SERMACS 2021 Technical Program

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

Maps are at the end of the technical program

WEDNESDAY AFTERNOON

Birmingham Jefferson Convention Center
East Exhibit Hall 1

Biochemistry

Poster Session

J. Zhang, Organizer

1:00 - 3:00

2. Investigation of Protein Complexes Involved in the Activation of Methyl-coenzyme m Reductase. S. Yavari


4. Screening of EndoV variants as a tool for mapping A-to-I editing. A. Scott, S. Knutson, A. Quillin, J.M. Heemstra


8. Expression, Purification, and Crystallization of a Putative Monooxygenase Key to Global Sulfur Cycling. **H.C. Frohock**, M. Culpepper, S. Bober


12. Ionic Liquid Loaded Nanoparticles to Deliver drug Candidates to Mammary Carcinomas. **G.S. Dasanayake**


20. Characterization of the substrate binding site for the poly(aspartic acid) hydrolase PahZ2 from Sphingomonas Sp. KT-1. **A. Jansch**, M. Weiland


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


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


31. **Ribonucleotide damage near a replication fork. Enzymatic and structural consequences.** **S.T. Brenden**, R.M. Brosh, M.W. Germann


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


41. Characterization of the Flavin-dependent Tryptophan 7-halogenase (PrnA) from Burkholderia ambifaria. M. Akter, M.R. Uddin, J. Emerson


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

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


48. Surface energy profiling of adhesin proteins. **P. Ayres Galhardo**, M. Phan, A. Brown


50. Exploring Microsphere Suspensions for High throughput detection of label-free RNA. **M.C. Adams**, V.T. Milam


55. Kinetic Mechanism of Translocation of ClpB, an Hsp100 Protein, on Protein Substrates. **J. Banwait**, A.L. Lucius


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


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


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 Withdrawn.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

64. Secondary Amine Selective Petasis 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. Miksovska

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

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

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

70. Recombinant Expression of Methyl-coenzyme M Reductase Reveals the Importance of Accessory Proteins for Proper Assembly. A. Gendron, K. Allen
Birmingham Jefferson Convention Center
East Meeting Room F

Bioinorganic Chemistry

B. S. Pierce, *Presiding*

1:00 Introductory Remarks.

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

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

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

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

R.E. Bachman, K. Wills, K. Barwick, G. Ferrence, K.A. Wheeler

2:45 Intermission.

3:15 76. Connecting Conformational Entropy Changes to Zinc(II) and Copper(II) Binding in Human Carbonic Anhydrase II. 
J. Emerson

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

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

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

**4:55** Concluding Remarks.

Birmingham Jefferson Convention Center  
East Meeting Room A

**Biophysics of Macromolecular Machines**

A. L. Lucius, *Presiding*

**1:00** Introductory Remarks.

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

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

**2:20** Intermission.

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

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

Birmingham Jefferson Convention Center  
East Meeting Room D

**Chemical and Biochemical Approaches to the Investigation of Lipid Membranes**
1:00 Introductory Remarks.


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.
Corinne E. Augelli-Szafran, Presiding

1:00 Introductory Remarks

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


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


3:05 Intermission

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


4:55 Concluding Remarks.

Birmingham Jefferson Convention Center
East Meeting Room L

General Session - Energy and Fuels
S. Pan, Organizer

1:00 Introductions.

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

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

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

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

2:30 Intermission.


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


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


4:40 Concluding Remarks.

Birmingham Jefferson Convention Center
East Meeting Room E
General Session - Environmental Chemistry

Financially supported by Nashville Local Section of the ACS

R. C. Wingfield, Presiding

1:00 Introduction.

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


1:45 111. 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


2:45 114. 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. Scearce, B. Holmes, A. Lee


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


Birmingham Jefferson Convention Center
East Ballroom B

High Performance Computing Applications in Chemistry 1

T. P. Straatsma, Presiding

1:00 Introduction .

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


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


4:15 125. Exploiting Graphical Processing Units (GPUs) to Enable Large-scale Quantum Chemistry of Molecules in Realistic Environments. F. Liu
Birmingham Jefferson Convention Center
East Meeting Room C

N-Heterocyclic Carbenes in Synthesis, Catalysis and Material Science

K. Marichev, Presiding

1:00 Introductory Remarks.


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


3:00 Intermission.


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.
General Session - Polymer Chemistry

V. Thomas, Organizer
D. Lerew, Presiding

1:00 Introduction.

1:10 133. Structure Property Relationships in Imidazolium Ionenes: 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 Ionenes. K. Watson, P. Rupar


2:40 Intermission.

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


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

Birmingham Jefferson Convention Center
East Meeting Room B

Single Molecule Approaches to Chemistry and Biology

K. Welsher, Presiding

1:00 Introductions.

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

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

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

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

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

2:55 Intermission.


3:50 151. 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


Birmingham Jefferson Convention Center
East Exhibition Hall 1

Analytical Chemistry

Poster session

A. Ghosh, S. Pan, Organizers

3:00 - 5:00


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

161. Label-free discrete frequency infrared imaging of beta sheet aggregates in Alzheimer’s Disease. **T.B. Maupin**


163. Withdrawn. Authenticating Aspirin Brands Through LC-MS/MS. **W. Than**


165. Withdrawn. Transferring Solid Phase Elution Methods from TomTec Quadra 4 SPE to Zephyr G3 SPE Workstation: Applications in HPLC. **S. Fisher**, L. Nguyen, C. Green, J. LaPalme, E. Bair, N. Epie


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


171. Interfacial Interaction Between cellulose nanofibrils (CNFs) and Fipronil. **S.W. Freij**, M.C. Iglesias, T. Ciaramitaro, M.S. Peresin

**WEDNESDAY EVENING**
Plenary

D. A. Dixon, *Presiding*

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

**THURSDAY MORNING**

Birmingham Jefferson Convention Center
East Meeting Room I

Contemporary Fluorine Chemistry in the Southeast 1

Cosponsored by FLUO
D. A. Dixon, T. Lectka, *Presiding*

8:00 Introductory Remarks.

