks.

Birmingham Jefferson Convention Center
East Meeting Room K

General Session - Polymer Chemistry

V. Thomas, *Organizer*

D. Lerew, *Presiding*

1:00 Introduction .

1:10 133. Structure Property Relationships in Imidazolium Ionenenes: Effects Of Linkage and Anion Structures. **S. Chatterjee**, J. Bridges, J.E. Bara, K.E. O'Harra, K.N. West

1:25 134. Anionic Ring-opening Copolymerizations of Sulfonylaziridines to Afford Previously Insoluble Linear Polysulfonylaziridines. **S. Sisk**, P. Rupar

1:40 135. Ion-Exchange Cellulose Nanoresins for Water Purification. **S. Schmal**, A. Sahu, S. Elmore, J.C. Poler

1:55 136. Upper Critical Solution Temperature Behavior of Linear and Star Polymers. **A. Aliakseyeu**, R. Hlushko, S.A. Sukhishvili

2:10 137. Synthesis and Characterization of Sulfonimide Based Anionic Ionenenes. **K. Watson**, P. Rupar

2:25 138. Anionic Polyimide Ionomers with Ionic Liquids Through Cation-exchanges for Gas Separation Membranes. **J. Chang**, G. Dennis, J.E. Bara, P. Rupar

2:40 Intermission.

3:00 139. Phenothiazine Based Polymer as a Mimic of Polyaniline for Optoelectronics Application. **H. Giri**, C.N. Scott

3:15 140. Synthesis of Branching-controlled Comb Polymers via Thiol-yne "click" Chemistry. **B.J. Curole**, A. Nadeem, W. Broussard, S.M. Grayson

3:30 141. Triphenylene-Enchained Perfluorocyclobutyl Aryl Ether Polymers: Blue-Light Emitters with High Thermal-Oxidative Stability. **E. Borrego**, B. Farajidizaji, S. Athukorale, C.U. Pittman, D.W. Smith

3:45 142. Synthesis of semi-fluorinated polyaryl ethers via direct Friedel-Crafts polymerization of aryl ethers and hexafluoroacetone hydrate. **G. Munoz**, K.M. Chamberlain, S. Athukorale, C.U. Pittman, D.W. Smith

4:00 143. Synthesis of Biobased Novolac Phenol-Formaldehyde Wood Adhesives from Biorefinery-Derived Lignocellulosic Biomass. **A. Bansode**, M.L. Auad

Birmingham Jefferson Convention Center
East Meeting Room B

Single Molecule Approaches to Chemistry and Biology

K. Welsher, *Presiding*

1:00 Introductions.

1:05 144. Single molecule imaging approaches to study the mechanochemistry of living systems. **K. Salaita**, H. Ogasawara, A. Blanchard, Y. Duan, Y. Hu, R. Ma

1:30 145. Active Feedback Three-dimensional Tracking of Single Polymer Particles in the Solution Phase. **D. Yu**, A. Garcia IV, S. Blum, K. Welsher

1:50 146. Covalently-Linked Rhodamine B Dimers: Stereochemistry and Photophysical Interplay. **K. Fogarty**

2:10 147. Indestructible Tension Probes for Measuring High-force Mechanical Events in Cells. **R.L. Bender**, Y. Duan, A.V. Kellner, B. Deal, J. Heemstra, Y. Ke, K. Salaita

2:30 148. Unraveling the Molecular Details of Bacterial Type 3 Secretion by Tracking Single Biomolecular Complexes in Living Cells. J. Prindle, O.I. de Cuba, Y. Wang, **A. Gahlmann**

2:55 Intermission.

3:05 149. 3D Intra-Organellar Transport of Toxins Inside Live BHK cells using Phase Engineered Optical Microscopy. **C. Dutta**, J. Zepeda O., A. Misiura, S. Sarkar-Banerjee, C.F. Landes

3:30 150. Recursive Bayesian Position Estimation for Active Feedback Single-Molecule Tracking in Complex Environments. **A.J. Niver**, K. Welsher

3:50 151. Chemical-to-mechanical Molecular Computation Using DNA-based Motors with Onboard Logic. **S. Piranej**, A. Bazrafshan, K. Salaita

4:10 152. Understanding Cells at the Molecular Level using Light Sheet Single-molecule Super-resolution Microscopy in 3D. **A. Gustavsson**

4:35 153. Single-Molecule Orientation Localization Microscopy: Visualizing Molecular Rotational Dynamics at the Nanoscale. T. Ding, T. Wu, **M.D. Lew**

Birmingham Jefferson Convention Center
East Exhibition Hall 1

Analytical Chemistry

Poster session

A. Ghosh, S. Pan, *Organizers*

3:00 - 5:00

154. Peroxidase-Like Activity of Platinum-Group Metal Nanoparticles. **H. Crawford,** A. Biby, X. Xia

155. Evaluating Structural Heterogeneities of Amyloid Aggregates in Alzheimer's Disease Tissues with Infrared Microscopy. **A. Foes,** S. Walker, J. Holmquist, A. Ghosh

156. Exploring the Biological Relevance of Some Synthesized Heterocyclic Compounds in Model Biomimetic Environment. **E.T. Fasusi,** S.M. Landge, D. Ghosh

157. Digestive Ripening Yields Atomically Precise Au Nanomolecules.. **S. Eswaramoorthy,** A. Antonysamy

158. Investigation of Polymerization Reactions via Dual Spray ESSI-MS. **J. Griggs,** M. Gilliland

159. Chemical Profiles of Weathered Ignitable Fluids Based on GC/MS, Raman, and Infrared Spectroscopic Analysis. R. Boyce, S. Perna, M. Zhang, **N.S. Chong**

160. Investigating the Photophysical Changes of a Prodrug in Cationic Micelles. **A. Merhar,** E. Dobson, K.S. Aiken, S.M. Landge, D. Ghosh

- 161.** Label-free discrete frequency infrared imaging of beta sheet aggregates in Alzheimer's Disease. **T.B. Maupin**
- 162.** Investigating Nanoscale Heterogeneities of Self-assembled Monolayers with AFM-IR for Area-selective Atomic Layer Deposition. **M. Hasan Ul Iqbal**, H. Yan, Q. Peng, A. Ghosh
- 163. Withdrawn.** Authenticating Aspirin Brands Through LC-MS/MS. **W. Than**
- 164.** Ionic Liquid-Solvated Indolizine Squaraine Sulfonate Dyes for Enhanced Emission in the Presence of Blood. **D.S. Darlington**, A.N. Mahurin, W.E. Meador, J.H. Delcamp, E.E. Tanner
- 165. Withdrawn.** Transferring Solid Phase Elution Methods from TomTec Quadra 4 SPE to Zephyr G3 SPE Workstation: Applications in HPLC. **S. Fisher**, L. Nguyen, C. Green, J. LaPalme, E. Bair, N. Epie
- 166.** Evaluation of a Targeted Multiple Reaction Monitoring Lipidomics Approach to Assess Various Sphingolipid Species. **S.C. Swiderski**, N.A. Chung, T.A. Clemons, R.A. Robinson
- 167. Withdrawn.** Gas Chromatography Rapid Automation and Quantitative Procedure for the Measurement of Hydrogen Cyanide in Whole Blood. **P. Brito**, J. LaPalme, E. Bair, N. Epie
- 168.** Analysis of Guanine Content on DNA detection, Induced Oxidative Damage, and Hydrolysis using Complementary Square Wave Voltammetry and LC-MS/MS. **T. Hindi**, **K. Cheek**, E. LaFave, E. Hvastkovs
- 169.** Morphological and Structural Studies of RGD and VEVE based-Tetraphenylalanines. **B.M. Almarwani**, A. Sunda-Meya, N. Phambu
- 170.** Energy Harvesting from Enzymatic Glucose Biofuel Cell Utilizing Meso-porous Two Dimensional Reduced Graphene Oxide. **M.H. Kabir**, W. GHANN, J. Uddin, M.M. Ali, H.Z. Msimanga, M. Thompson, A. Poyraz
- 171.** Interfacial Interaction Between cellulose nanofibrils (CNFs) and Fipronil. **S.W. Freij**, M.C. Iglesias, T. Ciaramitaro, M.S. Peresin

WEDNESDAY EVENING

Birmingham Jefferson Convention Center
East Ballroom B

Plenary

D. A. Dixon, *Presiding*

5:30 172. Drug Discovery and Development *via* structure and Mechanism Based Rational Design. **C. Zhan**

THURSDAY MORNING

Birmingham Jefferson Convention Center
East Meeting Room I

Contemporary Fluorine Chemistry in the Southeast 1

Cosponsored by FLUO

D. A. Dixon, T. Lectka, *Presiding*

8:00 Introductory Remarks.

8:05 173. Synthesis of Difluorinated Alcohols and Halohydrins. **D.A. Colby**

8:35 174. Advances in Trifluoromethoxylation and Electrophilic Fluorination. **G.B. Hammond**, T. Umemoto, Z. Lu

9:05 175.

C-F Bonds in tight spaces: Getting fluorine to do what it may not want to do. **T. Lectka**, S. Harry, M. Kazmin

9:35 Intermission.

9:50 176. New, One-step Synthesis of the Anesthetic Agent Sevoflurane, $(\text{CF}_3)_2\text{CHOCH}_2\text{F}$. X. Liu, C. Liu, A.V. Matsnev, P.V. Jog, M. Ulman, **J.S. Thrasher**

10:20 177. Real-time Dermal Sorption of ^{18}F -labeled Perfluorinated Alkyl Substances in Immunocompetent Mice. **J.L. Bartels**, S.R. Fernandez, M. O'Malley, G.F. Peaslee, S.E. Lapi

10:50 178. Direct Fluorination of Tetrafluoroethylene and the Effect of ^{60}Co γ -radiation on the Tetrafluoroethylene/ Perfluoro(methyl vinyl ether) Copolymer. **M.P. Confer**, S.R. Allayarov, D.A. Dixon

11:20 179. Comparison of [^{18}F]FDG with ^{18}F -labeled amino acids for PET imaging of breast cancer. **U. Akca**, P. Song, D.A. Devalankar, N. Yasui, A. Sorace, J.E. McConathy

Birmingham Jefferson Convention Center
East Meeting Room E

Frontiers in Nucleic Acids

K. L. Hayden, R. M. Wadkins, *Presiding*

8:00 Introduction.

8:10 180. Conjugation of the Synthetic Anthracycline Chemotherapeutic Pixantrone with an Apurinic Site in DNA. **M.P. Stone**, A.H. Kellum, P. Pallan, Y. Fu, J. Terrell, B. Noh, M.V. Voehler, C.J. Rizzo, M. Egli

8:30 181. Structural Effects of Incorporation 6-oxo- M_1dG DNA Adduct into DNA Duplex. **Y. Fu**, P. Kingsley, R. Richie-Janetta, L.J. Marnett, M.P. Stone

8:50 182. Coloring DNA Strands with Silver Clusters. **J.T. Petty**, D. Lewis, C. Couch, M. Branham, K. Thomas, Y. Zhang, B. Kohler, I. Santos, J. Brodbelt

9:10 183. Can anything Stabilize a DNA i-motif?. **R.M. Wadkins**

9:30 Intermission.

9:55 184. The Interaction of DNA with Gemini Surfactants. E. Boatwright, D. Aguilar, **R.D. Sheardy**

10:15 185. Programmable Approach for Specific Recognition of Adjacent GG Base Pairs by Modular Synthetic Diamidines. **A. Paul**, P. Guo, A. Farahat, D.W. Boykin, W. Wilson

10:35 186. Dynamic and Hydration Properties of DNA Site Selection by Nucleoproteins. **G. Poon**, J. Terrell

10:55 187. Influence of Pre- and Post-transition Baselines on the Uncertainty and Reliability of Thermal Denaturation Parameters Extracted from DNA Melting Curves. **R. Bishop**

11:15 Concluding Remarks.

Birmingham Jefferson Convention Center
East Ballroom B

High Performance Computing Applications in Chemistry 2

T. P. Straatsma, *Presiding*

8:00 Introduction .

8:10 188. Simplifying Multilevel Quantum Chemistry Procedures through Psi4 and QCArchive. **L.A. Burns**, C.D. Sherrill

8:45 189. Scalable GPU-accelerated Computational Infrastructure for Parallel Tensor Processing in Quantum Many-body Theory. **D. Lyakh**

9:20 190. Accelerating Density-Functional Tight-Binding Using Graphical Processing Units. **S. Irle**, V. Vuong, C. Cevallos, B. Aradi, C. Camacho

9:55 Intermission.

10:15 191. High-Performance Density Fitting Technology on Accelerated Computed Platforms. **E.F. Valeev**, A. Asadchev

10:50 192. GronOR: Scalable and Accelerated Non-Orthogonal Configuration Interaction for Molecular Fragment Wavefunctions. **T.P. Straatsma**

11:25 193. Withdrawn. Computational investigations of Aromatic Borylene-type Systems. **U. Gaillard**, K. Donald

Birmingham Jefferson Convention Center
East Meeting Room J

Inorganic Electron Transfer Reactions for Energy Storage

Financially supported by **Cell Reports Physical Sciences**

B. H. Farnum, *Presiding*

8:00 Introductory Remarks.

8:05 194. Advanced Scanning Electrochemical and Spectroelectrochemical Methods for Analyzing Surfaces of Catalytic Electrode Materials. **S. Pan**

8:25 195. Molecular Z-Scheme for H₂ Production via Dual Photocatalytic Cycles. **K. Hanson**, P.J. Avare, N. Watson, A.K. Vannucci

8:45 196. Characterization of a New Class of Platinum Bipyridyl Complexes with Blue to Cyan Emission. **J. McCarthy**, M.J. McCormick, J.H. Zimmerman, W.M. Thomas, P.S. Wagenknecht

9:05 197. Redox Hopping Promoted Water Oxidation by a Metal-Organic Framework. **A.J. Morris**

9:25 999. CHASE Hybrid Photoelectrodes for Water Oxidation **G. Meyer**

9:45 Intermission.

10:00 198. Improving 2e⁻ Redox Chemistry of Nickel Dithiocarbamates for Application in Redox-Flow Batteries. **B.H. Farnum**, M. Mazumder

10:20 199. Cr Complexes for the Electrocatalytic Reduction of Carbon Dioxide. S. Hooe, J. Moreno, A. Reid, **C.W. Machan**

10:40 200. Ligand-to-Metal Charge-Transfer Photochemistry and Photophysics of d⁰ Titanocenes. **H. London**, D. Pritchett, C. McMillen, G.C. Shields, P.S. Wagenknecht

11:00 201. Self-Sensitized Photocatalytic CO₂ Reduction by a Series of Ruthenium Complexes Under Visible-Light Irradiation. A. Devdass, K.M. McCardle, A. Dorris, D.K. Buettner, N. Hammer, J. Panetier, **J.W. Jurss**

11:20 202. Metalloenzyme Mimics: Iron Carbonyl Clusters Tethered to Non-Innocent Aromatic Ghiole Groups. **C.A. Mebi**

11:40 203. Excited State Proton Transfer and Electron Transfer in Complexes Exhibiting Intramolecular Reversible Energy Transfer. **F. Zhang**, J.J. Paul, R.H. Schmehl, J. Stash

Birmingham Jefferson Convention Center
East Meeting Room G

Measuring More than Mass: Innovations in Mass Spectrometry Experiments and Applications

Financially supported by **Mississippi State University**

A. L. Patrick, *Presiding*

8:00 Introductory Remarks.

8:05 204. Application of Liquid Chromatography Tandem Mass Spectrometry for Analysis of Complex Mixtures. **Z. Popovic**, L.C. Anderson, C. Weisbrod, H. Chen, D. Butcher, G.T. Blakney, X. Zhang, L. Babcock-Adams, R. Boiteau, N. Coffey, P. Morton, T.B. Kelly, A. Dispenzieri, S. Dasari, C.P. Hutchinson, P. Chance, C. Reimers, J. Li, B.N. Granzow, M. Acker, M.R. Stukel, D.R. Griffith, D.J. Repeta, R. Zubarev, D.L. Murray, D. Barnidge, A.M. McKenna, C. Hendrickson, A.G. Marshall

8:40 205. Determining the Structure of Neuregulin by Multi-dose FPOP Coupled with Computational Modeling. N.A. Khaje, C.K. Mobley, A. Eletsy, S.E. Biehn, S.K. Mishra, R.J. Doerksen, S. Lindert, J. Prestegard, **J.S. Sharp**

9:15 206. Comparing Lipid Normalization Methods for Label-free Quantitative Lipidomic LC-MS/MS. **L.S. Bailey**, K.B. Basso

9:50 Intermission.

10:10 207. Resolving Diagnostic Isomeric Lipids with Liquid Chromatography, Ion Mobility Spectrometry and Tandem Mass Spectrometry. **A.M. Hamid**

10:45 208. Derivatizing Reagents for Improved Analysis of Performance Enhancing Drugs with IM-MS. D.C. Velosa, S.P. Neal, **C.D. Chouinard**

11:20 209. Advancing Chemical Liability Assessments and Biogeochemical Interpretations of Aquatic, Soil, and Oil Organic Matter by FT-ICR MS. **J. D'Andrilli**, C. Romero, P. Zito, D. Podgorski, R. Payn, S. Sebestyen, A.R. Zimmerman, F.L. Rosario

11:55 Concluding Remarks.

Birmingham Jefferson Convention Center
East Meeting Room A

New Directions in Metal-Catalyzed Reactions 1

Financially supported by Organic Reactions, Biocryst, VWR

K. H. Shaughnessy, *Presiding*

8:00 Introductory Remarks.

8:05 210. Ruthenium-Catalyzed Enantioselective Functionalization of Carbon-Hydrogen Bonds. **X. Cui**

8:35 211. Metal-mediated Approaches Toward the Formation of the Synthetically Challenging 2-pyridyl bond. Z.Z. Gulledge, G.D. Waters, J.W. Cleveland, A. Chin, M.L. Tedder, **J.D. Carrick**

9:05 212. Applications of Platinum-Catalyzed Carbene Formation toward Heterocycle Synthesis. **E.M. Ferreira**

9:35 Intermission.

9:50 213.

Synthesis of Pyridyl Triazole Ligands With Transient Directing Groups For Meta and Para C-H Activation of Aryl Aldehydes, Ketones, and Aryl Amines. **T. Ricks**

10:20 214. Mechanistic Study of Enantiomer Selectivity C-H bond Functionalization catalyzed by Ruthenium complexes. **N. Le**, C. Hetti Handi, N. Udayanga, X. Cui, C.E. Webster

10:50 215. New Catalytic uses for Gallium in the Oxidation of Hydrocarbons. **C.R. Goldsmith**, A.C. Saunders

11:20 216. Pincer Ligand Cobalt Chromophores for Selective Radical Trifluoromethylations. **J.D. Soper**

Birmingham Jefferson Convention Center
East Meeting Room L

Electrocatalysts and Solar Cell For Clean Energy Conversion Part 1

S. Pan, *Presiding*

8:00 Introduction .

8:10 217. Bifunctional Nickel and Copper Electrocatalysts for CO₂ Reduction and the Oxygen Evolution Reaction. **H. Pan**, C. Barile

8:30 218. Photocatalytic Reduction of CO₂ to Formic Acid by Rhenium(I) Dicarbonyl Complexes. **E. Asempa**, E. Jakubikova

8:50 219. Photocatalytic Carbon Dioxide Reduction with Nickel Complexes Supported by Redox-active Macrocycles with Extended Conjugation. **S. Bhattacharya**, A. Devdass, J.W. Jurss

9:10 220. Electrocatalytic CO₂ Reduction with Nickel Complexes Supported by Redox-Active Macrocycles with Extended Conjugation. **A. Devdass**, A. Richmann, J.W. Jurss

9:30 221. Thickness Dependent OER Electrocatalysis of Epitaxial LaFeO₃ Thin Films. **A. Burton**, R. Paudel, B. Matthews, S. Spurgeon, M. Sassi, B.H. Farnum, R. Comes

9:50 Intermission.

10:10 222. Activation of Methane to Produce Methanol Over a Vanadium Single Site MCM-41 SiO₂ Amorphous Mesoporous Quantum Photocatalyst. **C. Evrard**, L.M. Thompson

10:30 223. Molybdenum Ditelluride and Sulfotelluride with Graphene Support as Cathodic material for hydrogen generation. **A. Ali**, S. Sarwar, D.R. Pollard, X. Zhang, A.J. Adamczyk

10:50 224. Electrochemical CO₂ Reduction and Water Splitting Reactions at NanoCOT Electrodes for Clean Energy Conversion and Storage. **A. Ashaduzzaman**, S. Pan

11:10 225. Automated Structure Generation and Theoretical Predictions for Potential Near-Infrared (NIR) Dye Sensitized Solar Cells. **T. Santaloci**, A. Wallace, R.C. Fortenberry

11:30 226. Highly Active and Robust Ruthenium Photocatalysts for CO₂ Reduction: Exploring Electronic and Steric Effects for both Sensitized and Self-Sensitized Catalysts. **E.T. Papish**, S. Das, C.E. Webster, J.H. Delcamp

Birmingham Jefferson Convention Center
East Meeting Room O

Polymer Assemblies: from Fundamental to Applications 1

E. P. Kharlampieva, G. Schneider, *Presiding*

8:00 Introductory Remarks.

8:05 227. Dynamics of Semiflexible Colloidal Polymer Chains. **S.L. Biswal**

8:30 228. Advanced Time-Temperature Scaling in Polymer Melts. K. Bichler, B. Jakobi, **G. Schneider**

8:55 229. Mesoscale Modeling of Controlled Degradation and Erosion of Polymer Networks. V. Palkar, **O. Kuksenok**

9:20 230. Unentangled Vitrimer Melts: Generalized Rouse Theory Reveals Influence of Cross-link and Backbone Chemistry on Linear Viscoelasticity. **R. Ricarte**, S. Shanbhag

9:45 Intermission.

10:00 231.

Polymer Salogels for Shape Stabilization of Inorganic Phase Change Materials. **S.A. Sukhishvili**, X. Zhu, K. Rajagopalan

10:25 232. Precision Synthesis of Acrylamide Block Polymers with Degradable Thioester Junctions. **W. Gutekunst**

10:50 233. Anionic Ring-Opening Polymerization in Ionic Liquids. **c. giri**, P. Rugar

11:05 234. Manipulating Structure and Membrane Properties of Nano-scale Model Membrane Systems of Amphiphilic Polymers and Lipids. **R.M. Perera**, G. Schneider

11:20 235. Development of Rapid, Colorimetric Sensors to Detect SARS-CoV-2 viral Particles in Environmental and Human Samples. **C.T. Stueber**, B. Cochran, J. Northcutt, P. Dawson, T.W. Hanks

Birmingham Jefferson Convention Center
East Meeting Room B

Small Molecules for the Disruption of Bacterial Processes 1

Financially supported by Clemson University

D. C. Whitehead, *Presiding*

8:00 Introductory Remarks.

8:10 236. Eradicating Resistant and Tolerant Bacteria with Phenazine Antibiotic Inspired Small Molecules. **R.W. Huigens**

8:45 237. Targeting Bacterial Polysaccharide Metabolism of Gut Microbes with Small Molecules. **D.C. Whitehead**

9:20 238. Slaying Superbugs One Natural Product at a Time. **W.M. Wuest**

9:55 Intermission.

10:10 239. Antiinfective Properties of Human Milk. **S.D. Townsend**

10:45 240. Disruption of Salmonella Biofilms In Vitro and In Vivo. **C. Melander**

11:20 241. Plant Natural Products as a Resource for Antibiotic Drug Discovery. **C. Quave**

Birmingham Jefferson Convention Center
East Meeting Room D

Structure-Property-Function Relationships in Polymers

C. Zhao, Presiding

8:00 Introduction .

8:10 242. Toughing the Elastomers, Go Beyond the State-of-Art. Z. Zhang, **P. Cao**

8:40 243. Structure-Property-Function of Polypentenamer Systems. **J.G. Kennemur**

9:10 244. Structure-property Relationships in Self-healable Ultra-stretchable Electronic Polymers for Wearable Strain Sensors. **E.K. Wujcik**

9:40 Intermission.

9:55 245. Investigation of the Doping Effects of Small Molecule Acids on Self-healable, Stretchable PANI/PAAMPSA Conductive Polymer Complexes. **N. Penners**, K. Webb, J. Jeon, Y. Lu, E.K. Wujcik

10:25 246. Solvent Vapor Annealing Processing to Control Properties of Semi-crystalline Polymers in Thin Films. **J. Albert**, S. Bliesner, J. Strzalka, Q. Zhang, T. Parker, G. Kelly

Birmingham Jefferson Convention Center
East Meeting Room K

Supramolecular and Biomolecular Chemistry

Financially supported by the Louisiana Local Section of the ACS and the Tulane Chemistry Department

J. Jayawickramarajah, *Presiding*

8:00 Introductory Remarks.

8:05 247. The Expansion of Bilingual Peptide Nucleic Acids: Decoding the Nucleic Acid and Protein interaction for the development of Self-Assembling and Stimuli-Responsive Biopolymers.. **H. Argueta-Gonzalez**, C. Swenson, S. Sterling, G. Song, J. Heemstra

8:20 248. Unravelling the Structural Organization of Individual Alpha-Synuclein Oligomers Grown in the Presence of Phospholipids. **D. Kurouski**

8:40 249. Development of Supramolecular Hosts Targeting Phospholipids Commonly Found in Gram-positive Bacteria. **N. Busschaert**

9:05 250. Recognition of GC rich Nucleic Acids. **D.P. Arya**

9:30 251. Carbon Monoxide: The Good, the Bad, and the Ugly. **B. Wang**

9:55 252. Synthesis, Self-Assembly, and Dynamic Behavior of DNA Sequences Appended with Supramolecular Host and Guest Moieties. **D. Walpita Kankanamalage**, S. Pandey, J. Jayawickramarajah, H. Mao, L.D. Isaacs

10:10 Intermission.

10:40 253. Increasing the Membrane Permeability of Carboxylic Acid-containing Drugs using Synthetic Transmembrane Anion Transporters. **R. Salam**, S. Marshall, N. Busschaert

10:55 254. Bilingual Peptide Nucleic Acids: Encoding the Languages of Nucleic Acids and Proteins in a Single Self-assembling Biopolymer. **J.M. Heemstra**

11:20 255. Supramolecular Assemblies as Key Contributors to the Origin of RNA. **N.V. Hud**

11:45 256. *RE*-SELEX: Restriction Enzyme-Based Evolution of Structure-Switching Aptamer Biosensors. **A. Sanford**, A.E. Rangel, T.A. Feagin, R. Lowery, H.S. Argueta-Gonzalez, J.M. Heemstra

Birmingham Jefferson Convention Center
East Meeting Room F

The Magic of Spectroscopy

Financially supported by ACS Division of Physical Chemistry, ThermoFisher Scientific

A. Gunn, *Presiding*

8:00 Introductory Remarks.

8:10 257. Theoretical Investigations of Oxygenated Hydrocarbons for Matrix Isolation Infrared Spectroscopy Experiments. **A. Gunn**, M. Sakalosh, A.L. Smalley, J. Dovi

8:35 258. Reactivity, Coordination Behavior, and DFT Challenges for Transition Metal-acetylene Complexes Revealed via Infrared Laser Photodissociation Spectroscopy.. **A.D. Brathwaite**, J. Marks, A. Batchelor, M.A. Duncan

9:15 259. Ultrafast Spectroscopy with Frequency Combs: Enabling new Measurements of Dilute Species in Molecular Beams. **M.A. Reber**, N.D. Cooper, W.M. Jones

9:55 Intermission.

10:10 260. Vibrational Fingerprints of Substituted Ketenes. E. Sparks, K. El-Shazly, K. Narkin, H. Legg, **L.R. McCunn**

10:50 261. Shining Light on the Avian Compass Sense: An Investigation of the Magnetic Sensitivity of Cryptochrome 4 from a Migratory Bird using Cavity-enhanced Spectroscopies. **L. Jarocho**, J. Xu, K. Henbest, C. Timmel, S. Mackenzie, H. Mouritsen, P. Hore

11:30 262. Vibrational Spectroscopy of Aqueous Solutions: A Tale of Two Bases. **C. Pibel**, J.D. Ametepe, B.S. Pibel

Birmingham Jefferson Convention Center
East Meeting Room C

Total Synthesis of Complex Molecules

J. M. Smith, *Presiding*

8:00 Introduction .

