

SERMACS 2021

WEDNESDAY AFTERNOON

Sheraton Birmingham Hotel
East Meeting Room MH and East Meeting Room N

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 metalloprotein 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-Azaauridine 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. 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. 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

Sheraton Birmingham Hotel
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. Karbalaie**, 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.

Sheraton Birmingham Hotel
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**

Sheraton Birmingham Hotel
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.

Sheraton Birmingham Hotel
East Meeting Room J

Discovery of Therapeutic Agents for Emerging Viruses

A. Centilli, *Presiding*

1:00 Intermission.

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 Introduction.

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.

Sheraton Birmingham Hotel
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.

Sheraton Birmingham Hotel
East Meeting Room E

General Session - Environmental Chemistry

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. 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

Sheraton Birmingham Hotel
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**

Sheraton Birmingham Hotel
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.

Sheraton Birmingham Hotel
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

Sheraton Birmingham Hotel
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**

Sheraton Birmingham Hotel
East Meeting Room N

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.** 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.** 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.** 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

Sheraton Birmingham Hotel
East Ballroom B

Plenary

T. P. Hamilton, *Presiding*

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

THURSDAY MORNING

Sheraton Birmingham Hotel
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

Sheraton Birmingham Hotel
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-M₁dG 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.

Sheraton Birmingham Hotel
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

8:10 189. Scalable GPU-accelerated Computational Infrastructure for Parallel Tensor Processing in Quantum Many-body Theory. **D. Lyakh**

8:45 190. Accelerating Density-Functional Tight-Binding Using Graphical Processing Units. **S. Irle**, V. Vuong, C. Cevallos, B. Aradi, C. Camacho

9:20 Intermission.

9:40 191. High-Performance Density Fitting Technology on Accelerated Computed Platforms. **E.F. Valeev**, A. Asadchev

10:15 192. GronOR: Scalable and Accelerated Non-Orthogonal Configuration Interaction for Molecular Fragment Wavefunctions. **T.P. Straatsma**

10:50 193. Computational investigations of Aromatic Borylene-type Systems. **U. Gaillard**, K. Donald

Sheraton Birmingham Hotel
East Meeting Room J

Inorganic Electron Transfer Reactions for Energy Storage

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**

9:25 198. Excited State Proton Transfer and Electron Transfer in Complexes Exhibiting Intramolecular Reversible Energy Transfer. **F. Zhang**, J.J. Paul, R.H. Schmehl, J. Stash

9:45 Intermission.

10:00 199. Improving 2e⁻ Redox Chemistry of Nickel Dithiocarbamates for Application in Redox-Flow Batteries. **B.H. Farnum**, M. Mazumder

10:20 200. Cr Complexes for the Electrocatalytic Reduction of Carbon Dioxide. **S. Hooe**, J. Moreno, A. Reid, **C.W. Machan**

10:40 201. Ligand-to-Metal Charge-Transfer Photochemistry and Photophysics of d^0 Titanocenes. **H. London**, D. Pritchett, C. McMillen, G.C. Shields, P.S. Wagenknecht

11:00 202. 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**

11:20 203. Metalloenzyme Mimics: Iron Carbonyl Clusters Tethered to Non-Innocent Aromatic Ghiole Groups.. **C.A. Mebi**

Sheraton Birmingham Hotel
East Meeting Room G

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

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. Eletsky, 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 Lability 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.

Sheraton Birmingham Hotel
East Meeting Room A

New Directions in Metal-Catalyzed Reactions 1

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**

Sheraton Birmingham Hotel
East Meeting Room L

Photocatalysts and electrocatalysts and electrochemistry methods for clean energy harvesting, conversion, and storage

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 Ditetelluride 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

Sheraton Birmingham Hotel
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 Vitriimer 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. Rupar**

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**

Sheraton Birmingham Hotel
East Meeting Room B

Small Molecules for the Disruption of Bacterial Processes 1

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**

Sheraton Birmingham Hotel
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. Kenemur**

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

Sheraton Birmingham Hotel
East Meeting Room K

Supramolecular and Biomolecular Chemistry

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

Sheraton Birmingham Hotel
East Meeting Room F

The Magic of Spectroscopy

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

Sheraton Birmingham Hotel
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

Sheraton Birmingham Hotel
East Meeting Room MH

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. 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