8:05 263. 21st Century Cope Rearrangements Inspired by the Historical Report.. **A.J. Grenning**

8:40 264. Innovative Reactions and Strategies for the Synthesis of Complex Natural Products. **J.G. Pierce**

9:15 265. Dearomative Alkaloid Synthesis. **J.M. Smith**

9:50 Intermission.

10:10 266. Venturing Outside Flatland: Formation of Hindered Bonds in Aliphatic Systems. **T. Qin**

10:45 267. Synthesis of Illudalic Acid and Analogous Phosphatase Inhibitors. **G.B. Dudley**

11:20 268. Photoassisted Total Synthesis of Architecturally Complex Diterpenes. **J. Frederich**

11:55 Concluding Remarks.

THURSDAY AFTERNOON

Birmingham Jefferson Convention Center
East Exhibit Hall 1

Environmental

Poster Session

R. C. Wingfield, *Organizer*

12:30 - 2:30

269. Investigating Adsorption Kinetics and Isotherm Studies of In-House Biochar for the Removal of Emerging Chemical Contaminant from Water. **J. Lennox**, L.D. Moore, A. Saha, P. Bhoi

270. Jar Test Studies on Simulated Raw Water Containing Microplastics: Monitoring Turbidity, pH and Added Metal Salts. J. Outten, **M.C. Koether**, A. Gruss

271. Withdrawn. Application of Microbial Communities for Bioremediation of Uranium Contaminated Sites. **J.R. Hoyle-Gardner**, V. Ibeanusi, G. Chen, V. Badisa, B. Mwashote

272. Modification of a Fast, Reliable Microplastics Quantification Method: Visualizing Plastic Particles in Freshwater with Nile Red. **J. Forakis**

273. Origin of Oxalate-rich Rock Coatings. **S. Ginsberg**, **L. Rayburn**, **A. Bray**, **F. Nuñez-Parker**, **A. Dowling**, J. Russ

274. GC/MS Analysis of Volatile Organic Compounds (VOCs) Emitted During Wildfires by Using Cryogenic and Sorbent Pre-concentration. **J. Mann**, S. Pham, Z. Li, M. Zhang, N.S. Chong

275. Boronic Acid-based ferrocene Complexes Towards Fluoride Ion Sensing. **P.I. Fernando**, **G. Kosgei**, M. Glasscott, G. George, E. Alberts, C. Bresnahan, L. Moores

276. Computational Study of the Thermal Degradation of Perfluoroalkyl Carboxylic Acids. **C. Paultre**, A.M. Mebel, K.E. O'Shea

277. Point-of-need Qualitative or Quantitative Detection of Trihalomethanes in Environmental Water Samples Using a Highly Sensitive and Selective Fiber-based Preconcentration System. H. Rouhi, C. Duprey, L. Terry, M. Elliott, **E.K. Wujcik**

278. Method Improvement of Microplastic Weathering Resulting in Improved Modeling of the Behavior of Heavy Metal Laden Microplastics through Drinking Water Treatment Plants. **S. Diehl**, M.C. Koether, A. Gruss

279. Nitric Acid and Base (Ammonia and Dimethylamine) Calculations of Gibbs Free Energies for Nucleation: A Computational Analysis for Aerosol Formation. **M. Joines**, T. Odbadrakh, G.C. Shields

280. A Computational Study of Atmospheric Aerosol Formation . **G. Mazaleski**, T. Odbadrakh, G.C. Shields

Birmingham Jefferson Convention Center
East Exhibit Hall 1

Organic

Poster Session

L. Yet, *Organizer*

12:30 - 2:30

281. “Real-World” Medicinal Chemistry is Possible with Undergraduate Research Students. **L. Yet**

282. Withdrawn Furan Synthesis via a One-Pot enol Silane Formation-alkylation-cyclization-aromatization Cascade. **C.W. Downey**

283. "Unzipping" a Corannulene Bowl: Harnessing Strain Energy for Promoting Novel Structural Transformations. **G. Leith**, N.B. Shustova

284. Rapid Synthesis of Primary Amines by Radical C-H Amination. **R.J. Comito**, M. Hu, S.K. Ghosh

285. Withdrawn. Ion-responsive Release of Contents from Liposomes for Cellular Delivery. **R. Sagar**, A. Watson, J. Lou, M. Best

286. Regioselective 6-*endo* or 5-*exo* Radical Cyclization of *N*-Hetrocycles via Photoredox Catalysis. **M. Maust**, S. Blakey, C. Hendy, N. Jui

287. Synthesis, Characterization and Antimicrobial Activity of N,N-substituted Triazolium Salts with Lipophilic Substituents on Triazole and Benzotriazole Rings. J. Wilson, Z. Lin, I.C. Rodriguez, D. Fico, S. Sanders, J. Gorden, M. Frazier, L. King, **K.S. Taylor**

288. NMR Studies of Temperature and Solvent Effects on Dimerization of 4-*tert*-butylnitrosobenzene. **C.H. Rogers**, S.C. Blackstock

- 289.** Mechanism of Thiol-catalyzed Hydrolysis of P-Nitrophenyl Acetate Ester: Towards Novel Method for Chemical Recycling of Polyesters. **A. Nisathar**, V. Popik
- 290.** Development of Inhaled PLGA Encapsulated Ivermectin for the Treatment of SARS-CoV-2. **S. Sood**, S. Jha, S. Rayalam, S. Taval, V.V. Mody
- 291.** Development of Inhaled PLGA Encapsulated Aloin for the Treatment of SARS-CoV-2. **S. Jha**, S. Sood, S. Rayalam, S. Taval, V.V. Mody
- 292.** The Development of a DNA Aptamer with Isozyme Selectivity for Human Carbonic Anhydrase II. **E.B. Atuk**, J. Jayawickramarajah, N. Beltrami, M.M. Ismail, D. Hook, Z. Pursell, M.F. Ali, N. Nguyen
- 293.** Exploring the Substrate Scope of the E1 subunit of the 2-oxoglutarate Dehydrogenase Complex for Abiological catalysis. **R. Peterson**, E. Reynolds
- 294.** Rhodium-Catalyzed Asymmetric Dearomatization Strategy for the Total Synthesis of Nuphar Alkaloids. **K.G. Ortiz**, R. Karimov
- 295.** Synthesis of (\pm)-Hibiscone C. **A. Wildgen**
- 296.** Efforts Toward the Development of Non-Nucleoside MraY Inhibitors for the Treatment of Tuberculosis. **T. Berida**, S. Chatterjee, S. Mckee, P. Pandey, C. Ducho, R.J. Doerksen, S. Roy
- 297.** Towards the Total Synthesis of Ambuic Acid and Analogues. **P.M. West**, A. Ustoyev, M.P. Croatt
- 298.** Bactericidal Urea Crown Ethers can Target Phosphatidylethanolamine Membrane Lipids. **S. Herschede**, N. Busschaert
- 299.** Stereoselective Desymmetrization of Nitriles to Lactones via the Pinner Reaction. **J. Frost**, K.S. Petersen
- 300.** Synthesis of Tetraarylphosphonium/Tetrakis(pentafluorophenyl)borate (TAP^R/TFAB, R=1,2,3-TriOMe, and R=3,5-DiOMe) salts as Non-aqueous Electrolytes for Organic Redox Flow Batteries. **G. Mandouma**
- 301. Withdrawn.** Heteroacene-based Amphiphilic Fluorescent Nanoparticles for Bioimaging. **T. Ranathunge**, M. Loku Yaddehige, J. Varma, C. Smith, W. Kolodziejczyk, N. Hammer, G. Hill, A. Flynt, D.L. Watkins

- 302.** Growth and Structure of Nitrosoarene Electron Donor-acceptor Co-crystals. **S.A. Kelley**, V. Shuger, S.C. Blackstock
- 303.** Design and Synthesis of Kekulé and non-Kekulé diradicaloids Utilizing Radical Peri-annulation Strategy. **F. Kuriakose**, I. Alabugin
- 304.** Synthesis of Organic Fluorophore Ph₂-IDPP for use in NIR-II Fluorescence Bioimaging. **K. McKinney**, D.L. Watkins, S.M. Vijayan
- 305.** Designer Liposomes for Phosphorylated Metabolite Triggered Release Through Conformational Changes of Synthetic Lipid Switches. **J. Lou**, J. Schuster, F. Barrera, M. Best
- 306.** Synthesis of Heterogeneous Green Catalysts for the Epoxidation Reaction. **J.C. Johnson**, M.H. San Soucie, S.M. Landge
- 307.** Design and Synthesis of pH-sensitive Benzothiazole Cyanine Dyes. **S. Casa**, M. Henary
- 308.** Synthesis of 6-(4-fluoro)-3,4-diphenylpyridazine. **T. Mallett**, J. Philp, A. Williams, C. Williams, V. Sittaramane, S.M. Landge
- 309.** New Molecular Designs for Solar Light Harvesting with Synthetic Bioinspired Pigments. **H. Jing**, N.C. Magdaong, C.R. Kirmaier, J.R. Diers, D.F. Bocian, D. Holten, J.S. Lindsey
- 310.** Rational Development of Activatable Donors for On-demand Delivery of HNO. **A. East**, R. Tapia Hernandez, N.W. Pino, J. Chan
- 311.** Killing Two Birds with One Stone: The Simultaneous Phosphorylation and Capturing of Phosphorylated Cyanide Ions Using a Single Fluorescent Chemodosimeter. **R. Mia**, K.J. Wallace
- 312.** Red Shifted Donor Acceptor Fluorophores as Potential Agents for Biomedical Applications. **G. Ersoy Ozmen**, Z. Essam, D. Setiawan, R. Hamid, R. El-Aalb, R. Aneja, D. Hamelberg, M. Henary
- 313.** Heterogeneous Catalysis: Cyclization Method via Self-assembled Monolayers. **A.H. Horchar**, K.S. Petersen
- 314.** Synthesis and Characterization of β -enaminoamides as Precursors for the Fabrication of ZnO Films for Application in the Microelectronic Industry. **G. Farris**

- 315.** Characterizing Biochemical Responses Originating from Leaf Pathogenic Stress: Spotlight on Red Spots. **B. McCormick, A. Ferraro**, M. Salley, N.M. Hughes, A.J. Wommack
- 316.** Synthesis of Phenylpropionic Acid using a Grignard Reagent. **A. Cronan**, R. Okoth
- 317.** Modification of a Hemicyanine Platform for Optimized Deep tissue Photoacoustic Imaging. **S. Gardner**, C. Brady, C. Keeton, A.K. Yadav, M.Y. Lucero, S. Su, J. Chan
- 318.** Stereoselective Synthesis of α -Allyl- α -Trialkylsilyl- γ -Alkyl- β,γ -Unsaturated Carboxylic Acids via an Ireland-Claisen rearrangement. **C. Massey**
- 319.** Epoxidation and Ring Opening of α -Trimethylsilyl- β,γ -Unsaturated Esters. **L.M. Fealy**, M.P. Jennings
- 320.** Synthesis and Screening of Near-infrared (NIR) Hemicyanine Dyes for Photoacoustic Imaging. **T. Tran**, W.M. MacCuaig, L. McNally, M. Henary
- 321.** Electrophilic Aromatic Substitution of Phenanthrene as a Precursor to Functional Porous Materials. **R.J. Van Demark**, B. Aguila
- 322.** Voltage-Sensitive Asymmetric Thiazolothiazole Dye for Molecular Probe Sensing Applications. **A.R. Brotherton**, N. Sayresmith, M.G. Walter
- 323.** Development of Novel Small Molecule Photosensitizers with Integrated Photoacoustic Readout. **C. Brady**, S. Gardner, J. Chan
- 324.** Activity-based Delivery of Chemotherapeutics and Imaging Agents to Target Cancer. **M.C. Lee**, M.Y. Lucero, J. Chan
- 325.** Donor-acceptor-donor NIR Xanthene-based Dye for Photoacoustic Imaging. **C. Rathnamalala**, N.W. Pino, C.N. Scott
- 326.** Boron-mediated Enantioselective Aldol Reactions of Substituted Phenylacetates. **J. Mather, S.K. Ferrufino Amador**, M.X. Yáñez Diaz, T.L. Walls III, P.B. Chanda
- 327.** Aluminum-catalyzed Intermolecular mono- and bis-hydroalkoxylation of Allenamides with Alcohols. **K. Alam**, T. Li, M.P. Croatt
- 328. Withdrawn.** Development of Photoactivated nanoMOF Drug Delivery Systems. **H.D. Cornell**, M. Nagai-Singer, I.C. Allen, A.J. Morris

- 329. Withdrawn.** Novel Synthesis of Macrophilones as Potential Treatments for Melanoma. **J. Cowan**, A. Sherwani, N. Yusuf, S.E. Velu
- 330.** Investigation of Self-assembling BODIPY-pyridine/imidazole acceptors with a Series of Zinc Porphyrin/phthalocyanine Donors and their Charge Separated States. **T. Blesener**, Y. Zatsikha, V. Nemykin, C. Bruckner, L. Harrison
- 331.** Aurones as *S. mutans* Gtf Inhibitors for Prevention of Dental Caries. **P. Ahirwar**, A. Law, B. Nijampatnam, E.M. Rojas, H. Wu, S.E. Velu
- 332.** An Efficient Synthesis of 3-Alkylpyridine Alkaloids Enables Their Biological Evaluation. **A. Kaplan**, C. Schrank
- 333.** Ligand Modification Strategies for the Synthesis of Cu(II) Catalysts for Allylic and Benzylic Oxidation Reactions in Water. **M. Guagliardo**, A.E. Gorden
- 334.** Design, Parallel Synthesis, and Crystal Structures of Biphenyl Antithrombotics as Selective Inhibitors of Tissue Factor VIIa complex: Structure Activity Relationship of the S' site. **A. Spaulding**, R. Krishnan, P. Chand, s. arnold, S. Gupta, R. Upshaw, A. Dehghani, B.G. Boudreaux, C. Parker, S. Bantia, Y. El-Kattan, T. Lin, S. Saini, Q. Zhang, S. Rowland, Y.S. Babu, P.L. Kotian
- 335.** Deaminative Nickel-catalyzed One-carbon Homologation of Alkyl Amines. **C. Twitty**, M.P. Watson
- 336. Withdrawn.** The Synthesis and Biocatalytic Reduction of Beta-keto Alkynes. **R.M. Francis**, B.D. Feske
- 1119.** Towards the Synthesis of Ambuic Acid & Analogues **A. Ustoyev**

Birmingham Jefferson Convention Center
East Meeting Room K

Centennial of the Discovery of Insulin

D. Rabinovich, *Presiding*

1:00 Introduction.

1:10 337. Insulin 100: A Brief Philatelic History. **D. Rabinovich**

1:40 338. History of Diagnosing Diabetes and Monitoring Blood Sugar.. **T. Whiteside**

2:10 339. The Past, Present and Future of Metformin.. **C.W. Padgett**

2:40 Closing Remarks.

Birmingham Jefferson Convention Center
East Meeting Room F

The Magic of Spectroscopy 2

Financially supported by ACS Division of Physical Chemistry, ThermoFisher Scientific

A. Gunn, *Presiding*

1:00 Introduction .

1:05 340. Quantum Chemistry and Spectroscopy: A Match Made in the Heavens. **R.C. Fortenberry**

1:45 341. Application of Polarization Modulated Infrared Spectroscopy to Model Prebiotic Chemical Systems. **H.L. Abbott-Lyon**

2:25 342. Rotational Constants and the Effect of Step Size on Quartic Force Field Calculations for Astrochemically Relevant, Cyclic, Aluminum-containing Compounds. **O.A. Harwick**, R.C. Fortenberry

2:50 Intermission.

3:05 343. Laboratory Analogs of Thermally Processed H₂O-rich Ices Containing NH₃ and CO₂ Relevant to Astrophysical Environments. **D. White**

3:45 344. Spectroscopic and Thermal Assessment of the Influence of Copper Loading on Calcium Phosphate Bio-relevant Glasses. **J.A. JimÃ©nez**

4:25 345. Hydrogen Binding and Dissociation in Metal Hydride Clusters. **J.T. Lyon**

4:50 Concluding Remarks.

Birmingham Jefferson Convention Center
East Ballroom B

Theoretical chemistry: Method development and applications 1

Financially supported by Auburn University
E. Miliordos, *Organizer*
J. V. Ortiz, *Presiding*

1:00 Introduction .

1:05 346. Quantum Chemistry and Computer Science: A Tightly Connected Parallel Development. **H.F. Schaefer**

1:35 347. Psi4Education: Free and Open-Source Programing Activities for Chemical Education with Free and Open-Source Software. **B. Magers**, V.H. Chávez, B.G. Peyton, D. Sirianni, R.C. Fortenberry, A. Ringer McDonald

2:05 348. New Developments in the Basis Set Exchange. **S. Lehtola**, B.P. Pritchard

2:25 349. Local Dispersion for Symmetry Adapted Perturbation Theory. **Z. Glick**, C.D. Sherrill

2:45 Intermission.

3:00 350. Accelerating the Convergence of Self-consistent Field Calculations using the Many-body Expansion. **K. Lao**, F. Ballesteros

3:30 351. Unraveling the Mechanism of the Hydroxide Transport between the Cobaltocenium groups in Polyelectrolytes. **S. Wickramasinghe**, T. Zhu, Y. Cha, C. Tang, Q. Wang, S. Garashchuk

3:50 352. Mechanistic Analysis on Non-enzymatic Dipeptide Hydrolysis and Applicability to Other Polyamide-based Materials and Composites. **K. Lawson**, A.J. Adamczyk

4:10 353. Computational UV Spectra for Amorphous Solids of Small Molecules.
A.M. Wallace, R.C. Fortenberry

Birmingham Jefferson Convention Center
East Meeting Room C

Methods and strategies for modern organic synthesis

Financially supported by **Oakwood Chemical, VWR, Auburn University**

M. Chen, R. Karimov, *Presiding*

1:15 Introductory Remarks.

1:25 354. Azadienes and Azatrienes for Catalytic Enantioselective Umpolung
Synthesis of Chiral Diamines – Methods and Mechanism. **S. Malcolmson**, X. Shao, P.
Zhou

1:55 355. Making Chiral Heterocycles Using Chiral Heterocycles as Ligands. **A.
Aponick**

2:25 356. Oxidative C-H Functionalization. **S. Blakey**

2:55 Intermission.

3:15 357. Polarity Reversal and Functionalization of Fluorinated Alkenes. **S. Roy**

3:45 358. Bisketene Equivalents as Diels–Alder dienes, and their Application in
Natural Product Synthesis. **C. Newton**

4:15 359. Dearomative Coupling of Heteroarenium Salts with Nucleophiles and
Electrophiles. **R. Karimov**

4:45 360. The Flip Side of Click Chemistry: Breaking Bonds Reliably. **M. Finn**

Birmingham Jefferson Convention Center
East Meeting Room J

Small molecule activation at biological or bio-inspired metal centers

Financially supported by Agilent Technologies, Quark Enterprises, Chemglass Life Sciences, Thermo Fisher Scientific, ACS Division of Inorganic Chemistry, M Braun Inc

J. D. Caranto, G. B. Wijeratne, *Presiding*

1:15 Introductory Remarks.

1:20 361. Cu-promoted Functionalization of C-H Bonds Using Directing Groups with Varying Denticity, Hydrogen Peroxide and Triethylamine.. **I. Garcia-Bosch**

1:45 362. Modulating O₂ Affinity and Reactivity in Sensor Globin Domains. **E.E. Weinert**

2:10 363. Towards Understanding why the TxtE {FeO₂}⁸ Intermediate Resists Reduction. **J.D. Caranto**, C.P. Martin, M. Chen, M. Martinez, Z. Ma, V.L. Davidson, Y. Ding

2:35 364. Native and Non-native Reactions Catalyzed by the Multifunctional Hemoglobin Dehaloperoxidase. **R.A. Ghiladi**, D. Yun

3:00 365. Kinetic, Thermodynamic, and Theoretical Investigations into Proton-coupled Electron Transfer Reactivities of Synthetic Heme Superoxide Intermediates. **P. Mondal**, G.B. Wijeratne

3:20 Intermission.

3:35 366. Superoxide Dismutase Mimicry Across the Third Row Metals. **C.R. Goldsmith**, J.L. Moore, L. Senft, R.S. Boothe, J. Oppelt, A. Franke, A. Scheitler, D.D. Schwartz, I. Ivanović- Burmazović

4:00 367. Protic Ruthenium Anticancer Compounds: Describing the role of Ligand Charge in both Photodissociation and Singlet Oxygen Production. **E.T. Papish**, O.E. Oladipupo, Y. Kim

4:25 368. De Novo Designed Artificial Cu Proteins (ArCuPs) as a New Generation of Biocatalysts for O-H/O-O/C-H Activation Reactions. **S. Chakraborty**, S. Mitra, D. Prakash

4:50 369. Bioinspired Heme Mediated Monooxygenation of Indoles. P. Mondal, **G.B. Wijeratne**

5:10 1903. The role of tyrosine-159 hydrogen bond donation on 3-mercaptopropionic acid dioxygenase (3MDO) catalysis: a combined catalytic, spectroscopic, and computational investigation. N. J. York, M. Lockart, A. Schmittou, **B. S. Pierce**

Birmingham Jefferson Convention Center
East Meeting Room E

Spatially resolved spectroscopy: Applications in Biomedical and Materials Imaging

A. Ghosh, *Presiding*

1:15 Introduction .

1:20 370. Phenotyping Extracellular Vesicles from Red Blood Cells Using Vibrational Spectroscopy and Imaging. **R.A. Dluhy**, A. Konutham, J. Oh, A. Gaggar, R. Patel

1:50 371. Discrete Frequency Infrared Imaging of Colorectal Cancer and Lipid Deposits in Alzheimer's Brain Tissue. **M.P. Confer**, A. Ghosh, R. Bhargava

2:20 372. Label-free Sensing and Imaging for Lipidome Analysis. **M.R. Gartia**

2:50 373. Disease Diagnosis using Mid-infrared Spectroscopic Imaging. **C. Gajjela**, R. Mankar, S. Afrose, D. Mayerich, R. Reddy

3:20 374. Simultaneous IR+Raman Microscopy Measurements, SIRRMM for the identification of microplastic contamination of <20 μ m. **J. Anderson**, M. Kansiz, F. Weston, C.A. Marcott

3:50 375. Nanoscale IR spectroscopy: From Principles to Nanoscale Imaging and Identification of Metal Soaps. **A. Centrone**

4:20 376. Challenges in Nanospectroscopy Techniques for Materials and Biological Applications. **J. Atkin**

4:50 377. Nanoscale Spatially Resolved Infrared Spectroscopy of Amyloid fibrils and Prefibrillar Aggregates. **A. Ghosh**

Birmingham Jefferson Convention Center
East Meeting Room I

Contemporary Fluorine Chemistry in the Southeast 2

Cosponsored by FLUO
M. Etzkorn, *Presiding*

1:30 Introduction .

1:35 378. Chemistry for Molten Salt Reactors – History and Perspectives. **S. Dai**

2:05 379. Semi-Fluorinated Aromatic ether Polymers from Step-growth Polymerization of Fluoroalkenes and Fluoroalkylation of Diphenyl Ether. G. Munoz, K.M. Chamberlain, K. Shelar, K.M. Mukeba, E. Borrego, S. Athukorale, C.U. Pittman, **D.W. Smith**

2:35 380. Fluorine's role in halogen bonding. **W.T. Pennington**, A. Peloquin, C.D. McMillan

3:05 381. Fluorinated Indene Derivatives as New Building Blocks for Organic Materials. **M. Etzkorn**, M.J. Elardo

3:05 Concluding Remarks.

Birmingham Jefferson Convention Center
East Meeting Room D

Design, Chemistry, and Application of Active, Functional Materials

A. Koh, *Presiding*

1:30 Introductory Remarks.

1:35 382. Electroactive Hydrogel actuators fabricated via Digital Light Projection Additive Manufacturing. Y. Wang, B. Beckingham, **M.L. Auad**

2:15 383. Photons, Electrons, and Polymer Design: Structure-processing-property Relationships for Radiation-induced Polymerization. **J.L. Jessop**

2:55 Intermission.

3:00 384. Shape and Structure in Active Biopolymer Droplets. **K.L. Weirich**, K. Dasbiswas, D. Scheff, F. Schwarzendahl, P. Ronceray, A. Patel, T.A. Witten, S. Vaikuntanathan, M. Gardel

3:40 385. Galinstan Multi-material Dispersions for Deformable Electronics. **E. Bury**, A. Koh

4:05 Intermission.

4:10 386. Mixed Heterocyclic Oligomers Based on Pyrazine, Thiophene, and Furan as Organic Semiconducting Building Blocks. **D. Karunathilaka**, D.L. Watkins

4:35 387. Enhancing the Sustainability of Pd-based Hydrogenation Catalysts. **A. Rahmani**, T. Jurca

Birmingham Jefferson Convention Center
East Meeting Room G

Ground truth: bridging knowledge gaps between computational and experimental enzymology

Financially supported by **University of Memphis College of Arts & Sciences, University of Memphis Department of Chemistry**

N. J. DeYonker, *Presiding*

1:30 Introductory Remarks.

1:35 388. Cassava as a Solution for Cancer: A Computational Approach. **S. Delwakkada Liyanage**, C. Ratnaweera, D. Gunasekera

1:55 389. Application of RINRUS in Studying Enzymatic Reactions. **Q. Cheng**, N.J. DeYonker

2:20 390. Structure-Guided Protein Engineering: Utilizing the *Sphingomonas* sp. KT-1 PahZ1 Structure to Create a Commercially Useful Bioreagent for Poly(aspartic acid) Degradation. **J.M. Miller**, T. Lamantia, A. Jansch, j. marsee, M. Weiland

2:45 391. Ensemble Docking and Exploration of the Coronavirus Protease Active Site: Developing Optimization Rules for SARS-CoV-2 M^{pro} Antiviral drug development. **S. Stoddard**

3:10 Intermission.

3:25 392. Coupling of Electrostatic Preorganization and Dynamic Allostery: Insights from Atomistic Modeling. M.M. Lawal, **V. Vaissier**

3:50 393. Ionic Atmosphere Effects: A Reminder to Consider Solution Ions in Computational Simulations. Y. Orozco-Gonzalez, B.D. Dratch, M. Kabir, G. Gadda, **S. Gozem**

4:15 394. A role for N99 in the “b-latch” regulatory mechanism of the type II cysteine desulfurase SufS from *Escherichia coli*. J.V. Conte, R. Gogar, J.A. Dunkle, **P.A. Frantom**

4:45 395. Ligand interactions that determine transcriptional outcomes. **C.D. Okafor**

Birmingham Jefferson Convention Center
East Meeting Room A

New Directions in Metal-Catalyzed Reactions 2

Financially supported by Organic Reactions, Biocryst, VWR

X. Cui, *Presiding*

1:30 Introduction .

1:35 396. Electronic Structure of RhO^{2+} , Its Ammoniated Complexes $(\text{NH}_3)_{1-5}\text{RhO}^{2+}$, and Mechanistic Exploration of CH_4 Activation by Them. **N. Khan**, E. Miliordos

2:05 397. Development of a Ni-catalyzed Larock Annulation. **D. Wilger**

2:35 398. Synthesis, Characterization, and Reactivity of Redox-Active Polymerization Catalysts. N. Taylor, L.N. Baker, M. Gordinier, K. Young, **T. Brewster**

3:05 Intermission.

3:20 399. Withdrawn. Copper-Catalyzed Aminoheteroarylation of Unactivated Alkenes through Distal Heteroaryl Migration. **Y. Kwon**, W. Zhang, Q. Wang

3:40 400. Enantioselective Lactonization by Pi-acid Catalyzed Allylic Substitution: a Complement to Pi-allylmetal Chemistry. **A. Kizhakkayil Mangadan**, J. Liu, A. Aponick

4:00 401. *E*-Substituted Polydentate Phosphine Complexes: Their Catalytic Activity and Incorporation into Metal Organic Frameworks. N.S. Abeynayake, L.J. Barrios, V. Ramkumar, C. Secrist, **V. Montiel-Palma**

4:30 402. Dipyridylarylmethane Ligands Enable Efficient Alkane C-H Borylation Catalysis. **N.D. Schley**

Birmingham Jefferson Convention Center
East Meeting Room L

Electrocatalysts, Solar cell and Electrochemical methods part 2

S. Pan, *Presiding*

1:30 Introduction .

1:40 403. Dye-Sensitized Solar Cells in Unbiased Water and CO₂ Electrolysis Systems. **J.H. Delcamp**, S. Pan, H. Cheema, J. Watson, R.R. Rodrigues, P. Shinde

2:05 404. *In situ* Surface Sensitive Vibrational Spectroscopic Probe of Catalyst Structures, Dynamics and Reaction Mechanisms at Electrochemical Interfaces. **T. Lian**

2:30 405. *Interfacing Photosystem I into Nanomaterials.* **D.E. Clifffel**, K. Wolfe, C. Stachurski, J. Williams

2:55 406. Electrocatalytic OER and ORR Studies with Single Crystal Perovskite and Spinel Oxides Grown by Molecular Beam Epitaxy. **B.H. Farnum**

3:20 Intermission.

3:35 407. Electrochemically Triggered Interfacial Deposition/Assembly of Aqueous-Suspended Colloids. **W. Zhan**

4:00 408. Nanointerface-localized Electrical Field Enhancement in Energy Harvesting and Ion Separation: From Single Nanopores to AAO Membranes. **G. Wang**, D. Baram, M.M. Kvetny, W. Brown

4:25 409. Electrochemical and Light-driven Carbon Dioxide Reduction by Molecular Manganese Catalysts: Exploring the Positional Effect of Second-Sphere Hydrogen-Bond Donors. S. Sinha Roy, K. Talukdar, **J.W. Jurss**

4:50 410. Investigating Oxygen Evolution Reaction over Layered Intermetallic Electrocatalysts. D.K. Mann, A. Díez, O. Lebedev, Y. Kolenko, **M. Shatruk**

Birmingham Jefferson Convention Center
East Meeting Room O

Polymer Assemblies: from Fundamental to Applications 2

Financially supported by the National Science Foundation

B. Beckingham, Y. C. Simon, *Presiding*

1:30 Introduction .

1:35 411. Supramolecular Crosslinking Strategies for Polylactone-based Nanocarriers for Theranostics. **D.L. Watkins**

2:00 412. Leveraging Connectivity in Block Copolymers to Control Assembly and Shape Transformation in Polymersomes.. **Y.C. Simon**, T. Chidanguro, L.D. Dugas, C.H. Liu

2:25 413. Responsive self-assembled nano- and microcapsules. **E.P. Kharlampieva**

2:50 414. Withdrawn. Incorporation of Polysaccharide Derivatives into Cellulose Particles for Enzyme Immobilization. L. Portilla Villareal, A. Bansode, J. Garcia Alonso, M.L. Auad, B. Via, **I. Vega Erramuspe**

3:05 Intermission.

3:20 415. Microcapsule-based Self-healing for Additive Manufacturing. **B. Beckingham**, V. Shinde

3:45 416. All-aqueous Assembly of Highly Hydrophobic, pH-responsive Polyelectrolyte Multilayers. **J. Brito**, K. Asawa, A.K. Andrianov, C. Choi, S.A. Sukhishvili

4:00 417. Star Polyelectrolytes in Multilayer Assemblies. **A. Aliakseyeu**, J. Ankner, S.A. Sukhishvili

4:15 418. Free-Standing Multilayer Hydrogels. **M. Dolmat**, V.A. Kozlovskaya, E.P. Kharlampieva

4:30 Concluding Remarks.

Birmingham Jefferson Convention Center
East Meeting Room B

Small Molecules for the Disruption of Bacterial Processes 2

Financially supported by Clemson University

D. C. Whitehead, *Presiding*

1:30 Introductory Remarks.

1:40 419. Exploration of a Synthetic Retinoid Scaffold for the Treatment of Persistent MRSA Infections. **C. Schrank**, A. Cheng, I. Escobar, B. Haney, E. Mylonakis, W.M. Wuest

2:05 420. A Novel Antibiotic Adjuvant Scaffold Identified Through Fragment Screening that Potentiates β -lactam Antibiotics in MRSA by Dampening Transcription of key resistance genes. **M.S. Blackledge**, H.B. Miller

2:30 421. Computationally-guided Design of Promysalin Analogues to Overcome Resistance in *P. aeruginosa*. **A. Mahoney**, J. Khowsathit, J. Karanicolas, W.M. Wuest

2:55 Intermission.

3:10 422. Synthesis and Characterization of Novel Diffusible Signal Factor Analogs for Analysis of Structure Activity Relationships. **R. Wiley**, D.L. Baker

3:35 423. Quantitative Analysis of Fatty acid diffusible signaling factors by HPLC-ESI-MS. **B. HOFFMAN**

4:00 424. Promysalin Analogs Reveal New Binding Cleft in Succinate Dehydrogenase. **S. Post**, C. Keohane, L.M. Rossiter, A. Kaplan, J. Khowsathit, K. Matuska, J. Karanicolas, W.M. Wuest

Birmingham Jefferson Convention Center
East Meeting Room N

How to Foster Diversity, Equity and Inclusion in the Chemical Sciences: Lessons Learned and Taught from the Stories of Recipients of the Stanley C. Israel Award

R. Joseph, *Organizer*
P. Gordan, *Presiding*

2:30 Introduction .

2:40 425. Transformation of the LSU Chemistry Department. **I.M. Warner**

3:05 426. Diversity and Excellence: The Role of Senior Faculty. **J.V. Ortiz**

3:30 427. A Cuban Campesino in Chemistry's Academic Court. **R. Hernandez**

3:55 428. DEIR in Teaching and Research: Some personal Experiences, Challenges, and Opportunities. **D. Rabinovich**

4:20 Panel Discussion.

Birmingham Jefferson Convention Center
East Meeting Room K

Chemical Education

The Plant Hunter

C. Quave, *Organizer*

3:00 Introduction.

3:10 429. Book Talk: "The Plant Hunter: A Scientist's Quest for Nature's Next Medicines". **C. Quave**

4:00 Discussion and Questions.

Birmingham Jefferson Convention Center
East Exhibit Hall 1

Inorganic

Poster session

J. E. Ritchie, *Organizer*

3:00 - 5:00

430. Loss of Chromium(III) from Mixed Cr(III),Fe(III) Serum Transferrins. K.C. Edwards, **D.R. Graham**, D. Keith, J.B. Vincent

- 431.** Hydrothermal Synthesis of Rare Earth Ruthenates. **B. Patel**, M. Kolambage, C.D. McMillen, J.W. Kolis
- 432.** Gas-phase Oxidative Coupling of Alcohols and Amines over Bimetallic Solid Catalysts. **A. Minne**, J.W. Harris
- 433.** Heterometallic Metal-Organic Frameworks as a Platform for Gas-Phase Heterogeneous Catalysis. **A. Mathur**, D. Shakya, D.A. Chen, N.B. Shustova
- 434.** Designing Sublimable Lanthanide-Based Precursors for Quantum Information Processing. **S. Bisht**, M. Gakiya-Teruya, J. Vellore Winfred, M. Shatruk
- 435.** One-electron Oxidation of Methanesulfinic Acid (MSA) by Hexachloroiridate(IV). **Y. Yang**
- 436. Withdrawn.** Light-activated ruthenium polypyridyl β -diketonate complex is Cytotoxic within the Photodynamic Therapy Window. **R. Ryan**, R.J. Mitchell, D. Havrylyuk, D.K. Heidary, J.P. Selegue, P.C. Glazer
- 437.** Photophysical and Electronic Properties of Photoresponsive Metal-organic Frameworks. **G. Wilson**, C.R. Martin, N.B. Shustova
- 438.** Pyrrophenes and Pyrropyridines: Hexadentate Coordination systems for Uranyl UO_2^{2+} . **J. Ducilon**, A.E. Gorden
- 439.** Syntheses and Characterization of Valence Tautomeric Cobalt Complexes with Magnetic Transition at Room Temperature. **P. Wang**, M. Shatruk
- 440.** Investigation of Well-Defined Donor–Acceptor Fulleretic Materials. **G. Thaggard**, G. Leith, N.B. Shustova
- 441.** Exploring Metal-organic Frameworks: Reversible Gas Adsorption and Catalytic Activity. **P. Kittikhunnatham**, N.B. Shustova
- 442.** Synthesis and Metalation of Two Redox-active Ligands Functionalized with a Terminal Alkyne for Applications in Flow Chemistry. **A. Yu**, J. Bacsa, C.E. MacBeth
- 443.** Magnetic Structure of Chain Antiferromagnets MBi_4S_7 (M = Mn, Fe). **I. Campbell**, M. Shatruk, O. Garlea
- 444.** Synthesizing Organometallic Polymers from Metal-sulfur Cubane Clusters. **J. Gillen**, C. Bejger

- 445.** Titanium-45 for Development of PET Radiopharmaceuticals. **F. shefali**, I. Chaple, S.E. Lapi
- 446.** Biomimetic-inspired Polyimidazole Manganese Chelates. **B. McIntyre**
- 447.** Superacidic Nanostructured Materials. A.A. Kuvayskaya, **A. Vasiliev**
- 448.** Water-soluble Rhodium (III) and Cobalt(III) Porphyrin Complexes for the Biological Inactivation of Fentanyl. **H. Pal**, **A. Nina**, O.K. Nag, E. Oh, A. Burkus-Matesevac, C.D. Chouinard, K. Maiello, J. Delehanty, D. Knight
- 449.** To activate or not to activate? Experimental and computational studies of small molecule activation by copper- and zinc-based frustrated Lewis pairs. **K. Bledsoe**, L.K. Bennett, K.M. Clark
- 450.** Dimethyl zinc complexes supported by TBAM ligands: Exploration of ligand exchange thermodynamics and the mechanism of protonolysis. **L.K. Bennett**, K.M. Clark
- 451.** Magnetic and optical properties of NaLnS_2 (Ln = La, Ce, Pr, Eu, Er, Yb, Lu). **F.I. Danladi**
- 452.** Production of ^{52}Mn using Natural and Enriched Chromium Targets with a Semi-Automated Purification System. **J. Pyles**, A.V. Massicano, J. Appiah, J.L. Bartels, A. Alford, S.E. Lapi, J. Omweri
- 453.** Radioscandium Isotopes of Clinical Interests: Production and Purification of High Purity $^{43,47}\text{Sc}$ Radioisotopes via Enriched $^{[46,50}\text{Ti}]\text{TiO}_2$. **S. Cingoranelli**, C.S. Loveless, J.L. Bartels, J.R. Blanoc, R. T, S.E. Lapi
- 454.** Mechanochemical Investigation of the Impact of Solvates on Organometallic Halide Metathesis. **H. DeGroot**
- 455.** Effect of Tethered, Axially Coordinated Ligands (TACLs) on Rh(II)-Catalyzed Cyclopropanation: A Linear Free Energy Relationship Study. **C. Zavala**, A. Darko
- 456. Withdrawn.** Ferromagnetic $\text{Cd}_{(1-x)}\text{Cu}_x\text{Cr}_2\text{S}_4$ Thin Films: Synthesis, Characterization and First-principles Calculations. **J. ABBASI**, S. Regmi, A. Gupta
- 457.** Inelastic Neutron Scattering Study of Magnetic Exchange Pathways in MnS and MnSe. **J. Roth**, V. Yannello, A. Samarakoon, C. Ross, M. Uible, O. Garlea, M. Shatruk

- 458.** Optimization of a Microwave-assisted Reaction Method to Synthesize Europium-based Calcium Fluoride Nanoparticles for Potential Optical Imaging. **M. Fratarcangeli**, M. Rathbone, C. De Silva
- 459.** Zr-MOFs as a Platform for Nuclear Waste Sequestration. **K. Park**, N.B. Shustova
- 460.** Dynamically and Statically Tailoring the Properties of Metal-Organic Frameworks. **C.R. Martin**, N.B. Shustova
- 461.** A Novel Magnetic Drug Screening Nanoplatform Based on Immobilized Transmembrane Proteins on Magnetic Superparticles. **S. Mansur**, J. Horne, S.E. Velu, Y. Bao
- 462.** Surface Functionalized Polyamidoamine (PAMAM) - Fatty Acid Amphiphilic Janus Dendrimers for Biomedical Applications. **M. Loku Yaddehige**, I. Chandasiri, D.L. Watkins
- 463.** Unprecedented Ag Doping and the Crystal Structure of $\text{Au}_{30-x}\text{Ag}_x(\text{S}-t\text{Bu})_{18}$. **K.H. Wijesinghe**, N. Sakthivel, T.C. Jones, A. Antonysamy
- 464.** Short-range Ordered 2D Phases and their Electronic Properties in $\text{Nb}_x\text{V}_{1-x}\text{O}_2$. **T. Rawot Chhetri**
- 465.** Structure-Function Correlation in InP-Based Quantum Dots. **S. Click**, J.R. McBride, K. Reid, S. Rosenthal
- 466.** Biodegradation of N-nitroglycine by the Heme Protein NnlA. **K.A. Strickland**, A. Holland, A. Trudeau, D.E. Graham, J.D. Caranto
- 467.** Reorganization Energy and Charge Transfer Rates from Quantum Dots to Cobalt Redox Mediators. **M. Fort**, S. Click, E.H. Robinson, F.M. He, P.V. Bernhardt, J. Macdonald, S. Rosenthal
- 468.** Synthesis and characterization of ultras-small superparamagnetic Iron Oxide Nanoparticles-encapsulated Liposomes as a Novel pH-responsive T1-weighted MRI Contrast Agent for Cancer Diagnosis. **S. Rahmati**

Birmingham Jefferson Convention Center
East Exhibit Hall 1

Multidentate Ligands in Inorganic Chemistry

Poster session

W. E. Lynch, *Organizer*

3:00 - 5:00

469. Synthesis, Characterization and Structure of a *tetra*(acetonitrile)ruthenium(II) complex, $[(\text{NCCH}_3)_4\text{RuPh}(\text{P}\{\text{OCH}_2\}_3\text{CET})][\text{BArF}']$ and its Reactivity with Multidentate Ligands. **G. Durrell**, J. Bazemore, B.P. Quillian

470. Synthesis of New Nickel(II) CNC-Pincer Complexes as Catalysts for Carbon Dioxide Reduction. **S.Y. Manafe**, **S. Das**, **D. Nugegoda**, **J.H. Delcamp**, **E.T. Papish**

471. Synthesis of Symmetric Water Soluble N-Heterocyclic Carbene Ligands for AuNPs. **R. Borsari**, S.L. Strausser, I.M. Jensen, D.M. Jenkins

472. Systematic Investigation of Halogen Bonding Interactions in Dye-sensitized Solar Cells Using Cobalt Redox Shuttles Bearing Halogen Substituents. **S. Bhattacharya**, D. Nugegoda, J.H. Delcamp, J.W. Jurss

473. Catalytic Activity of NU-1000 based Catalysts Grafted with a Ni Organometallic Complex. **L.J. Barrios**, C. Secrist, V. Montiel-Palma

474. Synthesis of Heterobimetallic Arene Ruthenium Complexes Incorporating Aromatic N-Heterocycles and a Group 13 Metal. **G. Sanchez Lecuona**, V. Montiel-Palma

475. Synthesis of C_2 -symmetric Chiral Diimidazoles for NHC Macrocyclic Construction for Catalytic Applications. **H. Brothers**, J.R. Russell, D.M. Jenkins

476. Light-responsive and protic ruthenium compounds bearing bathophenanthroline and dihydroxybipyridine ligands achieve nanomolar toxicity towards breast cancer cells. **O.E. Oladipupo**, S. Brown, R. Lamb, J. Gray, C. Cameron, A. DeRegnaucourt, N. Ward, F. Hall, Y. Xu, C. Petersen, F. Qu, A. Shrestha, M.K. Thompson, M. Bonizzoni, C.E. Webster, S. McFarland, Y. Kim, E.T. Papish

477. Investigation of Phthalocyanine Synthesis for Catalysis in Zeolites. **J. Enguita**, A. Shrestha, A. Chowdhury, M.G. Bakker

478. Synthesis of New Pincer Ligands for Forming Ruthenium Photocatalysts for Carbon Dioxide Reduction. **W. Silprakob**, S. Das, D. Nugegoda, J.H. Delcamp, E.T. Papish

479. Synthesis and Characterization of Tri- and Tetra-cobalt Complexes Supported by 2,6-bis[(trimethylsilyl)Amino]pyridine. **L. Nguyen**, J. Bates, G. Guillet

480. Catalytic Hydrodeoxygenation of Vanillyl Alcohol with Ruthenium and Iridium Catalysts in Water and Other Green Solvents. **W. Yao**, S. Das, A.K. Vannucci, E.T. Papish

481. Synthesis, Characterization, and Catalytic Performance of Ru(II) Complexes Bearing 2,2'-bis(diphenylphosphino)Biphenyl (BIPHEP) Derivatives. **M.J. Goldberg**, **I. Alam**, **J.R. Stryker**, R.E. Black

482. Synthesis and Characterization of the Second Triiron Extended Metal Atom Chain Complex with Fe-Fe Bonding. **C.E. Mullins**, J.E. Bates, G. Guillet

483. Cobalt Catalyzed Regioselective Trifluoromethylation of C–H bonds. **C. Kuehner**, C.F. Harris, J.D. Soper

484. Development of Multidentate, Mixed O/S-donor Imidazole Thione Ligands. **R. Wolsleger**, M. Wetzler, J.L. Brumaghim

485. Small Molecule Activation by Ruthenium (BB)-carboryne Complex. **H. Jayaweera**, D.V. Peryshkov

THURSDAY EVENING

Birmingham Jefferson Convention Center
East Ballroom B

Plenary

D. A. Dixon, *Presiding*

5:30 486. From Isotopes to Images: Development of Radiometal Agents in Medicine. **S.E. Lapi**

FRIDAY MORNING

Birmingham Jefferson Convention Center
East Meeting Room G

Research in Practice 1

Financially supported by Wilson Dam Local Section of the ACS

S. Love-Rutledge, *Organizer*
S. Johnson, *Presiding*

8:00 Introductory Remarks.

8:05 487. Evaluating peer-led team learning in an online context: Is it still effective?.
J.D. Young, S.E. Lewis

8:25 488. Uncovering the Chemistry behind Food: Intentional Course Design for Broadening Science Literacy in Nonmajors during a Global Pandemic. **J.A. Dabrowski**

8:45 489. How does task design affect student engagement in small group discourse?.
S. Fateh, Z. Kirbulut, J. Reid, G.T. Rushton

9:05 Intermission.

9:20 490. Uncovering Mindset Perspectives via Analysis of Undergraduate Views on Intelligence in Chemistry. **D. Santos**, H. Gallo, J. Barbera, S. Mooring

9:40 491. Socio-psychological Interventions to Promote General Chemistry Student Success. Y. Wang, G.A. Rocabado, J.E. Lewis, **S.E. Lewis**

10:00 492. Exploring the Relationship Between a Student's STEM Professional Identity and their Perception of Meaningful Learning in the chemistry Laboratory.
M.L. Head, D. Dayani, A. Alkawam, E. Pearman

10:20 493. "I Felt Like I was Losing Like, an Hour of my Time": Examining the Experiences of Pregnant and/or Parenting Women in STEM Doctoral Programs. **C. Wright**

10:40 Discussion.

11:00 Concluding Remarks.

Birmingham Jefferson Convention Center
East Meeting Room I

Classroom Chemistry: Innovations in Practice

Financially supported by Central Alabama Community College
J. M. Carr, *Presiding*

8:00 Introductory Remarks.

8:05 494. *Can Students Learn Chemistry on Their Phones? Opportunities and Challenges in Tech-Driven Learning.* **K.D. Revell**

8:35 495. Psi4Education: Free and Open-Source Programming Activities for Chemical Education with Free and Open-Source Software. **R.C. Fortenberry**, B. Magers, A. Ringer McDonald, C.D. Sherrill

8:55 496. Surveying Microplastic Pollution and developing Science Identity through Field Experience and Course-based Undergraduate Research. **J. Forakis**, J. March, M.A. Erdmann

9:20 497. Incorporating Concept Development Activities into a Flipped Classroom Structure: Reframing the Flipped Classroom as a Blended Learning Mode of Instruction. **J.F. Eichler**, E.J. Yeziarski

9:40 Intermission.

9:55 498. Withdrawn. Flipped Classroom in Organic Chemistry: Significant Effect on Final Grades. **C. Cormier**

10:15 499. Lennard-Jones Plot Construction in General Chemistry: How Well Do Semiempirical ΔH_f Values Accurately Estimate Covalent Bond Lengths in Simple Diatomics? **J.M. Carr**, C.A. Rock, Z. McClendon

10:35 500. Withdrawn. Model-Based Inquiry and Engineering Design in the Classroom. **C.A. Rock**, B.A. Whitworth

11:00 501. Online-simulation Modules as Pre-learning Material to Reduce Cognitive Overload in Guided Inquiry Labs. **D. Das**

11:20 Concluding Remarks.

Birmingham Jefferson Convention Center
East Meeting Room F

f-Element Chemistry and Applications

Financially supported by University of Tampa College of Natural and Health Sciences, ACS Division of Nuclear Chemistry and Technology

A. E. Gorden, E. J. Werner, *Presiding*

8:00 Introduction .

8:05 502. Alternative Methods to Generate High-Valent Transuranic Elements. M. Sheridan, J. McLachlan, J. Gonzalez-Moya, T.S. Grimes, **C. Dares**

8:25 503. Crystal Engineering with Imidophosphorane Ligands in High-valent Actinide Complexes. **J. Niklas**, J. Bacsá, H.S. La Pierre

8:45 504. Understanding tetravalent actinide oxide formation, stability, and dissolution under far field environmental conditions. **B.A. Powell**, K. Peruski, C.J. Parker, M. Maloubier, D. Kaplan, A. Kersting, M. Zavarin

9:05 505. Tailoring Redox Active Ligands for Probing the Reactivity of Actinides. **A.E. Gorden**

9:25 506. From Solution to Solid State: An Update on Hexavalent Actinide Co-Crystallization. **J.D. Burns**, J. Einkauf

9:45 507. Exploring the Nature of F-Element Soft Donor Interactions using Electronically Tunable Azolate Ionic Liquids. **R.D. Rogers**, H.B. Wineinger, G. Gurau

10:05 Intermission.

10:20 508. Withdrawn. Use of Bis-lactam-1,10-phenanthroline Ligands as Selective Holdback Reagents for Improved Adjacent Lanthanide Separation. **K. Johnson**, I. Popovs, S. Jansone-Popova

10:40 509. Technetium Complexation with Halides. **N.A. Wall**, C. Eiroa-Lledo

11:00 510. Clean-up after F-element chemistry: Savannah River Site Tank Closure Cesium Removal (TCCR) In-Situ Cs-137 monitoring. **T. Whiteside**, D.P. Diprete, K.M. Fenker

11:20 511. Why Formal Oxidation States do not tell the Story of Magneto-structural Phase Transitions in Ce- and Eu-containing Intermetallics. J. Roth, V. Yannello, A. Rogalev, V.O. Garlea, **M. Shatruk**

11:40 512. Meso-unsubstituted Expanded Porphyrins: Synthesis and Applications. **J.L. Sessler**

Birmingham Jefferson Convention Center
East Meeting Room D

Frontiers in Organic Synthesis and Catalysis 1

Cosponsored by ORGN
W. Santos, *Presiding*

8:00 Introductory Remarks.

8:05 513. Withdrawn. Nickel-Catalyzed Deaminative Cross-coupling Reactions. **M.P. Watson**

8:30 514. Multifunctional aza-crown Ether Catalysts for Selective Hydroxyl Functionalizations. **B. Kim**

8:50 515. Ring Distortion of Indole Alkaloids as a Synthesis Platform for Drug Discovery. **R.W. Huigens**

9:15 516. Heterogeneous acid- and base-catalyzed Conversion of Unprotected Aldose Sugars to Furan Derivatives via the Garcia Gonzalez Reaction. **S.A. France**

9:40 Intermission.

9:55 517. Leveraging Complex Molecule Synthesis as a Driver for Chemical and Biological Discovery. **J.G. Pierce**

10:20 518. Broadening Copper-catalyzed Boracarboxylation to include Unactivated α -olefins by using Xantphos as a Secondary Ligand: Preliminary Insights from Catalytic and Stoichiometric Reactivity Studies. **B.V. Popp**, S.W. Knowlden, C.H. Gordon, N.N. Baughman

10:40 519. Transition Metal-Free Stereoselective Borylation Reactions. **W.L. Santos**

11:05 520. Beyond Cp* - Mechanism guided design of a new rhodium complex for enantioselective C-H functionalization. **S. Blakey**

Birmingham Jefferson Convention Center
East Meeting Room L

Main Group Chemistry and Inorganic Materials

P. Rugar, *Presiding*

8:00 Introductory Remarks.

8:05 521. Coordination Chemistry of Aromatic Boracyclic Anions. **C. Martin**

8:25 522. Effects of Heteroatoms on the Chemical and Electrochemical Stability of Some Polyaniline Derivatives. **C.N. Scott**, M.N. Almtiri, H. Gigi

8:45 523. Tetraarylphosphonium: A Versatile Platform for Green Chemistry Applications. **B. Wicker**, B.A. Atwater

9:05 524. Synthesis and Optical Studies of 4-coordinate Borafluorenes. **M. Pennington**, P. Rugar

9:25 525. Redox-active Ligands for the Rational Design of Electronically Delocalized Materials. **K.M. Clark**

9:45 526. Metal-free Bond Activation by Carboranyl Diphosphine. **G. Gange**, D.V. Peryshkov

10:05 Intermission.

10:20 527. Accessing Structural Information across Different Length scales in Distorted Rutilites using Irreducible Representations and Total Scattering Methods. **J.M. Allred**, T.C. Douglas, M.A. Davenport, M. Krogstad, L.M. Whitt, T. Rawot Chhetri, R. Osborn, S. Rosenkranz

10:40 528. Connections between Synthesis, Physical Properties and Chemical Bonding in 3d Polar Magnets. **T.T. Tran**

11:00 529. Understanding Dendrite Formation in Mg-based Batteries. **R.D. Davidson**, A. Verma, S. Angarita-Gomez, F. Hao, J. Van Buskirk, O. Gonzalez, P. Balbuena, P.P. Mukherjee, S. Banerjee

11:20 530. Relationship between Local Crystallographic Order and Geometric Frustration within $V_{1-x}Mo_xO_2$. **T.C. Douglas**, M.A. Davenport, L.M. Whitt, T. Rawot Chhetri, M. Krogstad, S. Rosenkranz, R. Osborn, J.M. Allred

11:40 531. Possible Evidence for Incipient Magnetism in quasi-one-dimensional Chevrel Phases. **L.M. Whitt**, T.C. Douglas, S. Chi, K. Taddei, J.M. Allred

Birmingham Jefferson Convention Center
East Meeting Room K

Multidentate Ligand Systems in Inorganic Chemistry: Synthesis, Complexes, Structures and Reactions 1

W. E. Lynch, *Presiding*

Financially supported by ACS Division of Inorganic Chemistry, and the Coastal Georgia Local Section of the ACS

8:00 Introductory Remarks.