Sheraton Birmingham Hotel
East Meeting Room MH

Organic

Poster Session

L. Yet, *Organizer*

12:30 - 2:30

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

282. 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. 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.** 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.** Development of Photoactivated nanoMOF Drug Delivery Systems. **H.D. Cornell**, M. Nagai-Singer, I.C. Allen, A.J. Morris

- 329.** 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. Deghani, 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.** The Synthesis and Biocatalytic Reduction of Beta-keto Alkynes. **R.M. Francis**, B.D. Feske

Sheraton Birmingham Hotel
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.

Sheraton Birmingham Hotel
East Meeting Room F

The Magic of Spectroscopy 2

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. Jimenez**

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

4:50 Concluding Remarks.

Sheraton Birmingham Hotel
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

Sheraton Birmingham Hotel
East Meeting Room C

Methods and strategies for modern organic synthesis

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**

Sheraton Birmingham Hotel
East Meeting Room J

Small molecule activation at biological or bio-inspired metal centers

Financially supported by Agilent Technologies
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**

Sheraton Birmingham Hotel
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**

Sheraton Birmingham Hotel
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.

Sheraton Birmingham Hotel
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

Sheraton Birmingham Hotel
East Meeting Room G

Ground truth: bridging knowledge gaps between computational and experimental enzymology

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**

Sheraton Birmingham Hotel
East Meeting Room A

New Directions in Metal-Catalyzed Reactions 2

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. 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**

Sheraton Birmingham Hotel
East Meeting Room L

Photocatalysts and electrocatalysts and electrochemistry methods for clean energy harvesting, conversion, and storage

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. Cliffl**, 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**

Sheraton Birmingham Hotel
East Meeting Room O

Polymer Assemblies: from Fundamental to Applications 2

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. 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.

Sheraton Birmingham Hotel
East Meeting Room B

Small Molecules for the Disruption of Bacterial Processes 2

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

Sheraton Birmingham Hotel
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, *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.

Sheraton Birmingham Hotel
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.

Sheraton Birmingham Hotel
East Meeting Room MH

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. 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. Gordon
- 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. Bacsá, 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 NaLnS₂ (Ln = La, Ce, Pr, Eu, Er, Yb, Lu).
F.I. Danladi

452. Production of ⁵²Mn 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}Sc Radioisotopes via Enriched [^{46,50}Ti]TiO₂. **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. Ferromagnetic Cd_(1-x)Cu_xCr₂S₄ 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 Nanoplatfom 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. Antonyamy

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 ultrasmall superparamagnetic Iron Oxide Nanoparticles-encapsulated Liposomes as a Novel ph-responsive T1-weighted MRI Contrast Agent for Cancer Diagnosis. **S. Rahmati**

Sheraton Birmingham Hotel
East Meeting Room MH

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 Macrocycle 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

Sheraton Birmingham Hotel
East Ballroom B

Plenary

T. P. Hamilton, *Presiding*

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

FRIDAY MORNING

Sheraton Birmingham Hotel
East Meeting Room G

Chemical Education Research in Practice 1

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.

Sheraton Birmingham Hotel
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. 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. 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.

Sheraton Birmingham Hotel
East Meeting Room F

f-Element Chemistry and Applications

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. 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

Sheraton Birmingham Hotel
East Meeting Room D

Frontiers in Organic Synthesis and Catalysis 1

Cosponsored by ORGN
W. Santos, *Presiding*

8:00 Introductory Remarks.

8:05 513. 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**

Sheraton Birmingham Hotel
East Meeting Room O

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

Sheraton Birmingham Hotel
East Meeting Room K

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

W. E. Lynch, *Presiding*

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. Nessell, 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**

Sheraton Birmingham Hotel
East Meeting Room E

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

B. Beckingham, *Presiding*

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*-Diynyl 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.