8:05 532. Trisimidazolyl Phosphine, a Versatile Tridentate Ligand for Bioinorganic and Catalytic Studies. **W.E. Lynch**, C.W. Padgett, B.P. Quillian

8:30 533. Polydentate bis(amidines) as Selective Molecular Locks for Embedding Coinage Metal Fragments. **M. Stollenz**, J. Arras, O. Ugarte Trejo, C. O'Dea, A. Calderón-Díaz, N. Bhuvanesh, C.D. McMillen

8:55 534. Heterobimetallic Complexes of Ru, Rh and Ir Incorporating a Group 13 Element and Formation of bi- and Polydentate Phosphinogallyl Ligands. G. Sanchez Lecuona, N.S. Abeynayake, **V. Montiel-Palma**

9:20 535. Trimetallic Extended Metal Atom Chain Complexes of Fe(II) with Fe-Fe bonds, Variation of Properties Derived from Ligand Composition. **G. Guillet**, K.Y. Arpin, C.E. Mullins, J. Bates

9:45 Intermission.

10:05 536. The Generation of *Trans*-spanning Metallohedged Ligands. **J.A. Pienkos**, J.P. Lee, C.D. McMillen, S.L. McDarmont, L.D. Jaques, B.D. Nessel, S.E. Neglia

10:30 537. New hydroxy substituted Salen-type Pd and Pt complexes: Spectroscopical properties, Structural characterization, DFT calculations, and CO₂ reduction. **D.M. Pinero Cruz**, J.O. Rivera

10:55 538. Imidazole Thiones: Unique Sulfur-Containing Ligands for Metal Coordination. M.M. Kimani, M.T. Zimmerman, A.A. Gaertner, M.A. Abbas, R. Wolsleger, M. Wetzler, **J.L. Brumaghim**

11:20 539. Coordination Chemistry with Tridentate Pyridine/chalcogenone Mixed-donor Ligands. **D. Rabinovich**

Birmingham Jefferson Convention Center
East Meeting Room E

Polymer Membrane: Chemistry, Fabrication, and Application to Separations and Energy Devices

B. Beckingham, *Presiding*

Financially supported by Polymers

8:00 Introductory Remarks.

8:05 540. Tethered Electrolyte Active-layer Membranes (TEAMs): Expanding the Avenues for Polyelectrolyte Membranes. **C. Porter**, R. DuChanois, E. MacDonald, S. Kilpatrick, M. Zhong, M. Elimelech

8:35 541. Effect of PEGMA as a Comonomer in PEGDA Based Films for Controlling Fractional Free Volume and in Co-transport of Carboxylate Ions with Alcohols Through the Films.. **A. Mazumder, J. Kim, B. Hunter, B. Beckingham**

8:50 542. Advancing Forward Osmosis for Energy-efficient Wastewater Treatment towards Enhanced Water Reuse and Resource Recovery. **S. Zou**

9:20 Intermission.

9:30 543. MOF- Functionalized Membranes with Enhanced Antifouling and Selectivity for Efficient Water Treatment. **M.R. Esfahani**

10:00 544. Poly(4-vinylpyridine)-*block*-poly(*tert*-butylmethacrylate) as a Promising Precursor System to Charge Mosaics: Nanostructured thin Films of Oppositely Charged Domains.. **J.G. Kennemur**, R. Verduzco, T. Terlier, B.A. Fultz, B. Dunoyer de Segonzac

10:15 545. Leveraging Insights from Transport and Co-transport Behavior in Anion Exchange Membranes to Improve Membrane Performance for Direct Urea Fuel cells. **B. Beckingham, J. Kim**

10:45 Intermission.

10:55 546. Synthesis and Performance of New Vinylimidazolium Poly(Ionic Liquids) as Gas Separation Membranes. **S. Ravula**, J.E. Bara

11:10 547. Polynaphthalene Networks and High Yield Carbon-Carbon Composites via *Ortho*-Diyne Arene (ODA) Resins. E. Borrego, S. Athukorale, S. Gorla, A.K. Duckworth, W. Johnson, H. Ahmad, S. Kundu, C.U. Pittman, **D.W. Smith**

11:40 Concluding Remarks.

Birmingham Jefferson Convention Center
East Ballroom B

Theoretical chemistry: Method development and applications 2

Financially supported by Auburn University
E. Miliordos, *Organizer*
K. D. Vogiatzis, *Presiding*

8:00 Introduction .

8:05 548. Spin-forbidden processes and molecular magnetism: New theoretical tools for quantitative modeling and insight. **A. Krylov**

8:35 549. Flexible wavefunctions for strongly correlated systems: quasiparticle, coupled cluster, and seniority-based approaches. **R. Miranda Quintana**

9:05 550. Partitioning Correlation Mechanisms through Nonorthogonal Multiconfigurational Self-Consistent Field Theory. **L.M. Thompson**

9:25 551. New Method Developments for the Application of Correlated Electron Systems. **E. Kempfer-Robertson**, L.M. Thompson

9:45 Intermission.

10:05 552. Identifying domains of applicability of machine learning models of quantum-mechanical properties. **C. Sutton**

10:35 553. Density Matrix Embedding Theory Methods for Non-equilibrium Electron Dynamics in Extended Systems. **J. Kretchmer**

11:05 554. (T)+EOM Quartic Force Fields for Theoretical vibrational spectroscopy of electronically excited states.. **M. Davis**, R.C. Fortenberry

11:25 555. Global Searching of Self-Consistent Field Solutions Extended to Large Systems. **X. Dong**, L.M. Thompson

11:45 556. Modeling of Macromolecules with Electric Fields. Y. Zheng, **V. Vaissier**

Birmingham Jefferson Convention Center
East Meeting Room J

Women in Chemistry: Advances and Experiences in the Field A

Financially supported by **ACS Women Chemists Committee**

S. K. Hamilton, *Organizer*

X. Jiang, *Presiding*

8:00 Introduction .

8:05 557. Providing Students with Interdisciplinary Research in Organic Synthesis and Computational Chemistry. **J.A. Pigza**

8:35 558. Withdrawn. Elucidating Molecular Mechanisms of Mental Illness with Quantum Dots. **S. Rosenthal**

9:05 559. “It's not the warmest environment”: How Women Navigate Pregnancy and Parenting Throughout the STEM Doctorate. **C. Wright**

9:35 Panel Discussion.

Birmingham Jefferson Convention Center
East Meeting Room A

STEM Education in K-12

Financially supported by ACS Division of Polymer Chemistry, Alabama Science Teachers Association, Southern Research, Alabama Math Science and Technology Initiative, Birmingham Southern College

STEM K-12 1

E. Menard, C. Willingham, *Organizers*

9:00 560. Ironclad Chemistry – from Supernovae to the Red Mountain iron ore. **S. Brande**

10:00 Intermission.

10:10 561. Teaching Physical Science, Chemistry, and AP Chemistry in the Digital Realm. **K. Reeves, J. Firth, L. Swift**

11:10 Intermission.

12:40 562. Ask the Professor. **J. March, K.L. Hayden, M.S. Ponder, K.H. Shaughnessy, J. Harshman**

1:40 Intermission.

1:50 563. Particulate Diagrams in AP Chemistry. **L. McGaw**

2:50 Intermission.

3:00 564. Acids, Bases and Buffers in AP Chemistry. **L. McGaw**

Birmingham Jefferson Convention Center
East Meeting Room B

STEM Education in K-12

STEM K-12 2

E. Menard, C. Willingham, *Organizers*

9:00 565. The AMSTI/ASIM Program: An Overview. **A. Murphy**

10:00 Intermission.

10:10 566. REasons for Geographic and Racial Differences in Stroke (REGARDS).
G. Howard

11:10 Intermission.

12:40 567. Developing a Particle Model of Matter using Modeling Instruction. **C. Manor**

1:40 Intermission.

1:50 568. Proportional Reasoning to Describe (Qualitatively and Quantitatively) gas Behavior using Modeling Instruction. **C. Manor**

2:50 Intermission.

3:00 569. The Science of Sloss Furnaces. **T. Malugani**

Birmingham Jefferson Convention Center
East Meeting Room C

STEM Education in K-12

STEM K-12 3

E. Menard, C. Willingham, *Organizers*

9:00 570. Colorful and Sweet Chemistry. **A.A. Hazari**

10:00 Intermission.

10:10 571. Changing an Atom. **K. Williams**

11:10 Intermission.

12:40 572. Proficiency Scales in the Chemistry Classroom. **R. Poe**

1:40 Intermission.

1:50 573. Uses of Radioactive Isotopes in Pharmacy. **J.D. Burns**

2:50 Intermission.

3:00 574. FoodMASTER: Cooking with Chemistry. **T. Petrov**

Birmingham Jefferson Convention Center
East Exhibit Hall 1

Energy and Fuels

10:00 - 12:00

575. Analysis of Molten Salt Reactor Source Terms. **S. Creasman**, T.J. Harrison, L.H. Heilbronn

576. Copper Redox Shuttles Supported by Pentadentate Ligands for High Performance Dye-Sensitized Solar Cells. **A. Devdass**, J. Watson, J.H. Delcamp, J.W. Jurss

577. Electrochemical and Ce(IV)-driven Water Oxidation with Dinuclear Ruthenium Complexes Featuring Dipyridyl- or Dipyrimidyl-Pyridazine Bridging Ligands. **S. Sahil**, J.W. Jurss

578. Plasmon-Exciton Coupling Effect in Nanostructured Arrays for Optical Signal Amplification and Application in Nucleic Acid Detection. **F. Tukur**, **A. JAYAPALAN**, J. Wei

579. Novel Cobalt Oxide @ N-carbon Dots Core-shell Nanocomposite Synthesis as Efficient Electrocatalysts in Oxygen Reduction Reactions. **A. JAYAPALAN**, F. Tukur, J. Wei

580. MnO₂-MWCNT Nanocomposite for High Energy Supercapacitor Applications. **M.H. Kabir**, M. Thompson, W. GHANN, J. Uddin, A. Rodriguez, A. Poyraz

Birmingham Jefferson Convention Center
East Exhibition Hall 1

Undergraduate Research 2

Poster Session Undergraduate Research 2

J. A. Nikles, *Organizer*

10:00 - 12:00

- 581.** Surface Modification of Titanium to Support Soft Tissue Growth. **M. Roberts,** S.G. Dennis-Little, M. Yost, T.W. Hanks
- 582.** Effects of Co-doping and Alternate Sulfur Sources on Polyol Synthesized Cu-Sb-S Systems. **J.E. Daniel,** M. Jensen, T.R. MacAlister, M.E. Anderson
- 583.** Effect of Flanking Sequence on AT-hook peptide Motif Binding Action. **E.A. Durham,** M. Tedrick, K.L. Buchmueller
- 584.** Screening of a Small Library of Phenolic Compounds as Inhibitors of Melanoma and Non-melanoma Skin Cancer Cells. **M. Agbo,** S. Boateng, T. Roy, J. Chamcheu, J. Fotie
- 585.** Expression and Characterization of Lanthipeptide Components from the Marine Bacteria *Salinispora arenicola*. **A. Deen Sesay, D. Ellis,** E. Limbrick
- 586.** Stereoselective Hydrosilylation of Alkynes Catalyzed by Dichloro(ethylenediamine) Platinum(II) under Heterogeneous Conditions – a Mechanistic Study. **T. Tolar,** M. Agbo, C. Huff, **J. Fotie**
- 587.** A Comparative Study of Palladium on Charcoal and Palladium Nano-Dispersed in Organically Modified Silicate as Heterogeneous Catalysts for the Hydrosilylation of Aldehydes and Ketones. **H. Drago,** M. Agbo, T. Tolar, C. Huff, **J. Fotie**
- 588.** Cobalt, Nickel, Iron, Platinum and Palladium Individually Dispersed and Stabilized in Organically Modified silicate as Catalysts for a Reductive Functionalization of CO₂. **C. Huff,** M. Agbo, T. Tolar, H. Drago, **J. Fotie**
- 589.** Synthesis and Spectroscopic Analysis of Liquid State Hydantoin Derivatives. **B.C. Copeland,** O.A. Cojocar
- 590.** Synthesis and Analysis of Self-Assembling Small Organic Molecules for Rectifiers and Biosensors. **R. Ma,** M.E. Welker, R. Sullivan, O. Jurchescu
- 591.** Photochemical Annulation of 2-pyridone via Photocycloaddition–oxidative Cyclobutane Fragmentation. **E. Hardwick,** C. Slough, M.E. Daub
- 592.** Method Development of MC-LR Detection in the Liver and Brain of the Mummichog. **M.K. Klumb,** A. Aga, W. Silander, D. Hollis, J.F. Wheeler, S.K. Wheeler

- 593.** Mycoremediation of the herbicide Atrazine with Various White-rot Fungi via Ultra Performance Liquid Chromatography (UPLC). **J.S. Wirth**, M.K. Klumb, C.S. Webber, L.H. Olson, J.F. Wheeler, S.K. Wheeler
- 594.** Analysis of Atrazine Degradation and Metabolite Formation after Mycoremediation Utilizing the Fungus *Pleurotus ostreatus*. **J.R. Wilson**, H.E. Burney, L.H. Olson, J.F. Wheeler, S.K. Wheeler
- 595.** Atrazine Degradation in Soil by a Mixed Inoculum and White-Rot Fungi. **C.S. Webber**, **M.L. Schroder**, M.K. Klumb, J.S. Wirth, J.R. Wilson, L.H. Olson, J.F. Wheeler, S.K. Wheeler
- 596.** Quantification of Heavy Metals in Commercial Tuna. **M. McCormack**, J.D. Leyba
- 597.** Synthesis of Styrenes from Aldehyde-Aldehyde Aldol Coupling Products. **M. Rodriguez**, **T.G. Chong**, G. Dixon, C.W. Downey
- 598.** One-pot Synthesis of Furans from 3-(trimethylsilyl)propargyl Carboxylates. **A.V. Helbling**, D. Sklar, C.W. Downey
- 599.** Enol Silane Formation-allylation Reactions Promoted by Trimethylsilyl Trifluoromethanesulfonate. **R. Coyle**, E.D. Heafner, X. Lin, H. Zhong, C.W. Downey
- 600.** Addition of Indoles to Nitrones via Friedel–Crafts Silyloxyaminoalkylation. **H.L. Xia**, Z. Oracheff, C. Poff, S.E. Isaacson, C.W. Downey
- 601.** Synthesis of 2,3-Dihydroisoxazoles from Ketones and N-benzyl Nitrones. **R.M. Goodner**, C.W. Downey
- 602.** Determination of Cannabidiol in Tennessee Hemp Bud and Trim. **M.A. Lutey**, G.E. Potts
- 603.** Withdrawn
- 604.** Withdrawn
- 605.** Modifying SurMOF Thin Film Morphology: Examining the Effect of Deposition Parameters on Nucleation and Growth. **B.N. Diederich**, F.G. Gonzalez, A.M. Weeks, M.E. Anderson
- 606.** Correlating the Regioselectivity of Bromohydrin Formation from Unsymmetrical Alkenes with Bromonium ion C-Br Bond Lengths. N. Johansen, **B. Tutkowski**

- 607. Withdrawn.** Synthesis of Biaryl Phosphatrane Ligands for Transition Metal-Catalyzed Cross-Coupling Reactions. **Z.K. Abro, V.A. Osenga**
- 608.** Analysis of Hormone Agonists on the Differentiation of Oligodendrocytes Precursor Cells. **N. Campbell, M.C. Zupan, I. Parish, A. N.D. Punchi Hewage, M.D. Hartley**
- 609.** Ampicillin-induced Biophysical Changes of *Escherichia coli* Cells Over Multiple Generations. **A. Carranza-Parras, K. Dungey**
- 610.** Halogen Bonding Capable Functionalized Gold Nanoparticles – an Avenue for Molecular Detection Schemes. **Q. Dang, K. Lalwani, S.T. Gilmore, M.C. Leopold**
- 611.** Sintering-Based In-Situ Synthesis of Noble Metal Nanoparticles for Ceramic Glaze Color Control. **K. Lalwani, N. Dinh, M.C. Leopold, R. Coppage**
- 612.** Design and Application of an Immobilizable Protein Kinase. **T. Cope, D. Deane, T. Bennett, R.M. Hughes**
- 613.** Analysis of Commercial Glow Sticks. **T. Kanipe, H.E. Sasko, C.E. Dahm**
- 614.** Analysis of Colored Golf Balls. **J.A. Nolasco, C.E. Dahm**
- 615.** Colorimetric and Fluorometric Dual Sensor for the Detection of Copper and Aluminum Ions. **A. Foret, E. Fasusi, S. Westervelt, D. Ghosh**
- 616.** Suspension of Pt(II) Complexes in PMMA Films: Photophysical Effects. **J.H. Zimmerman, M.J. McCormick, P.S. Wagenknecht**
- 617.** Search for Blue Emitters with High Phosphorescence Quantum Yield. **W.M. Thomas, M.J. McCormick, J.H. Zimmerman, C.D. McMillen, P.S. Wagenknecht**
- 618.** Photochemistry and Computational Modelling of Titanocene Complexes. **T.J. Whittemore, H.C. London, A.G. Gale, G.C. Shields, P.S. Wagenknecht**
- 619.** Preparation and Analysis of Vanadium–Amoxicillin Complexes. **R. Overend, J.A. Dabrowski**
- 620.** Synthesis, Characterization, and Cytotoxic Activity of Asymmetric *N,N'*-bis-substituted 1,2,3- Triazolium Salts. **D. Fico, I.C. Rodriguez, J. Wilson, R.V. Clamor, S. Sanders, J. Gorden, M. Frazier, L. King, K.S. Taylor**

621. Reverse Engineering as a Freshman Chemistry Research Experience. **M. Morris**, N. Edge, J.K. Konzelman

622. Novel Synthesis of Gamma Lactones from Dinitriles. **K. Youngblood**, K.S. Petersen

623. *Selenium heterocycles and the enzymatic inhibition of SARS-CoV-2's M^{protease}.* **R.E. Panella**, M. Donahue, J. Kessler, F. Bai

624. Investigating the Role of Disulfide Interface in Metal Binding for Psoriasis Using Molecular Dynamics Simulations. **Y. Chen**, A. Acharya, D. Das

625. Synthesis, Characterization, and Reactivity of Copper Complexes Supported by a Tripodal Amidate Ligand. **Y. Zhang**, E. Liu, J. Bacsa, C.E. MacBeth

626. Developing a Biodegradable Collagen Mimic for Applications in Wound Healing. **A. Tarlton**, S. K. Hamilton

627. Recycling Plastic Materials by Solvent-targeted Recovery and Precipitation. **B. Martin**, C. Tirla, J. Locklear

628. The Chemical Depolymerization of Poly Lactic Acid (PLA) Plastic Accelerated by Microwave Heating. **B. Murphy**, J. Cooper, J. Konzelman

629. Withdrawn. Monitoring Ivyp1 Active Site Loop Structure and Dynamics using Variable Temperature NMR. **J. Durham**, K. Letsinger, T. Leeper

999. Synthesis and Reaction Pathways Cu-Sb-S Systems for Sustainable Energy Production. **M. Jensen**, T. MacAlister, M. Anderson

Birmingham Jefferson Convention Center
East Meeting Room J

Women in Chemistry: Advances and Experiences in the Field B

Financially supported by ACS Women Chemists Committee

S. K. Hamilton, *Organizer*
J. M. Murphy, *Presiding*

10:00 Introduction .

10:10 630. Thiosemicarbazone Inhibition on Topoisomerase II α . **X. Jiang**, W. Medawala, L. Ngo, W. Morris, E.C. Lisic, J. Deweese, E. Driggers

10:40 631. Bloom Where You are Planted: Growing Outreach Programs as an Early Career Chemist. **E.E. Hardy**

11:10 632. Encouraging Representation of Women in STEM: Organizing Arkansas' first Virtual Women in STEM Conference. **S.E. Hubbard, S.K. Hamilton**

11:40 Panel Discussion.

FRIDAY AFTERNOON

Birmingham Jefferson Convention Center
East Meeting Room G

Research in Practice 2

Financially supported by Wilson Dam Local Section of the ACS

S. Johnson, *Organizer*
S. Love-Rutledge, *Presiding*

1:00 Introductory Remarks.

1:05 633. Comparison of Laboratory Notebooks in Three Contexts - Traditional Laboratory, CURE, and Research. **A. Hagwood**, M.G. Koufas, W.E. Allen, **J.P. Walker**

1:25 634. Assessing the Scientific Practices: Lessons Learned about Content and Context. **J.H. Carmel**, E. Day, N.S. Stephenson, M. Cooper, D.G. Herrington

1:45 635. Using Classical Test Theory and Rasch Modeling to Improve General Chemistry Exams on a Per Instructor Basis. **K. Hanson**, B. Sorrenson

2:05 636. Engaging Metabolic Pathways: Infographics to Promote Creativity and Multimodal Learning in Biochemistry. **S.T. Love-Rutledge, S. Johnson**, J. Robinson

2:25 Intermission.

2:40 637. Understanding how Representations of Chemical Bonding Influence the Paths Students Engage in while Predicting Molecular Shape. **A. Farheen**, S.E. Lewis

3:00 638. Organic Chemistry students' Reasoning and Representational Competence Skills in the Context of Dash-wedge Diagrams and Newman Projections. **M. Popova**

3:20 639. Using EEG and Eye Tracking Data to Characterize Learner Cognitive Processes During 3D Modeling Tasks in General Chemistry. K. Barbee, T. Gordon, H. Knoefel, T. McCullough, A. Randolph, C. Terrell, **K.J. Linenberger Cortes**

3:40 Discussion.

4:00 Concluding Remarks.

Birmingham Jefferson Convention Center
East Exhibition Hall 1

COMP

Poster session

T. P. Hamilton, *Organizer*

1:00 - 3:00

640. Computational comparison of atmospheric clusters: $\text{H}_2\text{SO}_4\text{-HCOOH-H}_2\text{O}$ and $\text{H}_2\text{SO}_4\text{-HNO}_3\text{-H}_2\text{O}$. **L. Juechter**, S. Harold, T. Odbadrakh, G.C. Shields

641. Computational Analysis of Prebiotic Triglycine Formation in Atmospheric Microdroplets. **S. Harold**, S. Warf, T. Odbadrakh, G.C. Shields

642. Calculating the Concentrations of Hydrated Sulfuric Acid Clusters. **L. Kurfman**, S. Vanovac, T. Odbadrakh, G.C. Shields

643. Computational Study of Hydrated $\text{H}_2\text{SO}_4\text{-NH}_3\text{-(H}_2\text{O)}_n$ Clusters. **V. Fowler**, T. Odbadrakh, G.C. Shields

- 644.** Triglycine Formation in Atmospheric Nano Droplets of Water. **S.L. Warf**, S. Harold, T. Odbadrakh, G.C. Shields
- 645.** Computational Calculations of Radical pair EPR Parameters for Avian Magnetoreception. **C. Bready**, C. Kerpel, T. Odbadrakh, L. Jarocho, G.C. Shields
- 646.** Design and Computational Study of Cyanide Bridged Platinum-iron Complex as Anti Cancer Prodrugs. **A. Kaspi-Kaneti**, S. Bhandari, A. Schubert, S. Huang, B.D. Dunietz
- 647.** Generating Spin-orbit Couplings for x-ray Absorption Spectra using a Simplified LR-TDDFT/ZORA Approach. **S. Pak**, D. Nascimento
- 648.** Determination of the Binding Affinities of Acridinyl, Quinoliny, and Pyridinyl Benzenesulfonamides with Enzymes in the *Plasmodium Falciparum* folate Pathway using Docking and Molecular modeling studies. **A. Mallia**, N.Y. Forlemu
- 649.** Electron Donating Group Effects on Halogen Bond donor σ -holes. **D. Devore**, T.L. Ellington, K.L. Shuford
- 650.** σ -Hole Flexibility in Chalcogen Bond Donors. **K.A. French**, T.L. Ellington, K.L. Shuford
- 651.** Statistical Analysis of Protein Similarity Measures. **K. Orellana**, **C. Dyer**, A.L. Parrill-Baker, D.L. Baker
- 652.** QM/MM studies of Xanthine Oxidase Inhibitors. **Y. Maghsoud**, C. Dong, G.A. Cisneros
- 653.** Pursuing type II Heterostructures Using low Dimensional Material Composites for Enhanced Photocatalytic Activity. **U. De Alwis**, K.M. Weerawardene, T.L. Ellington, K.L. Shuford
- 654.** Conventional Strain Energies of Three-membered Heterocycles. **R.P. Ivey**, M.M. Case, D.H. Magers
- 655.** QM-cluster study of Reaction Energies in [Ni,Fe]-hydrogenase. **T. Suhagia**, T.J. Summers, Q. Cheng, M. Griffing, N.J. DeYonker
- 656. Withdrawn.** Feasibility Studies of High Speed Molecular Information Processing. **K. Williamson**, D. Herr, Y. Mo, H.P. Rathnayake

657. Computed vs. Experimentally Derived Oscillator Strengths: A Benchmark Study of Excited-state Quantum Chemical Methods. **J. Garcia Alvarez**, A. Tarleton, A. Wynn, C. Awbrey, T. Roberts, S. Gozem

658. Understanding the Effects of Non-bonding Interaction on the Flavin's Absorption Spectra. **M. Kabir**, Y. Orozco-Gonzalez, S. Gozem

659. Benchmarking Dimer Contributions to Crystal Lattice Energies in Small Organic Crystals. **C. Sargent**, C.D. Sherrill

660. Free energy of Fc/Fc⁺ redox process in Ferrocene-terminated alkanethiol self-assembled monolayers on Au(100). **J. Hymel**, J.G. McDaniel

661. Dissociation Dynamics of Water Molecule on the Core-excited Potential Energy Surface. **A. Datar**, D. Matthews

Birmingham Jefferson Convention Center
East Exhibition Hall 1

Physical Chemistry

Poster session

T. P. Hamilton, *Organizer*

1:00 - 3:00

662. Methane to Methanol Conversion Facilitated by Anionic Transition Metal Centers: The Case of Fe, Ni, Pd, and Pt. **S. Sader**

663. Development of Solvated Electrons Precursors as a Novel Catalyst: Functionalization of CO₂. **B. Jackson**, E. Miliordos

664. Benchmark Database of Accurate Nonadditive Interaction Energies of Three-body Complexes. **S. Ochieng**, K. Patkowski

665. Investigations into the Physical Properties of Gemini Surfactants. **D. Aguilar**, A. Wisner, S.J. Bachofer, R.D. Sheardy

- 666.** Temperature Dependence of Fluorescence Emission of Polyaromatic Hydrocarbons: Effect of Excitation Wavelength, Emission Wavelength, and the Sample Matrix. **M. Wamsley**, W. Peng, X. Cui, D. Zhang
- 667.** Eliminating Spurious Multipoles in Intramolecular Symmetry-adapted Perturbation Theory. **D. Luu**, K. Patkowski
- 668.** QM-cluster Modeling of Chorismate Mutase Based on Sampling MD Simulation. **D.A. Agbaglo**, **T.J. Summers**, Q. Cheng, N.J. DeYonker
- 669.** Guest-Host Raman Under liquid Nitrogen Spectroscopy (GHRUNS) for the acquisition of improved vibrational spectra of solids. **E.C. Lambert**, C. Smith, R.N. Compton, N. Hammer
- 670.** Tunable Attosecond Charge Migration in Functionalized Environmentally Persistent Free Radicals. **N. Luedman**, **C.T. Papszycki**, A. Osborne, V.B. Baron, A. Bruner
- 671.** Electron Paramagnetic Resonance Studies of Transition Metal Phthalocyanines. **G.R. Rana**, M.G. Bakker
- 672.** Probing mixed ionic-electronic conducting polymers using ultrafast spectroscopy. **C. Grieco**
- 673.** Plasmonic Coupling of Silver and Gold Nanoparticles in Dimer Systems: Investigating the Near-field Spectra. **S. Gomrok**, J. Barr, E. Chaffin, X. Huang, Y. Wang
- 674.** Pro-drug Encapsulation by Cyclodextrin in a Model Biomimetic System. **S.E. Westervelt**, K.S. Aiken, S.M. Landge, D. Ghosh
- 675.** Observing Belousov-Zhabotinsky Oscillating Reactions in Acoustically-Levitated Droplets. **K. Everitt**, H. McCardle, E.R. Duranty
- 676.** The Ideal Gas Thermodynamic Properties of PtC. **L. Biolsi**
- 677.** Solvent Polarity-induced SPAAC Rate Enhancement of the Most Reactive Cyclooctyne: Synthesis and Photo-click Kinetics of a Water Soluble Cyclopropenone-caged Triazole-fused Dibenzocyclooctyne. **C.J. Molnar**, V. Popik

678. Self-assembly, Gelation, and Mechanical Properties of Molecular Gels Based on Tyramine based Alkanamides and N-(4-hydroxyphenyl)alkanamides as Low Molecular Mass Gelators. **J. Miller, A. Mallia**

679. Investigation of Carbene Formation in Ionic Media with Physics-based, Neural Network Force Fields. **J. Stoppelman**

680. Exploring Excited States of Ruthenium Polypyridine Chromophores by Ultrafast Transient Absorption and 2D-spectroscopy. **S.E. Dominguez, M.A. Hermosilla-Palacios, L. Baraldo, V.D. Kleiman**

681. Helmholtz Capacitance of Aqueous Solution at Au (100) Electrode Under Applied Voltage. **S. Park, J.G. McDaniel**

682. Solid Lipid Nanoparticles of Cannabidiol (CBD): A Brief Survey on Emulsifying Ingredients. **M. Valizadehderakhshan, A. Shahbazi, A. Bhowmik, M. Azami, F. Khaleseh**

683. Effect of Deposition Parameters and Constrained Area on the Characteristics of Langmuir Films of Nanoparticles. **C.V. Nguyen, J.J. Weimer**

684. Preparation And Characterization Of Microcrystalline Cellulose From Raphia Farinifera Inflorescence. **E. Agboeze**

Birmingham Jefferson Convention Center
East Exhibition Hall 1

Polymer Chemistry

Poster session

V. Thomas, *Organizer*

1:00 - 3:00

685. Self-assembly of Single-chain Polymer–fluorophore Nanoparticles in Physiological Milieu. **S. Liu, J.S. Lindsey**

- 686.** Multilayer Hydrogel Particles for Controlled Delivery. **D. Inman**, M. Dolmat, V.A. Kozlovskaya, P. Dickens, E.P. Kharlampieva
- 687.** Simplifying the Synthesis of Conjugated Polymers Utilizing Dihydropyrrolo[3,2-b]pyrrole as a Novel, Tailorable Building Block. **K.J. Bell**, A.M. Kisiel, G.S. Collier
- 688.** Understanding the Solution Behaviors of Ionenenes in Ionic Liquids using Dynamic Light Scattering. **C. Patton**, J.E. Bara, K.E. O'Harra, G. Thompson
- 689.** Synthesis of new Diketopyrrolopyrrole Scaffolds for High-performance Organic Electronic Device Applications. **R. Wahalathantrige Don**, C.N. Scott
- 690.** Highly Swellable Hydrogels Prepared from De-aromatized Lignin. **J. Hwang**, D. Goodlett, M. Ganewatta, M. Kent, C. Tang
- 691.** Co-transport of Methanol and Carboxylates in Cation Exchange Membranes: Effect of Poly(ethylene glycol) Phenyl Ether Acrylate as a Blocking Group. **P. Parasakthi Aravindhana**, J. Kim, B. Beckingham
- 692.** Polyaddition with Dimaleimides and Aminomaleimides. **N.Z. Singleton**, T.I. Robinson, A.J. Caroland, **H.J. Schanz**
- 693.** Dimaleimidide: Synthesis and Polyaddition with Diamines. **K.M. West**, N.Z. Singleton, H.J. Schanz
- 694.** Main-chain Metallo-Polyelectrolytes for Alkaline Anion-Exchange Membranes. **H. Lin**, C. Tang
- 695.** General Access to Allene-containing Polymers using the Skattebøl Rearrangement. **N. Galan**, J.N. Brantley
- 696.** Effect of Bicyclohexyl Regioisomer Ratios on the Physical Properties of Poly(bicyclohexyldimethylene terephthalate). **A. Coley**, T.N. Thompson, M.D. Schulz

Birmingham Jefferson Convention Center
East Exhibition Hall 1

Polymer Materials Science and Engineering

Poster session

V. Thomas, *Organizer*

1:00 - 3:00

697. Capacitive Electrode Printed Using Silver Nano-Ink on Plasma Modified/Functionalized PET for Potential Organic Pollutants Sensing from Water. **R. RAJAN PILLAI**, S. Gardner, S. Sunilkumar, S. Sanas, M. Haider, V. Thomas

698. Crystallization Kinetics of Mixtures of Polypropylene Homopolymer and Impact Copolymer. **P. Wang**, S. Liu, Y. Peng

699. Effects of Functional Groups and Anions on the Properties of Polyamide-Ionenes. **J. Bridges**, S. Chatterjee, K.E. O'Harra, J.E. Bara

700. Optimizing polyHIPE Foams for PFAS Removal from Wastewater and Groundwater via the Implementation of Surfmers. **I. Dorsey**, A. Koh

701. Development of a Scalable, Organic Solvent-free Process for PCDA Liposome Formation. **M. Head**, T.W. Hanks

702. Chemical "Activation" of Polyvinyl Chloride for Upcycling and Depolymerization. **M. Bepari**, A. Alshaikh, J.E. Bara

703. Tröger's Base Containing Polymers Membranes For Separation of CO₂ From other gases
. **C. Baltier**, S. Chatterjee, J.E. Bara, C. Patton, K.N. West

704. Non-releasing, Enzymatic Layer-by-layer Coatings with Antibacterial Activity. **J. Brito**, I. Alvarado, A.K. Andrianov, S.A. Sukhishvili

705. Competition-Enhanced Aptamer Selection Against A Chiral Lipid. **S. Ochoa**, M.C. Adams, A. Saad-Falcon, D. Hufnagel, V.T. Milam

706. Processing Carbon-Carbon Composites from Ortho-diynylarene Resins. **W. Johnson**, E. Borrego, S. Gorla, S. Athukorale, A.K. Duckworth, H. Ahmad, S. Kundu, H. Toghiani, C.U. Pittman, D.W. Smith

707. Electrospinning Parameters and Chemical Additives in Fabricating PVA Electro Spray Fibers. **M. Ucak Astarlioglu**, T. Thornell, H. George, E. Alberts, K. Klaus, S.E. Morgan

- 708.** Dynamics of Bottlebrush Polymers. **K. Bichler**, B. Jakobi, G. Schneider
- 709.** Agglomeration Behavior in Case of Bottlebrush Polymer. **B. Jakobi**, K. Bichler, G. Schneider
- 710.** AFM Investigation of the Effects of Disinfection Treatments on Polypropylene Personal Protective Equipment (PPE) Materials. **T.G. Chambers**
- 711.** Renewable Semifluorinated Polymers. **K. Mills**, K. Shelar, K.M. Mukeba, D.W. Smith
- 712.** Bis-*ortho*-diynylarene Performance Optimization via Expansion of Processing Window and Post-Cures in Air. **A.K. Duckworth**, E. Borrego, S. Athukorale, S. Gorla, W. Johnson, C.U. Pittman, D.W. Smith
- 713.** Effect of Nanoparticle Size on Internalization and Transport Across the Corneal Barrier. **M. Azadi**, A.E. David
- 714.** Improved Nanoformulation of *Linear-Dendrimer Block-co-Polymer* Materials for Red Blood cell Hitchhiking with *Ionic Liquids*. **C. Hamadani**, I. Chandasiri, M. Loku Yaddehige, G.S. Dasanayake, I. Owolabi, A. Flynt, D.L. Watkins, E.E. Tanner

Birmingham Jefferson Convention Center
East Meeting Room J

Women in Chemistry: Advances and Experiences in the Field C

Financially supported by the Women's Chemist Committee of the ACS

S. K. Hamilton, *Organizer*
S. E. Hubbard, *Presiding*

1:00 Introduction .

1:05 715. From AP Certification to PhD in six (intense) years: Obstacles and Advantages to Second-career PhD Students in Chemistry. **J.M. Murphy**

1:35 716. Equity in Parental Leave? or You Have a Baby...In a Pandemic!. **S. Zingales**

2:05 717. Changing the Academic Culture as a Woman in STEM. **J.L. Brumaghim**

2:35 718. Empowering the Next Generation of Chemists Through Academic Advising, Mentoring, and Cohort Building. **A.J. Carroll**

2:35 719. Resilience of Women in Chemistry: Lessons Learned. **L. Tribe**

3:05 Panel Discussion.

3:35 Concluding Remarks.

Birmingham Jefferson Convention Center
East Meeting Room F

Women in STEM

Undergraduate Discussions: Women in STEM

Financially supported by UAB Department of Chemistry, UAB Educational Foundation

J. M. Meyers, *Presiding*

1:00 Introduction .

1:10 720. Career built on collaborative investigations of membrane protein structure, function, and ligand discovery. **A.L. Parrill-Baker**

1:35 721. Dance to central dogma with physical chemistry at the single molecule level. **H. Lee**

2:00 722. Chemical tools for selective detection of monomethyl lysine PTMs. **M. Raj**

2:25 Intermission.

2:40 723. How did I get here? From Chemistry to Biology and motherhood. **M. Frazier**

3:05 724. Biomolecules do amazing things and I get to work with amazing people. **J.M. Heemstra**

3:30 Panel Discussion.

Birmingham Jefferson Convention Center
East Meeting Room I

Active Learning Strategies in Remote Learning Environments: Successes and Lessons Learned

M. S. Reeves, *Presiding*

1:15 Introductory Remarks.

1:20 725. Remote Mentoring of Undergraduate Research Students (ReMentURS).
S.M. Ladge, E. Sargent, K. Marriott, D. Cannon-Rech, M.A. Lnu

1:45 726. Collaborative Classroom and Laboratory Experiences Incorporating Online Simulations and Animations for Gas Chromatography. **A. Le**

2:10 727. Online Hands-on First-Semester Biochemistry Lab Course: It is Possible.
K.R. Willian

2:35 728. From in-person to online: The Evolution of POGIL-PCL Workshops. **S.S. Hunnicutt**, A. Grushow, M.N. Muniz, R.M. Whitnell

3:00 Intermission.

3:15 729. Engaging Students in a Remote Learning Environment. **N.F. Campbell**,
T.L. Demeritte

3:40 730. What a great idea! Let's try it online.... **M. Tourne**

4:05 731. Flipped General Chemistry Instruction in the Time of COVID. **L. Hibbard**

4:30 732. Strategies for Making Feedback Useful in Online Courses. **S. Zingales**

4:55 Concluding Remarks.

Birmingham Jefferson Convention Center
East Meeting Room E

Optoelectronic Materials

Financially supported by Mississippi EPSCoR

C. N. Scott, *Presiding*

1:15 Introduction .

1:25 733. The Development of a Conjugated Polymeric Electrochemical Memristor for Neuromorphic Computation, Boolean logic, and Elementary Algebra. **B. Grant**, S.H. Foulger, I. Bandera

1:45 734. The Design, Synthesis and Application of Photoacoustic Imaging Probes for Companion Diagnostic Applications. **J. Chan**, M.Y. Lucero

2:05 735. Colloidal Quantum Dots and Gold Nanorods in Imaging and Photothermal Applications. **H.N. Jayawardena**

2:25 736. The Hole Problem. M. Fort, S. Click, A.D. Lacroix, K. Reid, E.H. Robinson, E.A. Hernandez-Pagan, S. Rosenthal, **J. Macdonald**

2:45 Intermission.

2:55 737. High Refractive Index and Fully Degradable Polymers Prepared Using Radical Polymerization. **W. Gutekunst**

3:15 738. Photo-Electroswitchable Arylaminoazobenzenes. **C.J. Saint-Louis**, D. Warner, K.S. Keane, M. Kelley, C.M. Meyers, S.C. Blackstock

3:35 739. Surface Functionalization for Mid-infrared On-chip Gas Sensing.. **D. Al Hussein**, J. Zhou, R. Gutierrez-Osuna, G. L. Coté, P. Lin, S.A. Sukhishvili

3:50 740. Solvent Effects on Properties and Spectra of Xanthene-based dyes - DFT studies. **J.M. Saloni**, C.N. Scott, W. Kolodziejczyk

4:10 Intermission.

4:20 741. Chromogenic Thiazolothiazole Hydrogel Devices Exhibiting Electrochromism, Electrofluorochromism, and Photochromism. **T.J. Adams**, A.R. Brotherton, M.G. Walter

4:35 742. Modular, Simple, and Efficient Synthesis of Electron-Rich Pyrrolopyrroles for Novel and Tailorable Conjugated Polymers. **G.S. Collier**, K.J. Bell, A.M. Kisiel, E.M. Wagner

4:55 743. Withdrawn. Enhanced Perovskite Solar Cells Performance by Organic Materials. **Q. Dai**

Birmingham Jefferson Convention Center
East Ballroom B

Theoretical chemistry: Method development and applications 3

Financially supported by Auburn University
E. Miliordos, *Organizer*
R. C. Fortenberry, *Presiding*

1:15 Introduction .

1:20 744. Exploiting GPU-Accelerated Ensemble Density Functional Theory to Enable Efficient Photochemistry Simulations of Large Molecules. **F. Liu**

1:50 745. Resonant Inelastic x-ray Scattering Simulations from Simplified Time-dependent Density Functional Theory Approaches. **D. Nascimento**

2:20 746. A Critical Comparison of Direct Methods for Computing Metastable States. **T. Sommerfeld**, J. Davis

2:40 747. Multi-surface Quantum Dynamics with the QTAG Method. **M. Dutra**, S. Wickramasinghe, S. Garashchuk

3:00 Intermission.

3:20 748. Strong Light-matter Interaction Effects on Molecular Systems. **R.F. Ribeiro**

3:50 749. Electronic spectroscopy of the $\tilde{A}-\tilde{X}$ transitions of jet-cooled calcium methoxide (CaOCH_3) and calcium ethoxide (CaOC_2H_5) radicals: Vibronic structure of nonlinear alkaline earth monoalkoxide radicals as candidates for direct laser cooling. A.C. Paul, K. Sharma, H. Telfah, A. Reza, T.A. Miller, **J. Liu**

4:10 750. Systematic Catalyst & Ligand Design for C-H Bond Activation: A Computational Approach. **E.E. Claveau**, E. Miliordos

4:30 751. F12-TZ-cCR: A Methodology for Faster and Still Highly-Accurate Quartic Force Fields. **A. Watrous**, B.R. Westbrook, M. Davis, R.C. Fortenberry

4:50 Concluding Remarks.

Birmingham Jefferson Convention Center
East Meeting Room D

Frontiers in Organic Synthesis and Catalysis 2

Cosponsored by ORGN
W. Santos, *Presiding*

1:30 Introduction .

1:35 752. Synthetic Methodologies Inspired by Complex Natural Products. **S.M. Wilkerson-Hill**, N.F. Cok, A.J. Zahara

2:00 753. Aerobic Oxidation Chemistry of Catalytically-relevant Cobalt-aminophenol Complexes. **J.M. Hoover**

2:25 754. Amine-Catalyzed Site- and Chemoselective C-H Hydroxylation. **M.K. Hilinski**

2:50 755. Determinants of Selectivity in Hydrosilylative Alkyl Ether Cleavage.. **N.D. Schley**

3:10 Intermission.

3:25 756. Developing New Alkene Difunctionalization Reactions. **Q. Wang**

3:50 757. Carbohydrate Derived Macrocycles in Catalysis. **G. Wang**

4:15 758. Forging Dissonant Functional Group Pairs through Cu-catalyzed Asymmetric Reductive Coupling Reactions of *N*-Substituted Allenes. **J.D. Sieber**

4:40 759. (3+2) Cycloadditions Using Photocatalysis Based on Earth-Abundant Metals with Heterocyclic Ligands. **E.M. Ferreira**

Birmingham Jefferson Convention Center
East Meeting Room K

Multidentate Ligand Systems in Inorganic Chemistry: Synthesis, Complexes, Structures and Reactions 2

W. E. Lynch, *Presiding*

Financially supported by ACS Division of Inorganic Chemistry, and the Coastal Georgia Local Section of the ACS

1:30 Introduction .

1:35 760. How a Pair of Extra “CH₂’s” Unlocks Stability Versus Reactivity for Macrocyclic Tetra-*N*-heterocyclic Carbene Complexes. J.F. DeJesus, X.B. Carroll, M.R. Anneser, K.M. Blatchford, G. Elpitiya, **D.M. Jenkins**

2:00 761. Nickel Complexes with Multidentate N/S-ligands as Synthetic Models of Nickel-containing Superoxide Dismutase (NiSOD). **T.C. Harrop**, P.T. Truong, L. Howell

2:25 762. Copper-based Redox Shuttles Featuring Preorganized Polydentate Ligands for Dye-Sensitized Solar Cells. A. Devdass, J. Watson, R.R. Rodrigues, J.M. Lee, N.S. Taylor, H. Cheema, L. Chen, R.C. Fortenberry, J.H. Delcamp, **J.W. Jurss**

2:50 763. Withdrawn. Ruthenium Complexes Supported by *bis*(pyrazolyl)acetate and its Derivatives: Synthesis, Structure, Characterization and Reactivity. **B.P. Quillian**

3:15 Intermission.

3:35 764. Structural Inspiration for New Opportunities with Azamacrocyclic Ligands: Rethinking their Synthesis and Facile Access to Multiple Substituents. M.M. Sibley, I. Ruohoniemi, M. Wasilewski, **M. Wetzler**

4:00 765. Tethered Axial Coordination as a Control Element on Dirhodium Paddlewheel Complexes. **A. Darko**

4:25 766. Poly(pyrazolyl)aluminates and their TM complexes. **M.A. Muñoz-Hernandez**

4:50 767. First Row Transition Metal Photocatalysts for CO₂ reduction: control of the coordination environment. **E.T. Papish**, C.M. Boudreaux, C.E. Webster, J.H. Delcamp

Birmingham Jefferson Convention Center
East Meeting Room L

Risk Management in Teaching and Research Settings

S. B. Sigmann, C. N. Situma, *Organizers*

Financially supported by ACS Division of Chemical Health & Safety

1:30 Introductory Remarks.

1:35 768. Data Analytics and Information Sharing as a Tool for Managing Safety in Academic Labs. **C.N. Situma**

2:05 769. Evolution of a risk Assessment Curriculum for Undergraduate and Beginning Graduate Student Researchers. **M.C. Box**, E.D. Blue

2:35 770. Staying Ahead of the Curve- Changing World of Laboratory Risk Assessment During Covid. **K. Jacob, J. McBride**

3:05 Intermission.

3:20 Discussion.

4:05 Concluding Remarks.

Birmingham Jefferson Convention Center
East Meeting Room M

Intellectual Property Basics

A. Hoehner, *Presiding*

2:30 Introduction.

2:40 771. Intellectual Property Basics. **A. Hoehner**

3:15 Discussion and Questions.

Birmingham Jefferson Convention Center
East Exhibit Hall 1

Chemical Education

Poster Session

3:00 - 5:00

772. Get involved with the ACS Division of Chemical Education. **S. Johnson, D.S. Boucher**

773. Determination of Caffeine in Beverage Samples using the Gas Chromatograph-Mass Spectrometer for an Undergraduate Non-majors Kitchen Chemistry Course.
H.V. Clontz, B. Xiong, N. Johansen

774. Studies of Photochemical Thiol-ene Cyclization in Biological Model Systems. **A. Purvis, A.J. Wommack**

775. Developments in Remote Teaching and Use of Instruments with Zoom's Remote Control Feature. **D.R. Zuidema**

776. Strategies for Enhancing the Virtual Lab Experience. M. Atteya, J. Caton-Williams, J. Gonzales-Roman, **V.A. Mativo**, D. Paschal, **L. Strange de Soria**, **A. Sukhu**, **M. Vanegas**

777. Comparison of Particle-in-a-Box Measurements with Molecular Modeling. **J.W. Hall**, S.K. Hutchison

778. Synthesis of Isoxazole and Isoxazoline Heterocycles as Potential Inhibitors of Lysyl Oxidase. **M. Goulart**, D.M. Solano

779. Video Assignments Improve Self-reported Sense of Community in an Online Undergraduate Chemistry Course. **S. Post**, C. Schrank, K.J. McKnelly

780. Synthesis and Characterization of Tripodal Amines. **A. Marsh**, L. Wonnum, K. Lupton, C.R. Whitlock

781. Investigation of Anti/pro-oxidant Effects of Carbon Nanodots (CNDs) Doped with Different Heteroatom Elements. **M. Azami**, J. Wei

782. Utilizing Student Attitude in Introductory STEM Courses: A Closer look into General Chemistry I (CH-131). **C. Glenn**, P. Clevenger, D. Williams

783. How Features of Molecular Representations Impact General Chemistry Students' Correct Prediction of Shape and Polarity. **A. Farheen**, S.E. Lewis

784. A Longitudinal Perspective on General Chemistry Students' Differentiation of Covalent Versus Ionic Models of Bonding. **S.E. Lewis**, K.A. Bowe, C.F. Bauer

Birmingham Jefferson Convention Center
East Exhibit Hall 1

Undergraduate Research 3

J. A. Nikles, *Organizer*
A. E. Gorden, *Presiding*

3:00 - 5:00

- 785. Withdrawn.** Systematic Approach to Evaluate Ruthenium-Based Anti-cancer Agents. **S. Robinson**, K. Enkhbold, L. Paul, M.R. Norris, J.A. Pollock
- 786. Withdrawn.** Expression, Purification, and Assay Development to Study STK1, a Kinase Implicated in Antibiotic Resistance. **M. Callender**, M.S. Blackledge, H.B. Miller, J.A. Pollock
- 787. Withdrawn.** Using Biochemical Tools to Probe the Complexity of MEMO1 Function. **C.A. Bayas**, **C.T. Corl**, S.T. Gilmore, M.C. Leopold, J.A. Pollock
- 788.** Photocatalytic removal of Tetracycline from Simulated Wastewater Lagoons using Compound Parabolic Reflectors. L. Borton, E.R. Gaston, **J.E. Boyd**
- 789.** Photocycloaddition–Cyclobutane Fragmentation for the Synthesis of Annulated Pyridones. **C. Slough**, E. Hardwick, M.E. Daub
- 790.** Development of an Oxidative [3+2] Photocycloaddition of 4-hydroxy-2-pyrones. **C. Sar**, J. Mackey, M.E. Daub
- 791.** Progress Towards an Oxidative [3+2] Photocycloaddition for the Synthesis of Furopyridone Natural Products. **J. Mackey**, C. Sar, M.E. Daub
- 792.** Removal of Cobalt(II) Aqueous Ions via Hydrogel Formation of Sodium Alginate in Synthetic Waters of Varying Harnesses. **P.N. Smith**, J.L. Hawk
- 793.** Using Sodium Alginate Hydrogels to Remove Cu^{2+} Contaminants from Various Aqueous Solutions. K. Spalding, **J.L. Hawk**
- 794.** Optimization and Characterization of Phosphonium Salts. B. Wicker, **M.B. Miller**
- 795.** Stereoselective Trisubstituted Alkene Synthesis Using Ni-catalyzed Alkyne Hydroarylation. **L.E. Hutchinson**, D. Wilger
- 796.** Electrostatic Tuning Maps: Intuitive Tools to Represent the Effect of an Environment on a Molecule's Properties. **J. Gay**, S. Gozem
- 797.** Isolation and Characterization of a Putative Dimethyl Sulfide (DMS) Monooxygenase in *Arthrobacter globiformis* . **T. Weishaar**, M. Culpepper
- 798.** DMSO Impacts the Reduction of the Metal Containing Anti-Cancer Drug KP1019. **M. Campbell**, E. Garrett, L.K. Stultz

- 799.** Suppression of Key Antibiotic Resistance Genes in MRSA with Small Molecule Adjuvants. **B. Viering**, T. Cunningham, A. King, M.S. Blackledge, H.B. Miller
- 800.** Molecular Dynamics Simulation of Poloxamer 188 and POPC Membranes. **D. Singhi**, S.G. Dennis-Little, M. Yost, T.W. Hanks
- 801.** Dopant Release from Polypyrrole Films and Nanoparticles Controlled by Poly(ethylene glycol) Surface Modification. **G. Richter**, T.W. Hanks
- 802.** Schlieren Effect Usage for Portable Qualitative Analysis. **J.A. Fields**, H. Park
- 803. Withdrawn.** Using CRISPR-Cas9 to Delete *stkI* in MRSA. **A. Anthony**, V. Federico, G. DiGiacomo, H.B. Miller
- 804.** Modulating the Properties of Iridium and Rhenium Complexes Using N-oxide Formation. **E. Stumbo**, J.A. Pienkos, C.D. McMillen
- 805.** Silver Cluster Luminescence. **K. Thomas**, J.T. Petty
- 806.** Silver Cluster Luminescence using $(C_2A)_6$. **M. Branham**, J.T. Petty
- 807.** DNA-Bound Silver Clusters using Modified Oligonucleotides. **C. Couch**, J.T. Petty
- 808. Withdrawn.** N-Heterocyclic Carbene Complexes of Nickel: An Examination of Synthetic Options and Targets. **M. Richter**, R.M. Meier
- 809.** Effect of CMPO Ligand Scaffold Variation on Lanthanide Extraction and Luminescence Properties. **B. Lake**, W. Larrinaga, S.M. Biros, E.J. Werner
- 810.** Synthesis, Scope, and Application of Tetra-aryl Phosphonium Salts. **D.J. Schwaibold**, **M.B. Miller**, B. Wicker
- 811.** Exploring the Scope of Pnictogenium Syntheses. **J.S. Davies**, B. Wicker
- 812.** Application of 1,8-ANS Fluorescent Probe to Identify Hydrophobic Patches on Surface of EF-hand Protein, Human Cardiac Troponin C (hcTnC) Upon Heavy Metal Binding. **O.R. Warfel**, A.M. Spuches
- 813.** Isolating the Opened and Closed Forms of a Rigid Dimer of the Fluorescent dye Rhodamine B. **A.J. Pierre**, P. Lundin, B. Stratton, K. Fogarty

- 814.** Efforts Towards the Design and Synthesis of a New Aminotroponimate Supported Zinc Complex for Hydroamination. **E.J. DiBlasio**, R.J. Harris
- 815.** Investigations on Organobarium Chemistry: Novel Carbon-Carbon Bond Formation, Novel Mechanistic Concepts and Synthetic Applications. **M. Gorman**, J.C. Donnelly, M.L. Smith, R.N. Salvatore
- 816.** Computational Study of the Structure, Vibrational Spectra, and Hydrogen Bonding of H_5O_2^+ and its Methylated Derivatives. **S. Sprouse, D. Herbert, B. Freeman, M. Kaledin**
- 817.** Synthesis of Hyperbranched Polymers via Metal-free Self-condensing ring-opening metathesis polymerization. **G. Dinges**, M.D. Schulz, H. Almuzaini
- 818.** Development of a Protecting Group Scheme for the Synthesis of Modified Deep-Cavity Cavitands. **T. Nsubuga**, M. Meadows
- 819.** Optimization of Synthesis and Spectroscopic Analysis of Vanadium–tetracycline Complexes. **S. Eastman**
- 820.** Effects of Pdr1 Phosphorylation Variants on Azole Resistance in *Saccharomyces cerevisiae*. **C.S. Burdette**, M.E. Breen
- 821.** Mapping Pho85-Pho80 Phosphosites in the *Saccharomyces Cerevisiae* transcription factor Pdr1. **R.E. Singer**, M.E. Breen
- 822.** Investigation of the Phosphorylation Status of the *Candida Glabrata* Pdr1 Transcription Factor. **J.R. McCallum**, M.E. Breen
- 823.** Detection of Nicotine Vapor through Photoacoustic Spectroscopy. **B. Freeman**, H. Park
- 824.** Development of Field Test for Identification of Cocaine with TLC. **E. Schrider**, J.O. Boles
- 825.** Predicting Protein Function in *Pythium Insidiosum* using Computational Techniques. **R.H. Gray**, S. Johnson
- 826.** Anion Effect on Octaethyltetraphenylporphyrin Protonation. **M. Swanson**, M. Ballester, V. Castro
- 827.** Recycling Plastic Materials by Solvent-targeted Recovery and Precipitation. **J. Locklear, C. Tirla, B. Martin**