Sheraton Birmingham Hotel
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**

Sheraton Birmingham Hotel
East Meeting Room J

Women in Chemistry: Advances and Experiences in the Field A

S. 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. 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.

Sheraton Birmingham Hotel
East Meeting Room A

STEM Education in K-12

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. Reaves, 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**

Sheraton Birmingham Hotel
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**

Sheraton Birmingham Hotel
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**

Sheraton Birmingham Hotel
East Meeting Room MH

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

Sheraton Birmingham Hotel
East Meeting Room N

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. Tailoring the Bottom-up Assembly of Surface-anchored Metal Organic Frameworks. **C.D. Fasana**, J.W. Wade, M.E. Anderson

604. Investigating surMOF thin film Growth via Alterations of Self-assembled Monolayers. **J.W. Wade**, C.D. Fasana, M.E. Anderson

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. 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. Whitemore**, 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^{pro}tease*. **R.E. Panella**, M. Donahue, J. Kessl, 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. Bacsá, C.E. MacBeth
- 626.** Developing a Biodegradable Collagen Mimic for Applications in Wound Healing. **A. Tarlton**, S. 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. Monitoring Ivyp1 Active Site Loop Structure and Dynamics using Variable Temperature NMR. **J. Durham**, K. Letsinger, T. Leeper

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

Sheraton Birmingham Hotel
East Meeting Room J

Women in Chemistry: Advances and Experiences in the Field B

S. 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. Dewese, 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

Sheraton Birmingham Hotel
East Meeting Room G

Chemical Education Research in Practice 2

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. Knoeferl, T. McCullough, A. Randolph, C. Terrell, **K.J. Linenberger Cortes**

3:40 Discussion.

4:00 Concluding Remarks.

Sheraton Birmingham Hotel
East Meeting Room N

COMP

Poster session

T. P. Hamilton, *Organizer*

1:00 - 3:00

640. Computational comparison of atmospheric clusters: H₂SO₄-HCOOH-H₂O and H₂SO₄-HNO₃-H₂O. **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 H₂SO₄-NH₃-(H₂O)_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, Quinolinyl, 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.** 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**

Sheraton Birmingham Hotel
East Meeting Room N

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 Cyclopropanone-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**

Sheraton Birmingham Hotel
East Meeting Room O

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. Dimaleimide: 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

Sheraton Birmingham Hotel
East Meeting Room O

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

Sheraton Birmingham Hotel
East Meeting Room J

Women in Chemistry: Advances and Experiences in the Field C

S. 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.

Sheraton Birmingham Hotel
East Meeting Room F

Women in STEM

Undergraduate Discussions: Women in STEM

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.

Sheraton Birmingham Hotel
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. Landge**, 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.

Sheraton Birmingham Hotel
East Meeting Room E

Optoelectronic Materials

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. Enhanced Perovskite Solar Cells Performance by Organic Materials. **Q. Dai**

Sheraton Birmingham Hotel
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.

Sheraton Birmingham Hotel
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**

Sheraton Birmingham Hotel
East Meeting Room K

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

W. E. Lynch, *Presiding*

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. 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

Sheraton Birmingham Hotel
East Meeting Room L

Risk Management in Teaching and Research Settings

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

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.

Sheraton Birmingham Hotel
East Meeting Room J

Intellectual Property Basics

A. Hoehner, *Presiding*

2:30 Introduction.

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

3:25 Discussion and Questions.

Sheraton Birmingham Hotel
East Meeting Room MH

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. Wonnun, 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

Sheraton Birmingham Hotel
East Meeting Room MH

Undergraduate Research 3

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

3:00 - 5:00

785. Systematic Approach to Evaluate Ruthenium-Based Anti-cancer Agents. **S. Robinson**, K. Enkhbold, L. Paul, M.R. Norris, J.A. Pollock

786. 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. 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 Cu²⁺ Contaminants from Various Aqueous Solutions. K. Spalding, **J.L. Hawk**

794. Optimization and Characterization of Phosponium 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.** Using CRISPR-Cas9 to Delete *stk1* 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 (C₂A)₆. **M. Branham**, J.T. Petty
- 807.** DNA-Bound Silver Clusters using Modified Oligonucleotides. **C. Couch**, J.T. Petty
- 808.** 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