- 828.** Gas-phase Acidities of Cyanobenzene and Dicyanobenzene Isomers. **R.A. Firth**, T. Dimino, W.K. Gichuhi
- 829.** Ethanolic Extraction of American Oak Wood. **N. Johansen, C. Baumgardner**, K.S. Kroeger
- 830.** Gas Chromatographic Analysis of Commercial Whiskeys. **C. Baumgardner**, K.S. Kroeger
- 831.** Synthesis, Characterization, and Evaluation of a Novel Coumarin Derivative as a Nerve Gas Sensor. T. Liontis, **S. Freitag**, A. Weerasinghe
- 832.** Preparation, Characterization, and Chemical/antimicrobial Activity of 6-ethoxy-6-phenyl-6H-chromeno[3,4-b]quinoxaline Derivatives. **G.R. Lee, H.N. Watkins**, A. Brown, S. Gremillion, B.P. Quillian
- 833.** A Metathesis Route Towards Sarcodictyin Analogs. **K. Estes**, N.M. Brandau, P. Wiget
- 834.** Synthesis, Characterization, and Reactivity of Phenylated *para*-cymene ruthenium(II) iodo Complexes Supported by Phosphorus Ligands. **K.D. Cartrette**, G. Durrell, B.P. Quillian
- 835.** Simple, Green, Applied Chemistry Research with Undergraduate Scientists of all Career Stages and Disciplines: the Construction and use of Silver Nanoparticle, Pencil Graphite Electrodes for the Detection of Milli-ampere Changes in Cell Solutions. **R. Brosky**, V. Sudhakar, A. Bramblett
- 836.** Hofmeister Anion Interactions with Coumarin. **O. Mumma**, Y. Zhang
- 837.** Solid-phase Extraction of Rare-earth Elements using Phosphonated Polymer Resins. **A. Fiorito**, S. Winn, W.R. Archer, M.D. Schulz
- 838.** Investigation of Quinolines as HIV-integrase Inhibitors. **J. Patterson**, M. Donahue
- 839.** Identification of Economical Cross-coupling Catalysts by Small Scale Reaction Screening with Gas Chromatography-Mass Spectrometry. **A.L. Akers**, P. Lundin, S. Geyer
- 840.** Synthesis and Characterization of New Earth-abundant Chalcogenide Perovskite Nanomaterials. **O. Parks**, D. Zilevu, S. Creutz

841. Grafting-through Synthesis of Aziridine-based Bottlebrush Polymers. **P. MacNicol**, G. Dinges, W.R. Archer, M.D. Schulz

842. Investigation of Pomalidomide-Derived HaloPROTAC Tool Compounds. **S. Nelson**, B. Ody, R. Liu, C. Dodd, J. Yin, M.L. Turlington

843. Metabolite-responsive Liposomes via a Synthetic Lipid Switch. **S.E. Bottcher**, J. Lou, M. Best

844. Analysis of the UVA/UVB Degradation of Lotions with Additives Through Raman Spectroscopy. **I. Dancer**, A. Wood, B. Sharma

1902. Methodology Optimization for the Synthesis of Novel Carbazole Derivatives Utilizing the Chan-Evans-Lam Coupling Reaction to Target Antibiotic Resistance. **J. Emrich**, S. Gregory, M.S. Blackledge

Birmingham Jefferson Convention Center
East Ballroom A

Undergraduate Research 4

J. A. Nikles, *Organizer*

3:15 - 5:15

845. Homology Modeling and Molecular Dynamics Studies of the CDK Pho85: a Possible Source of PDR1 Activation in *Candida Glabrata*. **J.M. Dudley**, T. Odbadrakh, M.E. Breen, K.N. Kirschner, G.C. Shields

846. Bioconjugation Studies of Polyethylene Glycol (PEG)-lysozyme and Small Laccase using ESI-MS and click-enabled Fluorescence. **H. Givhan**, W. Browning, M. Sullivan, B. McKinley, B.W. Gregory, C.M. Johnson

847. Metal-Organic Complexes for Hydrogen Sulfide Coordination. **E. Cain**, C.M. Wallen

848. Efforts Toward the Development of an N-heterocyclic Carbene Supported Zinc Catalysts for Hydroamination. **R.J. Alexander**, R.J. Harris

- 849.** Towards the Synthesis of a Simple Alkyl-substituted meta-poly(arylene ethynylene). **C. Bontempo, J. Faircloth, P. Lundin**
- 850.** qRT-PCR Assay Development for Campus-Wide Asymptomatic COVID-19 Screening on Undergraduate Campus. **M. McGuire, L. Evans, D. Manning, K. McKinney, R. Bishop, B. Magers, J. Neiswinger, S.A. Smith**
- 851.** Facile Chitosan Isolation for Heavy Metal Remediation. **R. Tikkala, B. Corbett**
- 852.** Investigating the C–H Arylation of Furan using a Carbazole Derivative as a Photocatalyst. **K. Ribeiro, A.R. Longstreet**
- 853.** A Carbazole Derivative as a Photocatalyst in the C–H Arylation of *N*-Methylpyrrole. **N.A. Reece, A.R. Longstreet**
- 854.** Storage of Carbon Dioxide in Basalt: An In-Depth Study of the Reaction Kinetics and Products of Enstatite Carbonation. **L.J. Hardee, B. Aguila**
- 855.** *Experimental analysis of double-stranded DNA cleavers on bacterial cells.* **T. Fraley, J. Heath, W. Yang**
- 856.** *Small molecules stabilizing the secondary structure of CCG repeat expansion.* **L. Wise, W. Yang**
- 857.** Effect of Initiator Structure on Poly(3-hexylthiophene) Polymerization and Aggregation Properties. **O.J. Armendarez, P. Lundin**
- 858.** Ionic Liquids to Enhance the Fluorescence of Organic Dyes for Bloodstain Detection. **A.N. Mahurin, D.S. Darlington, W.E. Meador, J.H. Delcamp, E.E. Tanner**
- 859.** Withdrawn
- 860.** Fabrication of Structures on Surfaces: From the Macro to the Molecular Scale. **P. Perdikis, B.H. Augustine**
- 861.** Joro Spider Webs as Bio-accumulators of Polycyclic Aromatic Hydrocarbons (PAHs) in North Georgia. **J. Casey, H. Cole, M. Smith-Roden, I. Agyekum, J. Driver**
- 862.** Evaluation of Polymer Surface Modification as an Inhibitor of Methicillin-resistant *Staphylococcus aureus* (MRSA) Biofilm Formation **M. Mauer, A. L. Akers, A. Copeland, M. S. Blackledge, P. Lundin**

- 863.** Determination of Metal Binding Specificity and Stoichiometry to a Monooxygenase Involved in Sulfur Cycling. **K. Zammit**, Z. Adamson, M. Culpepper
- 864.** Comparing Correlation Energy Approximations Derived from TDDFT within the Asymmetric Hubbard Dimer. **L. Everhart**, J.E. Bates
- 865. Withdrawn.** Fabrication of Microfluidic Devices Used for Electrophoretic Separations. **A. Wohlwend**, P. Lundin, K. Fogarty
- 866.** Withdrawn
- 867.** Time-resolved Protein-protein Interactions of Coronavirus nsp2 Constructs using a Trifunctional Small-molecule Probe. **M. Sullivan**, C. Cameron, L. Plate
- 868.** Synthesis of Biheteroaryls Through the Use of a Novel Imidazopyridine Phosphine Ligand in Pd-Catalyzed Suzuki-Miyaura Reactions. **A. Kantzler**, S.A. Jacoby, N.W. Harris, L. Yet
- 869.** Understanding the World at a Molecular-level: Use of the Johnstone Triangle to Determine if Students have Crossed the IMF Threshold. **D. Li**, B. Harmon, N.L. Powell
- 870.** Morphological Comparison of Grafted Bentonite to Various Nanoclays for Improvement of Fracture Toughness. **M.H. San Soucie**, M. Kimutai, J. Johnson, E. Koricho, S.M. Landge
- 871.** Hirshfeld and Void Surface Analysis in Halogen/chalcogen Bonded Crystalline Materials. **S. Alapati**, A. Peloquin, C. McMillen, **W.T. Pennington**, T.W. Hanks
- 872.** Understanding the Fluorescent Properties of Fluorescein Amide Derivatives. **R. King**, P. Lundin, K. Fogarty
- 873.** Reversible Colorimetric pH Sensors. **E. Callis**, **T.W. Hanks**
- 874.** Design and Antibiotic Activity of Novel Hair-pin Peptides. C. Rose, **I. Becerra**, **E. Roller**, **A. Dilorra**, **S.E. Collins**, **B. Jackson**, J.M. Meyers
- 875.** Introduction of Mindful Doodling into Chemistry Courses at Georgia Gwinnett College to help Reduce Stress and Improve Student Confidence in their Ability to Draw Chemical Images. **M.S. Morton**
- 876. Withdrawn.** Development and Optimization of microPADs for Iron Detection. **B. Kokes**, **A. Holmes**, M.E. Howard

FRIDAY EVENING

Birmingham Jefferson Convention Center
East Ballroom B

Plenary

A. E. Gorden, *Presiding*

5:15 877. From N-heterocyclic Carbenes to Dithiolene-based radicals: Recent Developments in Main Group Chemistry. **G.H. Robinson**

McWane Science Center

Student Chemistry Chapter Activities During Covid19 Poster Session at the McWane

Financially supported by UAB Department of Chemistry, UAB Educational Foundation, and Refresco

J. M. Meyers, J. A. Nikles, *Organizers*

7:00 - 9:00

878. Erskine Chapter of the ACS: Adapting During Uncertainty. **M. Clothier**

879. TNTech Student Chapter Activities During COVID-19. **C.E. LaPointe**, R.A. Firth, A.J. Carroll

880. Mississippi College student ACS chapter: Promoting chemistry during the pandemic. **L. Sisson**, **M. Stewart**, **B. Steen**, L.T. Ashley, E. Tullos, C. Stokes, T.D. Selby

881. Successes of the SMACS Chapter at Valdosta State University. **D.B. McKay**, K. Patel, L. De La Garza

882. Delivering Virtual Programming to Effectively Sustain Chapter Camaraderie and Educational Outreach During a Pandemic. **L. Jaskowski**, R. Adams, S. Hubbard, J.A. Nikles

883. Student ACS Chapter Activities During the COVID-19 Pandemic. **B. Robertson**

McWane Science Center

Undergraduate Research 1

Undergraduate Research at the McWane Center

Financially supported by UAB Department of Chemistry, UAB Educational Foundation, and Refresco

J. M. Meyers, J. A. Nikles, *Organizers*

7:00pm 884. Modeling and Investigating the Molecular Basis of Tay-Sachs Disease. **M. Denish**, K.M. Matera, T. Laakko Train

885. Developing an Alternative Diagnostic tool for Eosinophilic Esophagitis by Quantification of Modified Tyrosines in Urine Samples. **J. Germany**, M. Thomas, M. Gilliland

886. Physical Paper Modification for Detection of Antiretrovirals via Paper Spray Ionization Mass Spectrometry. **N. Cheyne**, M. Gilliland

887. Chemically Patterned Paper Substrates for Paper Spray Mass Spectrometry. **A. Arias**, M. Gilliland

888. Structural Expansion of a Novel Antibiotic Adjuvant Scaffold to Improve Aqueous Solubility and Biological Activity. **S. Gregory**, A. King, M.S. Blackledge

889. Method Developmental of High-throughput, Sensitive, Colorimetric Assay for Methanethiol Detection. **Z. Adamson**, C. Miller, M. Culpepper

890. Presumptive Forensic Test kit Differentiating Hemp and Marijuana. **C.E. LaPointe**, J.O. Boles

891. Chemical Investigations of Organics in the Chattahoochee River. **H. Carlisle**, K. Goodwin, E. Klar, K.S. Taylor

892. Optimizing Growth Conditions for the Recombinant Expression of P450 27A1. **J. Bartholomew-Schoch**, M. Reddish

893. Allosteric Inhibition of Cytochrome P450 27A1: A Potential Means for the Creation of Novel Cancer Therapies. **N.L. Arnold**, E. Harris, L. Snider, M. Reddish

894. Microfluidics-based Approach to PCDA Liposome Synthesis. **A. Chadwick**, T.W. Hanks

895. Exploring the Relationship Between a Student's STEM Professional Identity and their Perception of an Organic Laboratory Experience. M.L. Head, **D. Dayani**, **A. Alkawam**, **E. Pearman**

896. Naphthalimide-triazole Hybrid pH-sensitive Fluorescent Probe. **A. Powell**, R. Osbourn, D. McCall, E.A. Adogla

897. Ruthenium-catalyzed Microwave Oxidation of Benzyl Silyl Ethers and Analogues. **R. Peterson**, K. Darrigrand, K. Poythress, A. Cameron, B.C. Goess, S.K. Goforth

898. Iron Geochemistry at Glendale Shoals. **C. Hatchell**, **M. Santos**, C. Romanek, G. Lewis, G.E. Schwartz

899. The Impact of Iron Geochemistry on Carbon Degradation at Glendale Shoals. **M. Santos**, **C. Hatchell**, C. Romanek, G. Lewis, G.E. Schwartz

900. Synthetic Methods of 4,6- or 4,8-Disubstituted-quinoline-3-methylcarboxylates Inhibitors for HIV-1 Integrase (IN) Enzyme. **C. Glenn**, L.P. Dinh, L. Yet

901. Towards Transdermal Delivery of Thioridazine Double Salt Ionic Liquid Drugs. **C.E. Rust**, O. Cojocar

902. Spectroscopic, Elemental, and Surface Characterizations of Biochar made from Pine Biomass and Co-pyrolyzed with High-density Polyethylene. **L.D. Moore**, **J. Lennox**, A. Saha, N. Takas, P. Bhoi

903. Computational and Spectroscopic Studies of Nitrogen-containing Multipole-bound Anions. **N. Kruse**, N. Hammer

904. Infrared Reflection Spectroscopic Studies of UV-ozone Cleaning of Substrates for Self-assembly. **L.B. Spurgeon**, M. Milosevic, B.W. Gregory

905. Kinetic Characterization of GAPDH from Infectious Microorganisms. **M. Hurd, G. Thrash**, K.L. Hayden, D. Chattopadhyay

906. Phase Control in Cu_{2-x}Se Nanoparticles Through Tailored Selenium Reactivity Across Ligand Groups. **J. Macdonald, E.A. Ho**, A.R. Peng

SATURDAY MORNING

Birmingham Jefferson Convention Center
East Meeting Room G

Analytical Chemistry

Advanced materials and Surfaces for Analytical Chemistry

A. Ghosh, *Presiding*

8:00 Introduction .

8:10 907. Developed Ag@PANI/MWCNTs/MXene Nanocomposite as a High-performance Electrochemical Sensor for Simultaneous Determination of L-arginine and L-cysteine in Real Samples. **M. Mehmandust**, N. Erk

8:30 908. Transparent Ultramicroelectrodes for Studying Interfacial Charge Transfer Kinetics of Photoelectrochemical Water Oxidation at TiO₂ Nanorods with Scanning Electrochemical Microscopy. **X. Li**, S. Pan

8:50 909. Indirect Surface-Enhanced Raman Spectroscopic-Based Detection of Hormone Biomarkers Associated with Polycystic Ovarian Syndrome. **A. Wood**, I. Dancer, B. Sharma

9:10 910. Size Exclusion Chromatography: An Indispensable Tool for the Isolation of Monodisperse Gold Nanomolecules.. **S. Eswaramoorthy**, N. Sakthivel, V. Jupally, K.H. Wijesinghe, P. Nimmala, C. Kumara, M. Rambukwella, T.C. Jones, A. Antonyamy

9:30 Intermission.

9:45 911. Raman Spectroscopic Detection of Biosignatures in an Extraterrestrial Context. **G. Sarabia**, B. Sharma

10:05 912. Magnetic Fe₃O₄ Biochar Hybrid for Methylene Blue Removal: Effect of Porous Structure and Surface Chemistry. **S.N. Nawalage**, H. Samaraweera, T. Mlsna

10:25 913. Comparison of One-dimensional Plasmonic Gold Nanostructures for Colorimetric Sensing. **G. Chen**, B. Sharma, T. Egan

10:45 914. Investigation of Hydrogen Diffusion in High Hardness Steels. **R.F. Awoyemi**, W. Williams, H. Rhee, D. Wipf

Birmingham Jefferson Convention Center
East Meeting Room O

Biochemistry

General Session Biochemistry 1

J. Zhang, *Presiding*

8:00 Introduction .

8:05 915. Next Generation Disinfectants to Combat Resistance in the Post-COVID Era. K. Sommers, **M.E. Michaud**, C. Hogue, A. Scharnow, S.J. Post, R.A. Allen, K. Morrison, L. Amoo, A. Petersen, R.G. Carden, W.M. Wuest, K.P. Minbiole

8:25 916.

Combating Antibiotic Resistance in Septic Infections with Choline Carboxylic Acid-Based Ionic Liquids. **C. Chism**, E.E. Tanner, G.S. Dasanayake

8:45 917. Withdrawn. Biophysical Characterization of Orthogonal Conjugated Polymer Catalysis by Mutagenic Variants of T4 Lysozyme. **W.D. Turner**, T. Leeper

9:05 918. Utilizing Multi-scale Simulation to Reveal Mechanisms of Molecular Motors' Motility. **L. Li**

9:25 Intermission.

9:40 919. Experimental Predictions of Ribosomal Evolution. **J.W. Haynes**, K.A. Lanier, A. Petrov, L.D. Williams

10:00 920. Analyzing Interactions of Thermoresponsive Coacervate-forming biodegradable polyesters on protein structure and activity Utilizing Fluorescence and Nuclear Magnetic Resonance. **C. Casterline**, T. Leeper

10:20 921. Confirmed and Quantified *in vitro* glycosylation of Membrane Proteins. **G. Cook**

10:40 922. Biochemical and Therapeutic Actions of Cathepsin L (CatL) Inhibitors against Hepatocellular Carcinoma. **C. Olamide**, I.V. Ogungbe, F.K. Noubissi

11:00 923. Biochemical Characterization of the Radical SAM Methylase Involved in Tetrahydromethanopterin Biosynthesis. **J. McKinney**, T. Tunckanat, K. Allen

11:20 924. Hydrophobic Surface Patch Disruption to Produce Water-Soluble G-Protein Coupled Receptor Analogs. **C. Dyer**, A.L. Parrill-Baker, D.L. Baker

11:40 925. Withdrawn. Comparison of the Structure and Activity of *Pseudomonas aeruginosa* Proteins, Inhibitors of Vertebrate Lysozyme Classes I and II. **K. Letsinger**, T. Leeper

Birmingham Jefferson Convention Center
East Meeting Room K

Chemical Education Oral Presentations 1

J. March, *Organizer*

8:00 Introduction .

8:10 926. Teaching Design of Experiments for Method Development in Analytical Chemistry. **R. Thompson**, R. Saylor

8:30 927. Supporting the Motivation of Engineering Students with Design Challenges in General Chemistry Laboratory. **M. Korolev**, K. Crippen, L. Imperial, C. Payne, B. Phil, C. Wu

8:50 928. Upper-level Survey Course on Nanoscience for Chemistry Majors. **P. Lundin**, B. Augustine

9:10 Intermission.

9:30 929. Bridging Workforce Development to General Chemistry: Results from a Multi-Year Career Shadowing Program. **J.M. Carr**

9:50 930. A New Course to Increase the Success of Students in the First Semester of General Chemistry. **S.C. Blackstock**

10:10 Concluding Remarks.

Birmingham Jefferson Convention Center
East Meeting Room B

Engineering Solutions for Social Challenges: Renewable Materials and Resources 1

Financially supported by **Center for Sustainable Nanotechnology - UW Madison, and Surface Measurement Systems**

M. L. Curry, L. A. Lucia, M. S. Peresin, *Presiding*

8:00 Introductory Remarks.

8:10 931. Lignin Thermochemistry for Advanced Composite Materials. **C.E. Frazier**, S. Yazdi, L. Fang

8:55 932. On the Road to Developing Sustainable Alternative Materials for Long-lasting Insecticide Nets: Cellulose-based Insecticidal Fiber Yarn for Malaria Control. **S. Brake**, D. Gómez Maldonado, M.S. Peresin, S. Zohdy

9:25 933. Facile Preparation of Hydrophobic Papers Through Metal-ion-induced Modification of Conventional Hydrophilic Papers. **O.N. Rathnayaka Mudiyanse**laga, X. Zhang

9:55 Intermission.

10:15 934. Geologic Carbon Dioxide Storage Through Pyroxene Mineral Carbonation. **B. Aguila**

10:45 935. Fabrication and Thermal and Mechanical Characterizations of Cellulose-based UHP-Ionene Composites. **J. Mitchell**, K.E. O'Harra, J.E. Bara, M.L. Curry

11:15 936. Using Cyclodextrin Grafted Chitosan as Coating of Delignified Wood Aerogels for the Removal of Microcystin-LR. **D. Gomez Maldonado**, A. Reynolds, R.J. Babu, D.J. Burnett, M.N. Waters, M.S. Peresin

Birmingham Jefferson Convention Center
East Meeting Room J

Inorganic

General Session Inorganic 1 - Ligands and Metals in Catalysis

J. E. Ritchie, *Presiding*

8:00 Introduction .

8:05 937. Tuning Hydrosilylation and Dehydrogenative Silylation Upon the Choice of Metal Center: Rh and Ir Silylphosphine Catalysts. **N.S. Abeynayake**, V. Montiel-Palma

8:20 938. Redox-Active Heterobimetallic Catalysts for Polymerization of Polyolefins. **N. Taylor**

8:35 939. Enhanced Reactivity for C-H Bond Functionalization Using a Dinuclear Iron(III) Oxo-Bridged Catalyst and Hydrogen Peroxide. **Z. Turner**, J.W. Jurss

8:50 940. Modular Bimetallic Main Group Catalysts for Cooperative Polymerization of Lactones. **R.J. Comito**, Z. Gu, M. Tansky

9:05 941. Synthesis and Characterization of the Complete Series of Chlorine Substituted Cobalt Acetylacetonate Complexes—[Co(acac)_x(acac-Cl)_{3-x}], x = 0-3. **R.E. Bachman**, E.E. Joslin, E. Amason, M.H. Jones, C. Keuk, G. Ferrence

9:25 942. Synthesis of Zwitterionic-Alkenylammonio and Alkenylphosphonio Ligands in Dirhenium Carbonyl Complexes.. R.D. Adams, **M. Kaushal**

9:40 Intermission.

10:00 943. Ligand Aromatization/dearomatization in Pyridine and Pyrazine Diimine Complexes. **J.R. Billups**, S. Creutz

10:15 944. Effect of Donor Groups on Ruthenium CNC pincer Complex for Reduction of Carbon dioxide. **D. Nugegoda**, S. Das, F. Qu, C.M. Boudreaux, P. Burrow, M.T. Figgins, R. Lamb, C.E. Webster, J.H. Delcamp, E.T. Papish

10:30 945. Evaluating Photochemical C–H Bond Activation by Introducing Electronegative Substituents to W(VI) Dioxo Complexes. **S.M. Siddhharathi**, F. Fronczek, M.B. Chambers

10:45 946. Remote Directing Group for Para C-H Functionalization of Aromatic Aldehydes. **A. Mercado**, T. Ricks, N. Taylor, E. Vioria, T. Brewster

11:00 947. Asymmetric Ligand Design for Increased Volatility of Spin-crossover Complexes. **M. Gakiya-Teruya**, X. Jiang, A. Hebard, D. Le, T.S. Rahman, M. Shatruk

11:15 948. De Novo Designed Cu Peptides for Abiotic C-H bond Functionalization and Small Molecule Activation. **D. Prakash**, S. Mitra, P. Prasad, S. Chakraborty

Birmingham Jefferson Convention Center
East Ballroom B

Machine Learning in Computational Chemistry

S. Irle, *Presiding*

8:00 Introduction.

8:10 949. Machine Learning for Intermolecular Interactions. **C.D. Sherrill**

8:40 950. Genetic Algorithms for Inorganic Oxides. **E. Valencia**, R.C. Fortenberry

9:00 951. Reducing Uncertainty in Quantum Chemistry Discovery with Machine Learning. **F. Liu**

9:20 Intermission.

9:40 952. Recent Developments in CLIFF: A Component-based, Machine-learned, Intermolecular Force Field. **J.B. Schriber**, D. Nascimento, A. Koutsoukas, S. Spronk, D.L. Cheney, C.D. Sherrill

10:10 953. Data-driven Acceleration of Quantum Chemical Methods. **K.D. Vogiatzis**

10:40 954. Making use of Small Data in Machine-learned Binding Free Energy Prediction. **D. Metcalf**, Z. Glick, C.D. Sherrill

11:10 955. Deep Predictive Visual Proteomics. **D. Bhowmik**

11:30 Panel Discussion.

Birmingham Jefferson Convention Center
East Meeting Room A

Nanomaterials 1

S. Street, *Presiding*

8:00 Introduction .

8:10 956. Inorganic Nanoscale Unnatural Product Synthesis. C.G. Sharp, S. Sarkar, E.H. Robinson, A. Koziel, E.A. Ho, R.B. Goldfarb, A.R. Peng, A.D. Lacroix, E.A. Hernandez-Pagan, A.Y. Nuriye, **J. Macdonald**

8:30 957. Lewis Acid Catalyzed Synthesis of Metal Oxide Nanocrystals via Hydroxide Transmetallation. **B.H. Farnum**, A.R. Combs Breder, N.J. Gibson, N. Chakraborty

8:50 958. Metal Ion Doping in Lead Halide Perovskites for Efficient Blue and White LEDs. **M. Gangishetty**

9:10 959. Langmuir Methods to Cast Uniform Films of Nanoparticles. **J.J. Weimer**, C.V. Nguyen, J. Mitchell

9:30 Intermission.

9:50 960. Development of Solution-Based Synthetic Routes to Ternary Group 4-Containing Sulfides as Colloidal Nanomaterials. **S. Creutz**, D. Zilevu, N.E. Ingram, O. Parks, B. Jordan

10:10 961. High Temperature Synthesis of x-ray Luminescent Nanomaterials for Biomedical Applications. **E. Zhang**, A. Dickey, H.W. Jones, I. Foulger, I. Bandera, J.W. Kolis, S.H. Foulger

10:30 962. Intermediate Shell Formation and Anion Sublattice Rearrangement in the Cation Exchange from π -SnS to $\text{Cu}_{1.8}\text{S}$. **C.G. Sharp**, S. Sarkar, J. Macdonald

10:50 963. Synthesis and Characterization of Iron Complex-based Nanoparticles. **M. Hawkins**, Y. Bao

11:10 964. Chemical Ordering in Dimetallic Nanoparticles. **S. Street**, F. Acquaye, R. Mahat

Birmingham Jefferson Convention Center
East Meeting Room E

Organic

Natural Products/Biological Applications of Organic Synthesis/Heterocycles

L. Yet, *Organizer*

8:00 Introduction .

8:05 965. Biomimetic Cyclizations in Pursuit of Marine Natural Products. **E. Jones**, D. Lutin, S.A. France

8:20 966. Stereoselective Synthesis of Protected β -OH Dab Isomers for Natural Product Synthesis. **M. Dekarske**, W. Zhang, W.M. Wuest

8:35 967. Cyclic Thiosulfonates as Anticancer Agents: Structure-reactivity and Structure-activity Relationships. **A. Franceschini Ghilardi**, E. Yaaghubi, R. Ferreira, M.E. Law, M. Wang, B.J. Davis, Y. Yang, I. Ghiviriga, A.E. Roitberg, B.K. Law, R.K. Castellano

8:50 968. Semi-Synthesis of (5Z)-7-Oxozeaenol/Hypothemycin Analogues from Kinase Inhibition Towards Cancer Treatment. **T. Li**, M.P. Croatt, A. Ustoyev, P.M. West

9:05 969. Withdrawn. Design and Synthesis of New Modulators for the Downregulation of Liver Receptor Homolog-1. **R. Spurlin**, M.L. Cato, J. Cornelison, N. Jui, E. Ortlund

9:20 970. Targeting the Sphingosine-1-phosphate Transporter SPNS2 for the Treatment of Multiple Sclerosis. **D. Foster**, W.L. Santos, K. Lynch, R. Fritzemeier

9:35 971. Design and Synthesis of Taurine Conjugates as Potential Anticancer Agents. **K. Wyman**, S.S. Panda

9:50 Intermission.

10:05 972. Pyochelin Biosynthetic Metabolites Bind Iron and Promote Growth in Pseudomonads Demonstrating Siderophore-like Activity. **A. Kaplan**, J. Musaev, W. Wuest

10:20 973. Synthesis of Empetroxepin Derivatives and Bis-Nitrogenous Adjuvants and Subsequent Investigations into Biological Activity. **K. Murphy**

10:35 974. Development of Novel Fluorinated Amino Ester Prodrugs to Improve Detection of Brain Tumors. **D.A. Devalankar**, N. Yasui, U. Akca, A. Hjelmeland, J.E. McConathy

10:50 975. Fe(III)-Catalyzed Amidomethylative Nucleophile-free Tandem Reactions: Formal Substitution of Multiple C–H Bonds for Building Complexity of Styrenes. **X. Qian**, H. Zhou, C. Hetti Handi, J. Lucore, X. Cui

11:05 976. Synthesis of Achiral and Chiral CCC-NHC Pincer Complex and its Application in C-H Functionalization of Indoles. **M. Rawat**

11:20 977. Friedel–Crafts Additions of N-alkylated Indoles to Nitrones to Form 1:1 Products. **C.W. Downey**

11:35 978. Total Synthesis of the Reported Structure of Cahuitamycin A and Isomers. J.A. Shapiro, **S. Post**, M.E. Michaud, G. Smith, W.M. Wuest

11:50 979. Electrophile-Initiated Cyclization of Chiral, Non-Racemic Homoallylic *N*-tert-butanesulfonamide Carbamates and Bis-Boc/Cbz Protected Guanidines. **G.J. Rustin**, M. Donahue

Birmingham Jefferson Convention Center
East Meeting Room I

Physical Chemistry

General Session Physical Chemistry 1

M. G. Bakker, *Presiding*

8:00 Introduction .

8:05 980. Long-lived Ag₁₀⁶⁺ Luminescence and a Split DNA Scaffold. **D. Lewis**, S. Carnahan, D. Kim, J.T. Petty

8:25 981. Infrared Studies of the Effect of Hofmeister Ions on Model Drugs. **S.I. Busch**, G. Macdonald, Y. Zhang

8:45 982. EPR Spectroscopy to Probe the Incorporation of Phthalocyanines into Hierarchically Porous Carbon. M. Lockhart, R. Adhikari, **M.G. Bakker**, M.K. Bowman, K.H. Shaughnessy

9:05 983. Effect of Solvent, Time, and Mixing Speed on Self-Assembly of Thiols on Iron Microparticles for Improving the Colloidal Stability of Magnetorheological Fluids. **S. Thiagarajan**, A. Koh

9:25 984. Withdrawn. Investigation of Chemistry at Ice-Mineral Interfaces of Phosphorus-Containing Meteorite Analogues. **K.F. Meyberg**, H.L. Abbott-Lyon

9:45 985. Spectroscopic Investigation of Novel 3,4-ethylenedioxythiophene (EDOT) Derivatives and their Potential Aggregate Induced Emitter Behaviors. **A. Dorris**, N. Sparks, I. Chandasiri, D.L. Watkins, N. Hammer

10:05 Intermission.

10:20 986. Quantifying Emission of NIR-I and NIR-II dyes via Fluorescence Quantum Yield. **C. Smith**, D. Ndaleh, J.H. Delcamp, N. Hammer

10:40 987. Advances in CaLevIR: Observations of Droplet Heat Transfer via a High-Speed Thermographic Camera. **H. McCardle**, K. Everitt, K. Abbuhl, E.R. Duranty

11:00 988. Upconversion and Quantum Yield Studies of PdOEP-DPA System in the sPS/THF Polymer Gel. **A. Shaik**, B. Davis, Y.C. Simon, N. Hammer

11:20 989. Using 2D Spectroscopy to Explore Excited State Dynamics in Ruthenium Complexes. **M.A. Hermosilla-Palacios**, S.E. Dominguez, B. Aramburu-Trošelj, V.D. Kleiman, L. Baraldo-Victorica

11:40 990. Understanding the Microenvironment of Ionic Liquids. **S. Dutta**

Birmingham Jefferson Convention Center
East Meeting Room C

Polymer Materials Science and Engineering

General Session Polymer Materials 1 - Polymeric materials and composites

D. Dean, *Presiding*

8:00 Introduction .

8:00 991. Withdrawn.

8:15 992. Evaluation of the Dielectric Properties of Radar Absorbing Materials. **D. Wedgeworth**

8:30 993. Photomechanical Response from a Stilbene Polymer via Triplet Sensitization. **D. Beery**, E. Stanisauskis, G. McLeod, A. Das, W. Oates, K. Hanson

8:45 994. Covalent Anthracene Incorporation into Hydrogel Encapsulated Crystalline Colloidal Arrays for Radioluminescent Properties. **S. Mell**, H.W. Jones, I. Bandera, S.H. Foulger

9:00 995. Upcycling of Single-Use Polyethylene into High Strength Materials via Reactive Compounding. **A. Ghosh**, A.C. Kannan

9:15 Intermission.

9:25 996. Synthesis of Alicyclic Polyesters: Examination of the Effect of Regioisomer Ratios on Physical Properties. **T.N. Thompson**

9:40 997. Semi-fluorinated Arylene Vinylene Ether (FAVE) Telechelic Polymers from Polycyclic Aromatic Hydrocarbon Bisphenols and Trifluorovinyl Aryl Ethers. **K.M. Mukeba**, B. Farajidizaji, K. Shelar, C.U. Pittman, D.W. Smith

9:55 998. Pretreatment of Asphaltene for Carbon Fiber Development. **J. Hinkle**, N. Alizadeh, A. Bansode, A. Bass, J. Thornhill, N. Tram, F. Leiva, E. Triggs, R. Farag, M.L. Auad

10:10 999. Isosorbide-based Semifluorinated Polymers. *Where Green meets Mean..* **K. Shelar**, K. Mills, K.M. Mukeba, D.W. Smith

10:25 1000. Dynamic Mechanical and Mechanical Analysis of Ionic Liquid Regenerated Cellulose Aerogels Loaded with Hexagonal-Boron Nitride (h-BN). M. Arafat, B.L. Sadiku, **S. Chakraborty**

Birmingham Jefferson Convention Center
East Meeting Room F

Synthesis of Fluorescent Probes and Their Applications from Sensing to Imaging

M. Henary, *Presiding*

Financially supported by Molecules, De Gruyter

8:00 Introductory Remarks.

8:10 1001. Illuminating Biological Copper with Synthetic Fluorescent Probes. **C.J. Fahrni**

8:40 1002. Imaging and Tracking mRNA in Live Mammalian Cells via Fluorogenic Photoaffinity Labeling. **J.M. Heemstra**

9:10 1003. Bifunctionality of Neodymium (III) Complexes as Luminescent and Single Molecule Magnets (SMMs). R. Vincente, A. Tubau, S. Speed, F. Mautner, F. Bierbaumer, R. Fischer, **S.S. Massoud**

9:40 Intermission.

9:50 1004. Fluorescent Detection of Protein Lysine Acetyltransferase Activities. **Y. Zheng**

10:20 1005. Fluorescence and Electroluminescence Spectroelectrochemistry Studies of Perovskite Quantum Dots. **S. Pan, J. Yadav**

10:50 1006. Synthesis and Applications of Near-Infrared Fluorescence Probes Based on Cyanine Dyes. **M. Henary, H. Choi**

11:20 Concluding Remarks.

Birmingham Jefferson Convention Center
East Meeting Room D

Project SEED

A. Mallia, D. Masterson, *Presiding*

8:30 Introductory Remarks.

8:35 1007. History, Progress, and Outlook of the Project SEED Program. **B.W. Boudouris**

9:00 1008. Implementation of Project SEED in a small two-year college. **J.W. Hartman**

9:25 1009. Withdrawn. A Divergent and Persistent Approach to Educating Economically Advantaged Students. **C. Tang**

9:50 1010. How to Leverage Science Competitions with Project SEED Students and Funding Opportunities. **D.S. Masterson**

10:15 1011. Assessing the ACS Project SEED Virtual Summer Camp for High School Students: Can a Virtual Program Increase STEM Identity, Professional Identity, and College Preparation?. **L.S. Nadelson**, R.C. Jamison, E. Soto, D.L. Warner

10:45 Panel Discussion.

11:45 Concluding Remarks.

Birmingham Jefferson Convention Center
East Exhibit Hall 1

Undergraduate Research 1

Poster Session

J. A. Nikles, *Organizer*

10:00 - 12:00

1012. Characterization of Dewatered Nanocellulose for Commercial Application. **E. Pearson**, M.C. Iglesias, T. Ciaramitaro, A. Alawode, I. Vega Erramuspe, B. Via, M.S. Peresin

1013. Dynamic Patterns of Particle Size Distribution of Nonliving Natural Organic Matter. **K.E. Slamen**, K.N. Mealio, H.A. Stretz, M.J. Wells

1014. Synthesis and Computational Study of Semi-fluorinated Polyaryl Ethers via Friedel-Crafts Polymerization of Aromatic Hexafluoropropanol Derivatives. **K.M. Chamberlain**, G. Munoz, S. Athukorale, C.U. Pittman, C.E. Webster, D.W. Smith

1015. Metal Thiolate N-heterocyclic Carbenes for the Reductive coupling of Carbon Monoxide. **C. Carpenter**, N. Dodd, J.P. Sadighi

1016. Does the Environment Around the Carotenoid Change its Oxidation Potential and Thus its Scavenging Ability?. **D. Fountain**, A.L. Focsan

1017. LC-MS Identification of Serum Proteins Adsorbed onto Ionic Liquid-Coated Nanoparticles. **A.M. Hoang**, E.E. Tanner

- 1018.** Analysis of Different Types of Alcohol using gas Chromatography. A.C. Gaquere, **A. Cormier**, A. Watson
- 1019.** Theoretical Studies of Benzoquinone Reactivity in Acidic and Basic Environments. **N. Majoras**
- 1020.** Role of the Cation in Ionic Liquid-Facilitated Transdermal Transport. **A.N. Hunter**, E.E. Tanner
- 1021.** Synthesis of Nano Carbon Microspheres (nCMS) from Natural Materials for the Removal of Water Pollutants. **E. Banks**, M.M. Moyer
- 1022.** Forensic Odontology: Cleaning Chemicals on Molar Remnants Using Infrared Spectroscopy. **A.E. Kelly**, J. McCutcheon
- 1023.** Antioxidant Properties of a Zinc Complex With a Macrocyclic Redox-active Ligand. **A. Jordan**, S. Karbalaei, C.R. Goldsmith
- 1024.** Improved LC-MS Methodology for Determination of Endocrine-disrupting Chemicals (EDCs) in Southwest Florida Waterways. **M. Sciancalepore**, D. Paull, N. Demers
- 1025.** Designer Ionic Liquids for in situ Red Blood Cell Hitchhiking. **J. Randall**, C. Hamadani, E.E. Tanner
- 1026. Withdrawn.** Diffusion of Nanoparticles in Mucus for Nasal Drug Delivery. **J. Marzette**, E.E. Tanner
- 1027.** Incorporating a Collagen Analog and a Bioengineered Protein into Modern Wound Dressings. **J. Spiva**, S.K. Hamilton
- 1028.** Towards the Study of Flow and Mass Transport of Species in a Two-phase Flow Inside a Microreactor using Computational Fluid Dynamics. **O. Ayeni**
- 1029. Withdrawn.** New Electron Donor-acceptor (DA) Complexes of Pyridine-N-oxides Donors with Electron Poor Olefin Acceptors. **C. Fricken**, S.C. Blackstock
- 1030.** Regioselective Asymmetric Akynylation and Arylation of Pyridiniums. **A. Subhit**, T.A. Grigolo
- 1031.** Optimizing Rhodamine B Encapsulation in ZIF-8 Metal Organic Frameworks. **E. Stravolo**

1032. Computational Studies of Properties of 10,11-Diphenylcyclobuta[5,6]pyrazino[2,3-f][1,10]phenanthroline. **J. Powell**, R. Saadein, S. Nkomo

1033. Europium-based Nanoparticles Functionalized with Melanocortin Stimulating Hormone-4 peptide for Potential Cellular Imaging. **M. Rathbone**, M. Fratarcangeli, C.R. De Silva

1034. Exploring Hydrogen Fuel Production using a Ruthenium-platinum Complex. **F.C. Wilson**, G.B. Ray

1035. Phytoremediation of Copper and Iron by Water Hyacinth (*Eichhornia crassipes*) and American Water Willow (*Justicia americana*). **R. Moore**, M. Hage, S. Nkomo

1036. Self-assembly, Gelation, and Spectroscopic Studies of 4-hydroxy-1-anthraquinonylalkanamides. **B. Dang**, J. Ivbaze, A. Mallia

1037. Synthesis, Characterization, and Spectroscopic Studies of Acridinyl and Quinolinylnyl Derivatives of Aminobenzenesulfonamides. **K. Figueroa**, N.Y. Forlemu, A. Mallia

1038. Modeling, Characterization and Analysis of Human WNT1-inducible-signalling pathway and Netrin receptor protein. **N. Luthcke**, G. Calderon, K. Edwards, K. Kasetty, S. Stoddard, K. Whalum, S. Stoddard

1039. Derivatives of 1,2,3-triazoles as Potential Drug Candidates. **G.S. Blount**, V.S. Smith, R. Dodson, A. Henderson, N. Nkengbeza, A. Stewart, J. Kocerha, R.R. Ramoutar, K.S. Aiken

1040. Characterization of a Novel Model for Rotational Acceleration-induced Traumatic Brain Injury. **R. Adams**, A. Umfress, J. Bibb

1041. Simulating the Two-dimensional Electronic Spectra of Organic dyes with vibronic coupling and internal solvation dynamics. **V.A. Suarez**, M.A. Hermosilla-Palacios, V.D. Kleiman

1042. Spectroscopic and Electrochemical Characterization of Iron(III) Oxide Electrodes for Photoelectrochemical Cells. **D.B. McKay**, L. De La Garza

1043. Gold Nanoparticle Immobilization for Photodynamic Therapy in Cancer Cells. **S. Crowder**

- 1044.** Synthetic Pathway Toward Generation of α -ketoalkynes. **J. Gonzalez, B.D. Feske**
- 1045.** Novel Analogs of Sildenafil to Prevent Colorectal Cancer.. **C. Miller, M. Williams, D. Lyons, H. Ramos, I. Lebedyeva**
- 1046.** Development of Sildenafil Analogs as Selective PDE5 Inhibitors.. **H. Ramos, D. Lyons, C. Miller, M. Williams, I. Lebedyeva**
- 1047.** Photocatalytic Degradation of Imidazolium Based Room Temperature Ionic Liquids. **A. Parris, M. Moscatelli, T.R. Hayden**
- 1048.** Designing an undergraduate forensic chemistry experiment on the levels of amphetamine in urine using two different methods. **M. Teigen, M. Popkin, W. Medawala**
- 1049.** Developing a Synthetic Strategy Toward β -ketoalkynes. **K. Glorioso, R. Francis, B.D. Feske**
- 1050. Withdrawn.** Computational contributions to the design of new metal-organic framework materials (MOFs) with improved opto-electronic properties. **C. Crawford, D.A. Clabo**
- 1051. Withdrawn.** Computational Investigations of the Stereoselective Reduction of Dicarboxyls with Borohydride. **J. Butler, D.A. Clabo**
- 1052.** Supported Ionic Liquid Strategy for Emergent Liquid Asthma Medications. **D.M. Cotter, O.A. Cojocar**
- 1053.** Hydrogen Production Using Nickel Complexes with Substituted Thiosalen Ligands. **A. Hemphill, J.m. Briant, N.T. Hames, W.T. Eckenhoff**
- 1054.** Investigation of Group 6 M(III) Complexes with Diimine Ligands for Solvatochromism. **M.A. Davis, E.E. Dove, S.D. Helland, W.T. Eckenhoff**
- 1055.** Investigation of $\text{Ni}(\text{EtImPDI})^{2+}$ as a Catalyst for Light-driven Hydrogen Production. **R.G. Musicante, L.M. Rhodes, W.T. Eckenhoff**
- 1056.** Nickel Complex with Pyridinediimine Ligands Bearing Pendant Base for Light-Driven Hydrogen Production. **S.A. Wicker, M. Kiker, W.T. Eckenhoff**

- 1057.** Progress toward the Synthesis of Antibacterial Aomounds to Avoid efflux-mediated resistance in Gram-negative bacteria. **G. Krisanic**, J.D. Greenberg, E.J. Chow, E.A. Fontana, L.W. Peterson
- 1058.** Using Extended DLVO Theory to Characterize Primary Colonization of Bacteria. **N. Pathak**, T.B. Cavitt
- 1059. Withdrawn.** Fluorinated molecularly imprinted polymer: monomer and polymer synthesis for PFOA sorption. S.M. Durbin, A.M. Loucks, J.C. Meyer, **S.T. Hobson**
- 1060.** Optimization of Synthesis of 3, 4-dihydroxycinnamic acid Analogues to Test Dioxygenase Activity. **J. Steiner**, G. Xhafkollari, R. Marasco, M. Betonio, K.L. Colabroy, L.W. Peterson
- 1061.** Screening quaternary ammonium and phosphonium cations as precursors for juglone ionic derivatives. **R. Paris**, O.A. Cojocar, T.W. Majors
- 1062. Withdrawn.** Effect of dietary supplements and flavonoids of N-methyl-N-nitrosourea mediated methylation of guanine. M. McCoy, C.H. Rippey, L.B. Autrey, **S.T. Hobson**
- 1063.** Use of a full-color 3D printer to create chemical objects for research and teaching. **K. Floyd**, D.A. Clabo
- 1064.** Reaction Mechanism of *Streptomyces sclerotialus* L-DOPA dioxygenase with Varied Substrates. **K. Klugh**, P. Jones, D. Muxue, L.W. Peterson, K. Colabroy
- 1065.** 3,6-dimethoxyxanthone from 2,2',4,4'- tetrahydroxy-benzophenone via Microwave-Assisted Annulation. R.E. Lee, **F.R. Rosario**, **S.E. Knisely**, **S.F. Gebeyehu**, P.E. Heiple
- 1066. Withdrawn.** Uncovering Determinants of Temperature Specificity in Extremophilic Bacterial Type II Topoisomerases. **A. Schoeffler**, **T. Littleton**, **A. Byrd**
- 1067.** Design and Synthesis of Fluoroquinolone Conjugates as Potential Antimicrobial Agents. **A. Rocque**, S.S. Panda
- 1068.** Design and Synthesis of Potential Drug Candidates for SARS-CoV-19. **R. Dobaria**, **J. Moore**, P. Surapaneni, K. Wyman, S.S. Panda

1069. A Salivary Hormonal study on Individuals of African Ancestry living in Different Socioeconomic Environments, in order to Understand Etiology of Prostate Cancer. **B. Jones**, R. Cundey, E. Kaninjing, W. Medawala

1070. Withdrawn. Synthesis of 4-(4-nitrophenoxy)-cyclohexanone and Preliminary Spectroscopic Analysis in its Reaction Towards Nucleophiles.. **H. Walker**, P. Wiget

1071. Energetics of the Ligand-binding Activities of Human Serum Albumin.. **B. Robertson**, **R. Bishop**

SATURDAY AFTERNOON

Birmingham Jefferson Convention Center
East Meeting Room J

Inorganic

General Session - Inorganic Chemistry 2 - Materials, Electrochemistry, and Solar Energy Conversion

J. E. Ritchie, *Presiding*

1:00 Introduction .

1:05 1072. Solvent Dependent Spectroscopic and Electrochemical Studies of Nickel (II) Diethyldithiocarbamate for Energy Storage. **R. Islam**, B.H. Farnum

1:20 1073. 2D Magnetism: from Layered Intermetallics to Exfoliated Ultrathin Magnets. **G. Sasi Kumar**

1:35 1074. Physical and Electrochemical Properties of Synthetically Optimized p-type CuCrO_2 . **A. Chown**, B.H. Farnum

1:50 1075. Fabrication and Application of Zinc Oxide Modified Cellulose Networks as Gas Separation Membranes. **A. Kinnebrew**, **C. Rhoades**, **M.L. Curry**

2:05 1076. Electronic Properties and Thermodynamics Investigation of Heterometallic Actinide-Based Metal–Organic Frameworks with Retrievable-Structure. **J. Yu**, N. Shustova

2:25 Intermission.

2:45 1077. Improving the $2e^-$ Reversibility of a Ni(IV/II) Redox Couple for Application in Redox Flow Battery. **M. MAZUMDER**, B.H. Farnum

3:00 1078. Polyimidazole Manganese Complexes for Oxidation Catalysis of Water. **G. Mu**

3:20 1079. Impact of Ethyl Cellulose on Defining the Structural and Electrochemical Properties of CuGaO_2 Mesoporous Nanocrystalline Thin Films. **H. Yeasmin**, A.R. Combs Bredar, B.H. Farnum

3:35 1080. Photophysics and Electronic Studies of Acceptor-Integrated Covalent-Organic Frameworks. **B. Yarbrough**, N.B. Shustova

3:50 1081. Nickel(II) Bis(diethyldithiocarbamate) as a Novel Redox Mediator in Dye-sensitized Solar Cells. **N. Dalpati**, B.H. Farnum

Birmingham Jefferson Convention Center
East Meeting Room F

Synthesis of Fluorescent Probes and Their Applications from Sensing to Imaging

2

M. Henary, *Presiding*
Financially supported by Molecules, De Gruyter

1:00 Introductory Remarks.

1:05 1082. The Force is Within You: Fluorescent Probes to Map the Molecular Forces in Cells. **K. Salaita**, Y. Duan, Y. Hu

1:35 1083. Chemical Sensing through Fluorescence Modulation in Conjugated Polymers. **M. Bonizzoni**

2:05 1084. Excited State Proton Transfer Dye with an Emission Quantum Yield up to 60% upon Zn²⁺ Coordination. **K. Hanson**, S. Ayad, E.S. Knorr

2:35 1085. Characterization and Applications of Binding of Cyanine Dyes to Biomolecules. **G. Patonay**, M. Henary, P. Ali

3:05 Intermission.

3:25 1086. Development of Chemical Tools to Decipher the Role of Reactive Nitrogen Species in Cancer Progression. **J. Chan**, A.K. Yadav, M.Y. Lucero, M.C. Lee, A. East, S. Su

3:55 1087. Characterization of the Reactivity and Optical Properties of an Amide Dimer of Rhodamine B. **P. Lundin**, **K. Fogarty**

4:25 1088. Tuning Asymmetric Xanthene-based Sensors via Modification of the Xanthene Moiety. **C. Stephenson**, M. Bratton, R. Brown, I. Andonie, M. Ohakwe

4:55 Concluding Remarks.

Birmingham Jefferson Convention Center
East Meeting Room E

Organic

Organic Probes/Methodology/General

L. Yet, *Organizer*

1:15 Introduction .

1:20 1089. Highly Adaptable ¹⁵N-tag motif for Development of Novel Hyperpolarized Magnetic Resonance Imaging Probes. **H. Park**, G. Zhang, J. Bae, W.S. Warren, Q. Wang

1:35 1090. Photoacoustic Probe for biopsy-free Assessment of Copper Status in Murine Models of Wilson's disease and liver metastasis. **M. Lucero**, S. Su, J. Forzano, J. Chan

1:50 1091. SWIR Emissive Rosindolizine Dyes as Fluorescence Imaging Materials. **W.E. Meador**, S. Chatterjee, C. Smith, I. Chandasiri, M. Farid Zia, J. Nguyen, A. Dorris, A. Flynt, D.L. Watkins, N. Hammer, J.H. Delcamp

2:05 1092. Unique Reactivity of Meso-nitrile Oxide BODIPYs. **B.R. Schrage**, Y. Zatsikha, V. Nemykin

2:20 1093. Synthesis of Novel Xanthene Based NIR I Dyes to Develop as Biosensors. **I.N. Rajapaksha**

2:35 1094. Analysis of Torrefied Wood by Forrier-Transform Infra-red (FTIR) Spectroscopy, Atomic Absorbance, X-ray Diffraction, and Elemental Analysis. **G.W. Durrell**, A. Hulette, L. Richa, Y. Lin, F. Leconte, B. Colin, A. petrissans, W. Chen, M. Petrissans, R.L. Quirino

2:50 1095. Withdrawn. Molecularly Imprinted Polymer Based Real-time Sensor for PFOA. **S.T. Hobson**

3:05 Intermission.

3:25 1096. Enantioselective Synthesis of Secondary Propargyl Amines. **K.N. Weeks**, A. Aponick

3:40 1097. (Diethylamino)Sulfur Trifluoride (DAST): A Versatile Reagent in Organic Synthesis. **M.A. Lnu**

3:55 1098. The Fascinating World of Nitrosobenzenes. **S.C. Blackstock**

4:10 1099. Radical Chain Reduction via Carbon Dioxide Radical Anion. **C. M Hendy**, G. Smith, Z. Xu, T. Lian, N. Jui

4:25 1100. Development of Sequence Defined Oligomers using Photo-SPAAC. **S. Sharma**, S. Minko, V. Popik

4:40 1101. Withdrawn. Ligand-Controlled Regiodivergence for Catalytic Stereoselective Semireduction of Allenes. **M. Hajiloo Shayegan**, Z. Li, X. Cui

4:55 1102. An Enantiomeric Excess Determination Using $^1\text{H-NMR}$ of Isotope Labeled Substrates. **T.A. Owens**, D.S. Masterson

Birmingham Jefferson Convention Center
East Meeting Room G

Analytical Chemistry

Advanced Analytical Chemistry Studies of Biomolecule and Tissue Systems

A. Ghosh, S. Pan, *Presiding*

1:30 Introduction .

1:40 1103. Studying the Photophysical Modulation of Small Organic Molecules in Drug Delivery Vehicles. **D. Ghosh**, K.S. Aiken, S.M. Landge

2:00 1104. Analysis of Microplastics (MPs) and Perfluoroalkyl Substances (PFAS) in Marine Animal Tissues. **C. Navarathna**

2:20 1105. Mass Spectrometry Characterization of Deep Eutectic Solvents and their Impact on Protein Structure and Dynamics. J. Stewart, P. Gambill, M. Wewers, C. White, K. Galvez, M. Rahman, **M. Halim**

2:40 1106. X-ray Excited Luminescence Chemical Imaging (XELCI) based pH sensor for non-invasive Monitoring of Implant Associated Infections. **A. Rajamanthrilage**, C. Taylor, U. Uzair, J. Tzeng, J.N. Anker

3:00 Intermission.

3:25 1107. Enhancing the Antioxidant Activity of Carotenoids-the Bioavailability Improvement. **A.L. Focsan**, Y. Gao, N. Polyakov, L. Kispert

3:45 1108. Fundamental Gas-Phase Chemistry of Beta2-agonists Using Mass Spectrometry: From Dissociation to Stereoisomer Discrimination. **M. Carlo**, A.L. Patrick

4:05 1109. UV-vis Extinction by Aggregated Proteins: Optical Absorption Induced by Charge Transfer or Light Scattering by the Protein Aggregates?. **P.D. Wathudura**, M. Wamsley, K.R. Carter, D. Zhang

4:25 1110. Optimization of a Prototype Analyzer for Trihalomethanes in a Drinking Water Distribution System. **M. Alfonso**, N. Boppana, M.A. Brown, P.S. Simone, G.L. Emmert

4:45 Concluding Remarks.