Sheraton Birmingham Hotel
East Meeting Room N

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.** Examining the Impact of BHT inhibitor on the Microstructure of Spun-cast Nanoporous Films of PMMA Exhibiting High Surface Areas. **S. Flagg, M.T. Knippenberg, B.H. Augustine**
- 860.** Fabrication of Structures on Surfaces: From the Macro to the Molecular Scale. **P. Perdakis, 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.** Withdrawn

- 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.** Fabrication of Microfluidic Devices Used for Electrophoretic Separations. **A. Wohlwend**, P. Lundin, K. Fogarty
- 866.** Evaluation of Small Molecules as Antibiotic Adjuvants to Combat Vancomycin Intermediate *Staphylococcus aureus* (VISA) and Vancomycin Resistant *Staphylococcus aureus* (VRSA). **A. King**, N. Kirby, A.L. Akers, M.S. Blackledge
- 867.** Time-resolved Protein-protein Interactions of Coronavirus nsp2 Constructs using a Trifunctional Small-molecule Probe. **M. Sullivan**, C. Cameron, L. Plate
- . Synthesis of a Focused Library of Loratadine Analogs and Evaluation of Their Antibiotic Adjuvant Activity in MRSA.. **R. Day**, N.C. Kirby, A. King, R. Ulrich, M.S. Blackledge
- 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. Development and Optimization of microPADs for Iron Detection.. **B. Kokes, A. Holmes,** M.E. Howard

FRIDAY EVENING

Sheraton Birmingham Hotel
East Ballroom B

Plenary

T. P. Hamilton, *Presiding*

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

Sheraton Birmingham Hotel
McWane Science Center

Student Chemistry Chapter Activities During Covid19

Activities Poster Session at the McWane

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**

Sheraton Birmingham Hotel
McWane Science Center

Undergraduate Research 1

Undergraduate Research at the McWane Center

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

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

7:00 885. Developing an Alternative Diagnostic tool for Eosinophilic Esophagitis by Quantification of Modified Tyrosines in Urine Samples. **J. Germany**, M. Thomas, M. Gilliland

7:00 886. Physical Paper Modification for Detection of Antiretrovirals via Paper Spray Ionization Mass Spectrometry. **N. Cheyne**, M. Gilliland

7:00 887. Chemically Patterned Paper Substrates for Paper Spray Mass Spectrometry. **A. Arias**, M. Gilliland

- 7:00 888.** Structural Expansion of a Novel Antibiotic Adjuvant Scaffold to Improve Aqueous Solubility and Biological Activity. **S. Gregory**, A. King, M.S. Blackledge
- 7:00 889.** Method Developmental of High-throughput, Sensitive, Colorimetric Assay for Methanethiol Detection. **Z. Adamson**, C. Miller, M. Culpepper
- 7:00 890.** Presumptive Forensic Test kit Differentiating Hemp and Marijuana. **C.E. LaPointe**, J.O. Boles
- 7:00 891.** Chemical Investigations of Organics in the Chattahoochee River. **H. Carlisle**, K. Goodwin, E. Klar, K.S. Taylor
- 7:00 892.** Optimizing Growth Conditions for the Recombinant Expression of P450 27A1. **J. Bartholomew-Schoch**, M. Reddish
- 7:00 893.** 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
- 7:00 894.** Microfluidics-based Approach to PCDA Liposome Synthesis. **A. Chadwick**, T.W. Hanks
- 7:00 895.** 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**
- 7:00 896.** Naphthalimide-triazole Hybrid pH-sensitive Fluorescent Probe. **A. Powell**, R. Osbourn, D. McCall, E.A. Adogla
- 7:00 897.** Ruthenium-catalyzed Microwave Oxidation of Benzyl Silyl Ethers and Analogues. **R. Peterson**, K. Darrigrand, K. Poythress, A. Cameron, B.C. Goess, S.K. Goforth
- 7:00 898.** Iron Geochemistry at Glendale Shoals. **C. Hatchell**, **M. Santos**, C. Romanek, G. Lewis, G.E. Schwartz
- 7:00 899.** The Impact of Iron Geochemistry on Carbon Degradation at Glendale Shoals. **M. Santos**, **C. Hatchell**, C. Romanek, G. Lewis, G.E. Schwartz
- 7:00 900.** 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