Birmingham Jefferson Convention Center
East Meeting Room O

Biochemistry

General Session Biochemistry 2

J. Zhang, *Presiding*

1:30 Introductory Remarks.

1:35 1111. Surface Adsorption and Structure-Function Characterization of Autolysin-Amidase from *S. epidermidis*. **R. Yadav**, S. Yang, R. Somarathne, N.C. Fitzkee

1:55 1112. Understanding Binding Properties of Staphylococcal Autolysin Domains with Polystyrene. **R. Somarathne**, E. Chappell, Y. Perera, R. Yadav, J. Park, N.C. Fitzkee

2:15 1113. Synthesis, Characterization, Biological Analysis, and Molecular Docking Studies of DPDPE, a Delta Opioid Receptor Agonist and a Cyclic DPDPE Derivative Containing a Sonogashira Linkage. **K.R. Wilson**, M. Goertzen, J.C. Ouellette, T. McGomery, A. Williams, S. Majumdar

2:35 1114. Intrinsically disordered electronegative clusters improve stability and binding specificity of RNA-binding proteins. **J. Zhang**

2:55 Intermission.

3:15 1115. Crystal Structure of a Mycobacteriophage Immunity Repressor Bound to DNA Sheds New Light on Transcriptional Silencing. **J. Wallen**, R. McGinnis, C. Brambley, B. Stamey, W.C. Green, K.N. Gragg, E.R. Cafferty, M. Hammel, T. Hollis, J.M. Miller, M.D. Gainey

3:35 1116. Withdrawn. Extending a Promising Aptamer Screening Platform to Gold Nanosphere Targets. **V.T. Milam**, M. Tapp, M.C. Adams, P. Dennis, R. Naik

3:55 1117. Asymptomatic COVID-19 Screening and Contact Tracing on an Undergraduate Campus. **S.A. Smith**, B. Magers, J. Neiswinger, R. Bishop, K. McKinney, L. Evans, M. McGuire, D. Manning

4:15 1118. Withdrawn. Targeting a Conserved Structural Element from the SARS-CoV-2 Genome Using Mirror Image Aptamers. **J. Li**, J.T. Szczepanski

4:35 1119.

Impact of Multivalency and Encapsulation of Affinity Reagents and Catalysts. **B. Manuel**, A. Sanford, S. Das, J. Heemstra, M. Finn

Birmingham Jefferson Convention Center
East Meeting Room K

Chemical Education

J. March, *Organizer*

Chemical Education Oral Presentations 2

1:30 Introduction .

1:40 1120. Improving Student Attitudes Towards General Chemistry I Laboratory as an Effect of Switching Lab Partners. **L. Smith**, D. Mlsna, T. Wei

2:00 1121. Measuring Internalized Stereotype Threat in Introductory Chemistry Courses Using a Customized Implicit Association Test (IAT). **T. Blue**, T.L. McGill

2:20 1122. Emerging Stronger through Resources Developed During the Pandemic. **B. Casselman**

2:40 Intermission.

3:00 1123. Pre-COVID and during-COVID: A comparison of general chemistry instruction at the University of Florida. **M.T. Sumner**, S. Benjamin, S. Harris, S. Lopez, M. Veige

3:20 1124. Effects of a Preparatory Adaptive Module on Student Performance in General Chemistry I at University of Florida. **S. Benjamin**, S. Harris, S. Lopez, M.T. Sumner, M. Veige

3:40 Concluding Remarks.

Birmingham Jefferson Convention Center
East Meeting Room B

Engineering Solutions for Social Challenges: Renewable Materials and Resources 2

Financially supported by **Center for Sustainable Nanotechnology - UW Madison, and Surface Measurement Systems**

M. L. Curry, L. A. Lucia, M. S. Peresin, *Presiding*

1:30 Introductory Remarks.

1:35 1125. Biobased Particles in Superstructured and Multiphase Materials. **O.J. Rojas**

2:20 1126. Cellulose Nanofiber-based Hydrogels for Rapid Removal of Methyl Blue dyes in Water. **Y. NAN**

2:50 1127. Effects of Hydrophobic-modified Cellulose Nanofibrils (CNFs) on the Physical and Chemical Properties of UHP PMDA Membranes. **M. Fair**, J. Mitchell, K.E. O'Harra, J.E. Bara, M.L. Curry

3:20 Intermission.

3:40 1128. Downed Timber Degradation of Loblolly Pine in South Alabama and Potential Recovery of Natural Polymers for Value-added Applications. **J.A. Hernandez-Diaz**, M. Musah, B. Via, M.S. Peresin

4:10 1129. A Novel Method for Uniform Suspension of CNFs and Its Impact on the Fabrication and Thermal Stability of Cellulose-based Polymeric Composites. **D.H. White**, M.S. Islam, B. Frank, E. Laudadio, J.T. Buchman, E.M. Jackson, H. Fairbrother, R.J. Hamers, C.L. Haynes, M.L. Curry

4:55 Concluding Remarks.

Birmingham Jefferson Convention Center
East Meeting Room N

Industrial Careers in Chemistry

Undergraduate Discussion: Industrial Careers in Chemistry

Financially supported by Refresco
J. A. Nikles, *Organizer*

1:30 Introduction .

1:40 1130. The Unconventional Career path of a Chemist in Industry. **H.L. Davis**

2:05 1131. Technical challenges facing the food and beverage industry. **D.E. Ragland**

2:30 Intermission.

2:40 1132. Chemistry Leads Beyond – Creating Your Career. **T. Tice**

3:05 1133. From a PhD in Biochemistry to the Director of Marketing: A Look at a Non-Traditional Career for your STEM Degree. **K. Sims**

3:30 1134. Successful Careers in the STEAM Field. **Y. Crawford**

3:55 1135. Transitioning from Academic Studies to an Industrial Career. **T.R. Totsch**

4:20 Panel Discussion.

Birmingham Jefferson Convention Center
East Meeting Room A

Nanomaterials 2

S. Street, *Presiding*

1:30 Introduction .

1:40 1136. Polymer Functionalized Zeolite - Green and Sustainable Ion Exchange Material. **J.C. Poler**, S. Elmore, C. Reid, S. Schmal

2:00 1137. Ionic Liquids as Antifouling Polymeric Nanoparticle Coatings. **E.E. Tanner**

2:20 1138. Using NMR to understand Protein Binding and Structure on Nanoparticle Surfaces. **N.C. Fitzkee**, J. Xu, R. Yadav, R.P. Somarathne, D.L. Amarasekara, Y. Perera

2:40 1139. Effect of Mass Transport Limitations on Gas Adsorption in Hierarchically Porous Carbons. **M.G. Bakker**, R. Adhikari

3:00 1140. Enhanced Harmonic Generation from Coupled Plasmonic Nanoparticle Films. **N. Spear**, J.M. Queen, S. Bailey, R.F. Haglund, J. Macdonald

3:20 Intermission.

3:40 1141. A Facile Benchtop Reactor Design using Dendrimer-templating Technology for the Fabrication of PEI-coated CuO Nanoparticles on the Gram Scale. A. Ethridge, M.J. Gallagher, N. Hudson-Smith, D. Finley, A. Ahsan, H. Fairbrother, C.L. Haynes, R.J. Hamers, **M.L. Curry**

4:00 1142. Metal-Organic Frameworks: From Bulk to Thin Films. **A. Bajpai**, D. Speed, G.J. Szulczewski

4:20 1143. Characterization of Metal-organic Framework Thin Films using Laser Desorption/ionization Mass Spectrometry. **D. Speed**, A. Bajpai, G.J. Szulczewski

4:40 1144. Transport Features of Network Materials Built with Carbon Nanotubes Despite of Chiralities and Other Shape Factors. **S. Tang**

Birmingham Jefferson Convention Center
East Meeting Room I

Physical Chemistry

General Session Physical Chemistry 2

T. P. Hamilton, *Organizer*

1:30 1145. Insights into Possible Halogen Bonding Effects in Dye Sensitized Solar Cells Studied via Nanosecond Transient Absorption Spectroscopy. **L. Hunt**, c. curiac, M. Sabuj, Q.Y. Li, A. Baumann, H. Cheema, y. zhang, N. Rai, N. Hammer, J.H. Delcamp

1:50 1146. Computational Analysis of the Spin-trapping Properties of Lipoic Acid and Dihydrolipoic Acid. **M. Bonfield**, S.J. Kirkby

2:10 1147. Correlating Stability of Substituted Cobaltocenium [bis(cyclopentadienyl)cobalt(III)] with Molecular Properties. **S.T. Wetthasinghe**, C. Li, H. Lin, T. Zhu, C. Tang, Q. Wang, V. Rassolov, S. Garashchuk

2:30 1148. Investigations of CF^+ using High Accuracy Electronic Structure Theory Methods. **G. McCarver**, R.J. Hinde

2:50 1149. Computer Modeling of Size Effects in $V_{1-x}M_xO_2$ (M = Mo, Nb). **J. Phillips**, T.C. Douglas, J. Allred, M. Krogstad, T. Rawot Chhetri, M.A. Davenport

3:10 Intermission.

3:30 1150. Understanding The Structural And Dynamical Properties Of Lignin Polymer In DmsO And DmsO/water Binary Mixtures. **N. Jahan**

3:50 1151. Transition-potential Coupled Cluster. **M. Simons**, D. Matthews

4:10 1152. Unusual Intramolecular Contacts in 2,3-Epoxy-cyclopentanol and their Analogs: Theoretical Evidence for Hydrogen Bonding. **J.M. Carr**, G.S. Tschumper

4:30 1153. Insight into Subsurface Adsorption from a Lattice-gas Model and Monte Carlo Simulations of Atomic Oxygen on the Silver Surface. **C. Mize**, L.D. Crosby, S.B. Isbill, S. Roy

Birmingham Jefferson Convention Center
East Meeting Room C

Polymer Materials Science and Engineering

General Session Polymer Materials 2 - Polymeric Materials for Biological and Environmental purposes

V. Thomas, *Presiding*

1:30 Introduction .

1:40 1154. Poly(amino acid)s and PEGylated poly(amino acid)s in Biological Applications. U. David, J. Sanchez, **C. Scholz**

2:00 1155. Polymeric Tissue Scaffolds that Mimic the Structure, Composition and Function of the Extracellular Matrix. **D. Dean**, J. Ayariga

2:20 1156. Plasma Assisted Surface Polymerization Process for Nanoparticles Modified 3D Printed Polymer Scaffolds for Tissue Engineering Applications.. **V. Vijayan**, V. Thomas

2:35 1157. Supramolecular DNA Photonic Hydrogel for on Demand Control of Coloration with High Spatial and Temporal Resolution. **Y. Dong**, K. Salaita

2:50 1158. Differential Stiffness of Electrospun PLA Scaffolds Modulate Chondrocyte Behavior *in vitro*.. **J.A. Ayariga**

3:05 Intermission.

3:15 1159. Synthesis and Characterization of PDMAEMA-g-CNT Composites. **T.L. Thornell**

3:30 1160. Recycling and Upcycling of Waste Plastics with Hemp Fibers. **Z. Wang**, Z. Vickery, E. Strickland

3:45 1161. Single-step Protease Immobilization in Solution Blown Polyethylene Oxide Nanofibrous Nonwoven Webs. **F. Asaduzzaman**, S.I. Salmon

4:00 1162. Fully Organic, X-ray Radioluminescent Crystalline Colloidal Arrays: Fine-tuning Color Characteristics via Photonic Bandgap Control and a Cascade of Energy Transfers. **H.W. Jones**, I. Bandera, E. Zhang, S.H. Foulger

4:15 1163. Anti-solvents Effects on Properties of Regenerated Cellulose from 1-butyl 3-methyl Imidazolium Chloride. **B.L. Sadiku**, C. Emehel, J.R. Alston

Birmingham Jefferson Convention Center
East Exhibit Hall 1

Undergraduate Research 5

J. A. Nikles, *Organizer*

1:30 - 3:30

1164. Exploiting Metallohedged *trans*-Bidentate Ligands for Cross-Coupling Reactions. **B. Nessell**, C.D. McMillen, J.A. Pienkos

1165. Biological Activity of Palladium Thiosemicarbazone. **E. Travers**, E.C. Lisic, J. Kim

1166. Attempts Toward Highly Electron-deficient Diimine Ligands and Expanding the Coordination Compounds of *N,N'*-bis(pentafluorophenyl)-2,3-butanediimine. **B. Newell**, J.P. Lee

1167. SDS-PAGE Studies on pH Dependent Lysozyme Modifications Induced by Naphthoquinones. **D. Madeksho**, J. Ewald, T.V. Albu, J. Kim

1168. Synthesis of Substituted Oxocanes to Probe Inductive Effects on Long-Range Hyperconjugation. **L. Middleton**, **J. Rivers**, **J. Hallford**, P. Wiget

1169. Pharmaceutical Drug Ligand Binding to Human Serum Albumin with Quantum Chemical Methods. **J.B. Baker**, A. Farmer, E. Mitchell, R. Bishop, B. Magers

1170. (Diethylamino)Sulfur Trifluoride (DAST) Mediated Oxidation of Alcohols and Amines to Carbonyl cCompounds. M.A. Lnu, **B. White**

1171. Synthesis of Trifluoromethyl Ketones by (diethylamino)sulfur trifluoride (DAST)-mediated nucleophilic trifluoromethylation of benzoic acids. M.A. Lnu, **M. Vescio**

1172. The Detection and Discrimination of Endocrine Disrupting Chemicals. **a. richardson**, M. Meadows

- 1173.** Defining the Mechanism of Inhibition of Thiosemicarbazone-metal Complexes on Topoisomerase II Alpha. **C. Greer**, K. Lyons, W. Morris, E.C. Lisic, J.D. Conner, X. Jiang
- 1174. Withdrawn.** Construction of an Instrument Capable of Two-color Fluorescence Correlation Spectroscopy:. **A. Lawrence**, K.H. Fogarty
- 1175.** Synthesis of Bioactive Juglone Compounds *via* aromatic Ammonium Cations. **H. Suddeath**, O.A. Cojocararu, T.W. Majors
- 1176.** Synthesis of α,β -unsaturated lactams via oxidative-elimination using NaIO_4 . **D. Toman**, J.M. Plummer
- 1177.** Discovery of the Cryptic Allosteric Site on the CB1 Receptor. **D. Hunnicutt**, **A. Lee**, J. Shim
- 1178.** Potentiating Antibiotics to Target Multidrug Resistant ESKAPE Pathogens. **B.O. Allen**, R. Day, M.S. Blackledge
- 1179.** Theoretical Study of $\text{Au}_{25}(\text{SCH}_3)_{18}^-$ and its Activation of O_2 Molecules. **J. Pinkerton**, S. Havenridge, C. Aikens
- 1180.** Computational Investigations into Tetrahalogenated Tricyclooctanes and Tricyclodecanes. **R.A. Davy**, R.L. King, J.R. Boone, E.W. Reinheimer, C. Clinger
- 1181.** Synthesis and Characterization of Zeolite-Encapsulated Organometallic Complexes that Catalyze Selective Alkane Oxidation. **J.L. Groeber**, C.R. Diemer, E.P. Iaia, J.W. Harris, M.G. Bakker, G.R. Rana
- 1182.** Role of Quenching and Diffusion in the Magnetic Sensitivity of Micellar Thionine-aniline Radical Pairs. **A. McHorse**, A. Markham, D. Sowood, C. Timmel, L. Jarocho
- 1183.** Effects of Hydrophobic Modification and Electrostatic Interactions on the Sensitivity of Flavin-ascorbic Acid Radical Pairs to Weak Magnetic Fields. **E. Dowker**, E. Evans, C. Timmel, L. Jarocho
- 1184. Withdrawn.** Separation of Chiral Amino Acids Using Mass Spectrometry and Ion Mobility. **K.D. Hernandez Gomora**, H. Dossmann, S. Alves, D. Lesage
- 1185.** Seasonal Comparison of Metal Concentrations along the Alafia and Hillsborough Rivers. **R. Vernarsky**, K.A. Deister

- 1186.** Preparation of Macrocyclic Polyphenylethynylarene Ethers. **B. Steen**, T.D. Selby
- 1187.** Synthesis of Macrocyclic Diaminopolyphenylethynylarenes and Diaminopyridinylethynylarenes. **M. Stewart**, T.D. Selby
- 1188.** Functionalizing Zeolite to Remove Hydrophilic Contaminants in Drinking Water. **S. Elmore**, S. Schmal, J.C. Poler
- 1189.** Campus-wide COVID Screening Provides Non-Traditional Clinical and Laboratory Experiences for Students During Pandemic. **D. Manning, R.G. Ayres**, L. Evans, M. McGuire, K. McKinney, A. Farmer, M.L. Ayres, C.C. Bishop, E. Campbell, O. Haney, K. McKinney, M. Meadows, S. Roberson, R. Bishop, J. Neiswinger, B. Magers, S.A. Smith
- 1190.** Chemical Analysis and Biototoxicity Assessment of Plastic Bioremediation using Tenebrio Molitor Larvae. **L. Sisson**, C. Stokes, S. Melton, T.D. Selby, S. Hearst
- 1191.** Shear Rate Effects on Particle Size Distribution of Nonliving Natural Organic Matter. **K.N. Mealio**, K.E. Slamen, H.A. Stretz, M.J. Wells
- 1192.** Protection of Alcohol Dehydrogenase Activity by a Tardigrade Cytosolic Abundant Heat Soluble Protein. **A. Burgess**, B.E. Christian
- 1193.** Effect of Novel Fluoroquinolone-derived Inhibitors on DNA Gyrase Activity. **C. Plantz**, A. Rocque, S. Panda, A.C. Spencer
- 1194.** A New Extraction and Quantification Method to Detect Polystyrene Plastics in Biological and Environmental Samples. **C. Stokes**, S. Melton, L. Sisson, T.D. Selby, S. Hearst
- 1195.** Stabilization of Proteins in Solution by a Tardigrade Cytosolic Abundant Heat Soluble Protein. **L. Vaughn**, B.E. Christian
- 1196.** Conventional Strain Energies of Thiaziridine and the Thiazetidines. **J.D. Gramm**, D.H. Magers
- 1197.** Joro Spider Webs as Bioaccumulators of Heavy Metals in North Georgia. **M. Smith-Roden**, J. Casey, H. Cole, J. Driver, I. Agyekum

- 1198.** Boron-mediated diastereoselective aldol reactions of *N,N*-dialkylphenylacetamides. **B. Peco**, A. McCullough, **S. Reliford**, S.W. Primeaux, D.J. Cambre, P.B. Chanda
- 1199.** Analysis of Electronic Cigarette Liquids. **M. Deen**, L. Butler, V. Geisler
- 1200.** Influence of Spring Water on Two Rivers in Tampa Bay, Florida. **P. Mead**, K.A. Deister
- 1201.** Regioselectivity of Acid-catalyzed Epoxide Ring-opening Reactions. **B.R. Chastang**, D.H. Magers
- 1202.** The Conventional Strain Energies of Cyclopropylborane, Borirane, Boretane, the Diboretanes, Borolane, the Diborolanes, Borinane, and the Diborinanes. **K.E. Hood**, R.M. Rocray, D.H. Magers
- 1203.** Relative Stabilities of Derivatives of 9-methylanthracene and 9-methylene-9,10-dihydroanthracene and Derivatives of 6-methylpentacene and 6-methylene-6,13-dihydropentacene. **E.P. Sullivan**, A.W. Plunkett, D.H. Magers
- 1204.** Ab Initio Analysis of Polarizability in Molecular Piezoelectric Response for Organic Dimer Systems. **D.L. Zetterholm**, D.H. Magers
- 1205.** Prediction of Chiroptical Spectroscopic Properties of Chiral Beta-lactone Heteroaromatics by Equation-of-Motion Coupled-Cluster Theory. **O. Haney**, H. McAlexander, R. Bishop, B. Magers
- 1206.** Design and Development of a Homogenous Protein-based Assay for the Detection of Organophosphates by Utilizing a Fusion Protein Between Organophosphorus Hydrolase (OPH) and Enhanced Green Fluorescent Protein (EGFP). **C.R. Schlaline**, **S. Knier**, L.G. Puckett
- 1207.** Structural Characterization of a Mutagenic 6-oxo-m1dg Adduct in DNA. **C.L. Wessel**, Y. Fu, L.J. Marnett, M.P. Stone
- 1208.** Comparison of Six Different Iron-Gall Ink Mixtures with Respect to Value of the Wet and Dried Inks as Determined using a Munsell Scale and Other Physical Properties. **M.S. Morton**, **J. Quesada**
- 1209.** Spin Trapping Reactive Oxygen Species Produced by X-ray Scintillating Nanoparticles. **I. Weaver**, E. Zhang, C. Kerpel, S.H. Foulger, L. Jarocho

- 1210.** Synthesis of Silver Phosphate Complexes. **T. Hussain**, N. Dodd, J.P. Sadighi
- 1211.** Characterization of Gamma Ray Imaging System for Use in Depleted Uranium Remediation Efforts: Shielding the Gamma Ray Imaging System. **C.E. McCormick**, B.P. Crider, R.J. Unz, L. Allen, B. Henkel, S. Lusby, S. Sansing, D.H. Magers
- 1212.** Synthesis of Homoepibatidine Derivatives for Smoking Addiction. **G. Womack**, S. Slauson
- 1213.** Are Halogenated Amino Acids from Plasma Proteins Correlated with Pediatric Eosinophilic Esophagitis?. **M. Thomas**, J. Germany, M. Gilliland
- 1214.** Using NMR Titrations and DFT Computational Modeling to Assess Halogen-Bonding Strength as a Function of Molecular Structure. **Q. Dang**, J. Simpson, C.A. Parish, M.C. Leopold
- 1215.** Biofouling Resistant ICP Films for Biologically Triggered Dopant Release. **A. Knepper**, P. Molino, T.W. Hanks
- 1216.** Nitrile Homoepibatidine Synthesis. **N.N. Al-Saadi**, S. Slauson
- 1217.** Characterizing *Brucella* FtrB: A New Class of Cupredoxin. **A. Kerkan**, S. Banerjee, D. Martin, S. Roy, B. Garcia, R. Roop
- 1218.** Analyzing Spectral Data of Rhodamine B dimer and related compounds. **B. Stratton**, A. Wolwhend, K. Fogarty, P. Lundin, A.J. Pierre
- 1219.** Mechanisms of Linoleic Acid Oxidation by Myeloperoxidase. **C. Powell**, K.M. Matera
- 1220.** Vapor Deposition Synthesis of Semiconducting Molybdenum Disulfide. **J. Arce**, P. Parajuli, A. Rao, R.E. Lee
- 1221.** Spartan18 QSAR Analysis of Ebselen-Type Heterocycles for the Inhibition of SARS-CoV2. F. Bai, **D. Cooper**, M. Donahue, J. Kessel
- 1222.** Resolution of Racemic Alcohol through the use of Mosher's Reagent for use in the Synthesis of Enantiopure Allosteric Inhibitors for HIV-1 Integrase. **L. Evans**, K. Patel, J. Patterson, J.A. Pigza, M. Donahue, J. Kessl
- 1223.** Effects of Self-assembled Monolayer Structure on Conjugated Polymer Morphology. **E. Silver**, P. Lundin

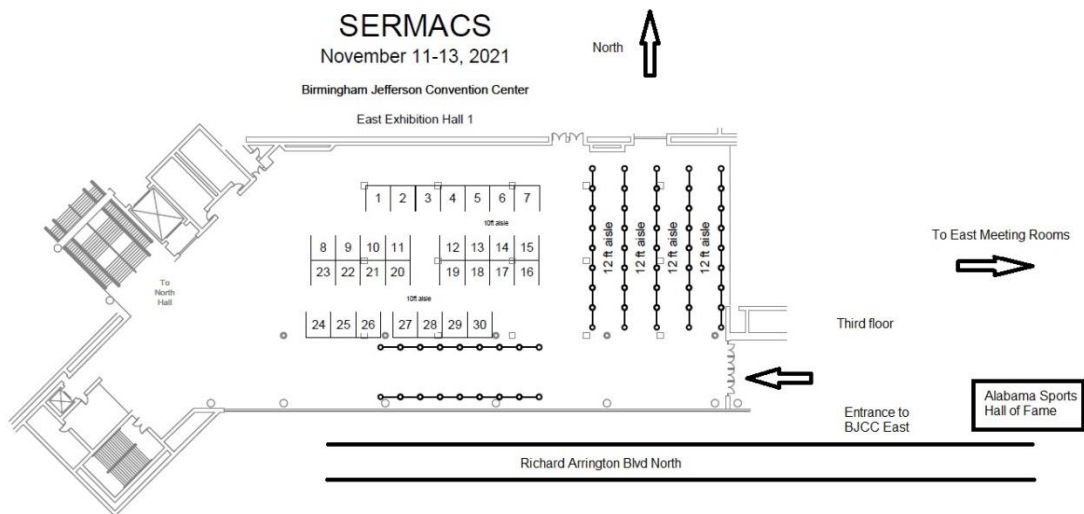
SATURDAY EVENING

Birmingham Jefferson Convention Center
East Ballroom B

Plenary

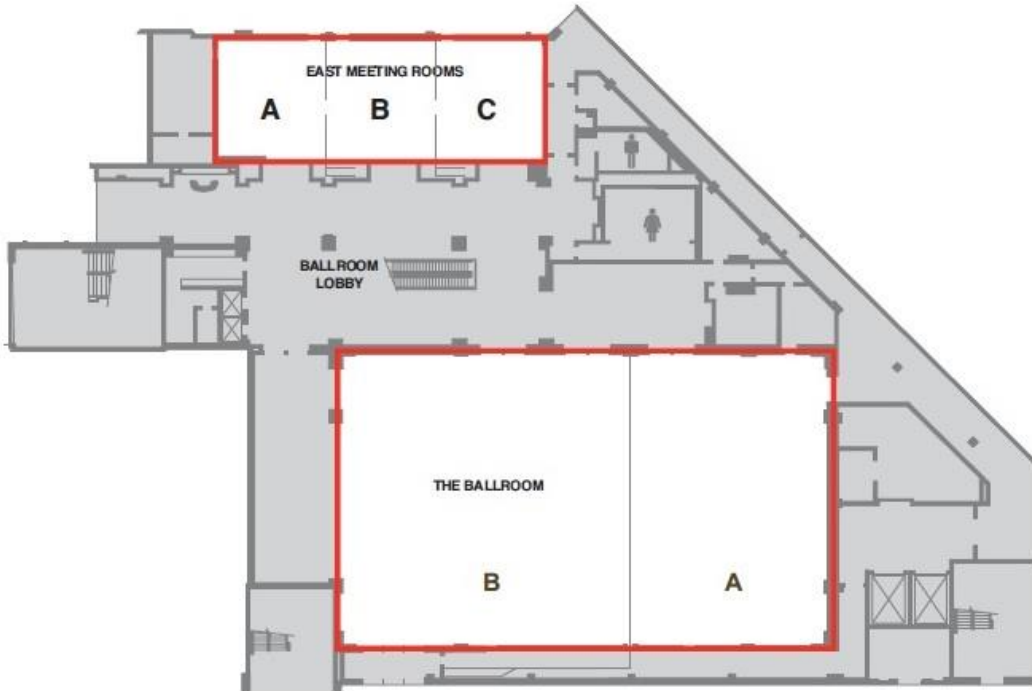
T. P. Hamilton, *Presiding*

5:30 1224. A Career in Science: Expect the Unexpected. **L.J. DeLucas**





Third Floor East Meeting Rooms



First Floor East Meeting Rooms

P5 is the recommended Parking Deck
Meetings are in East Meeting Rooms

Sheraton and Westin Hotels are also circled
Elevated walkway from Sheraton to Third Floor East