7:00 901. Towards Transdermal Delivery of Thioridazine Double Salt Ionic Liquid Drugs. **C.E. Rust**, O. Cojocar

7:00 902. 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

7:00 903. Computational and Spectroscopic Studies of Nitrogen-containing Multipole-bound Anions. **N. Kruse**, N. Hammer

7:00 904. Infrared Reflection Spectroscopic Studies of UV-ozone Cleaning of Substrates for Self-assembly. **L.B. Spurgeon**, M. Milosevic, B.W. Gregory

7:00 905. Kinetic Characterization of GAPDH from Infectious Microorganisms. **M. Hurd, G. Thrash**, K.L. Hayden, D. Chattopadhyay

7:00 906. 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

Sheraton Birmingham Hotel
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. Antonysamy**

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**

Sheraton Birmingham Hotel
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. 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. Comparison of the Structure and Activity of *Pseudomonas aeruginosa* Proteins, Inhibitors of Vertebrate Lysozyme Classes I and II. **K. Letsinger**, T. Leeper

Sheraton Birmingham Hotel
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.

Sheraton Birmingham Hotel
East Meeting Room B

Engineering Solutions for Social Challenges: Renewable Materials and Resources 1

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 Mudiyansele,** 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. Gómez Maldonado,** A. Reynolds, R.J. Babu, D.J. Burnett, M.N. Waters, M.S. Peresin

Sheraton Birmingham Hotel
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— $[\text{Co}(\text{acac})_x(\text{acac-Cl})_{3-x}]$, $x = 0-3$. **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. Nuggeoda, 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. Siddhicharathi, 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. Vilorio, 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**

Sheraton Birmingham Hotel
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.

Sheraton Birmingham Hotel
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 Bredar, 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

Sheraton Birmingham Hotel
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. 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

Sheraton Birmingham Hotel
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. Directing the Assembly of Surface-anchored MOF-14. **M.E. Anderson**

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**

Sheraton Birmingham Hotel
East Meeting Room F

Synthesis of Fluorescent Probes and Their Applications from Sensing to Imaging

M. Henary, *Presiding*

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.

Sheraton Birmingham Hotel
East Meeting Room N

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. 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.

Sheraton Birmingham Hotel
East Meeting Room MH

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.** 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.** 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.** Computational contributions to the design of new metal-organic framework materials (MOFs) with improved opto-electronic properties. **C. Crawford, D.A. Clabo**
- 1051.** 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.** 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.** 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 sclerotialis* *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.** 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. 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

Sheraton Birmingham Hotel
East Meeting Room I

Physical Chemistry

General Session Physical Chemistry 1

M. G. Bakker, *Presiding*

8:00 Introduction .

8:05 980. Long-lived Ag_{10}^{6+} 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. 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**

Sheraton Birmingham Hotel
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 CuCrO₂. **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 CuGaO₂ 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**

Sheraton Birmingham Hotel
East Meeting Room F

Synthesis of Fluorescent Probes and Their Applications from Sensing to Imaging

2

M. Henary, *Presiding*

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.

Sheraton Birmingham Hotel
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. 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. 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

Sheraton Birmingham Hotel
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.

Sheraton Birmingham Hotel
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. 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. 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

Sheraton Birmingham Hotel
East Meeting Room K

Chemical Education

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.

Sheraton Birmingham Hotel
East Meeting Room B

Engineering Solutions for Social Challenges: Renewable Materials and Resources 2

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.

Sheraton Birmingham Hotel
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.

Sheraton Birmingham Hotel

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**

Sheraton Birmingham Hotel
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

Sheraton Birmingham Hotel
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

Sheraton Birmingham Hotel
East Meeting Room MH

Undergraduate Research 5

J. A. Nikles, *Organizer*

1:30 - 3:30

1164. Exploiting Metallohedged *trans*-Bidentate Ligands for Cross-Coupling Reactions. **B. Nessel**, 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.** 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. Cojocar, 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. Iai, 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.** 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

Sheraton Birmingham Hotel
East Ballroom B

Plenary

T. P. Hamilton, *Presiding*

5:30 1224. A Career in Science: Expect the Unexpected. **L.J. DeLucas**