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


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.


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


Birmingham Jefferson Convention Center
East Meeting Room E

**Frontiers in Nucleic Acids**

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

8:00 Introduction.


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**


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

11:15 Concluding Remarks.

Birmingham Jefferson Convention Center
East Ballroom B

High Performance Computing Applications in Chemistry 2

T. P. Straatsma, Presiding

8:00 Introduction.

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

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

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

9:55 Intermission.

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


Birmingham Jefferson Convention Center
East Meeting Room J

Inorganic Electron Transfer Reactions for Energy Storage

Financially supported by Cell Reports Physical Sciences

B. H. Farnum, Presiding

8:00 Introductory Remarks.

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

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


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

9:45 Intermission.

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


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


Birmingham Jefferson Convention Center
East Meeting Room G

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

Financially supported by **Mississippi State University**

A. L. Patrick, *Presiding*

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**8:00 Introductory Remarks.**


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


11:55 Concluding Remarks.

Birmingham Jefferson Convention Center
East Meeting Room A

New Directions in Metal-Catalyzed Reactions 1

Financially supported by Organic Reactions, Biocryst, VWR

K. H. Shaughnessy, Presiding

8:00 Introductory Remarks.

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


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

9:35 Intermission.


11:20 216. Pincer Ligand Cobalt Chromophores for Selective Radical Triflouro methylations. J.D. Soper

Birmingham Jefferson Convention Center
East Meeting Room L

Electrocatalysts and Solar Cell For Clean Energy Conversion Part 1

S. Pan, Presiding

8:00 Introduction.

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

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

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

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


9:50 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


Birmingham Jefferson Convention Center
East Meeting Room O

**Polymer Assemblies: from Fundamental to Applications 1**

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

8:00 Introductory Remarks.

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

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

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


9:45 Intermission.
10:00 231. Polymer Salogels for Shape Stabilization of Inorganic Phase Change Materials. S.A. Sukhishvili, X. Zhu, K. Rajagopalan


Birmingham Jefferson Convention Center
East Meeting Room B

Small Molecules for the Disruption of Bacterial Processes 1

Financially supported by Clemson University

D. C. Whitehead, Presiding

8:00 Introductory Remarks.

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

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

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

9:55 Intermission.

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

10:45 240. Disruption of Salmonella Biofilms In Vitro and In Vivo. C. Melander
11:20 241. Plant Natural Products as a Resource for Antibiotic Drug Discovery. C. Quave

Birmingham Jefferson Convention Center
East Meeting Room D

Structure-Property-Function Relationships in Polymers

C. Zhao, Presiding

8:00 Introduction.

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


9:40 Intermission.


Birmingham Jefferson Convention Center
East Meeting Room K

Supramolecular and Biomolecular Chemistry

Financially supported by the Louisiana Local Section of the ACS and the Tulane Chemistry Department
J. Jayawickramarajah, Presiding

8:00 Introductory Remarks.


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


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


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


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

The Magic of Spectroscopy

Financially supported by ACS Division of Physical Chemistry, ThermoFisher Scientific

A. Gunn, *Presiding*

**8:00** Introductory Remarks.


**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*


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


9:50 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


11:55 Concluding Remarks.

THURSDAY AFTERNOON

Birmingham Jefferson Convention Center
East Exhibit Hall 1

Environmental

Poster Session

R. C. Wingfield, Organizer
12:30 - 2:30


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


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


Birmingham Jefferson Convention Center
East Exhibit Hall 1

**Organic**

**Poster Session**

L. Yet, *Organizer*

12:30 - 2:30

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


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


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


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 (±)–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**


308. Synthesis of 6-(4-fluoro)-3,4-diphenylpyridazine. T. Mallett, J. Philp, A. Williams, C. Williams, V. Sittaramane, S.M. Landge


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


318. Stereoselective Synthesis of \( \alpha \)–Allyl–\( \alpha \)–Trialkylsilyl–\( \gamma \)–Alkyl–\( \beta,\gamma \)–Unsaturated Carboxylic Acids via an Ireland–Claisen rearrangement. C. Massey

319. Epoxidation and Ring Opening of \( \alpha \)-Trimethylsilyl–\( \beta,\gamma \)-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


325. Donor-acceptor-donor NIR Xanthene-based Dye for Photoacoustic Imaging. C. Rathnamalala, N.W. Pino, C.N. Scott


327. Aluminum-catalyzed Intermolecular mono- and bis-hydroalkoxylation of Allenamides with Alcohols. K. Alam, T. Li, M.P. Croatt


336. Withdrawn. The Synthesis and Biocatalytic Reduction of Beta-keto Alkynes. R.M. Francis, B.D. Feske

1119. Towards the Synthesis of Ambuic Acid & Analogues A. Ustoyev

Birmingham Jefferson Convention Center
East Meeting Room K

Centennial of the Discovery of Insulin

D. Rabinovich, Presiding

1:00 Introduction.
1:10 337. Insulin 100: A Brief Philatelic History. D. Rabinovich

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

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

2:40 Closing Remarks.

Birmingham Jefferson Convention Center
East Meeting Room F

The Magic of Spectroscopy 2

Financially supported by ACS Division of Physical Chemistry, ThermoFisher Scientific

A. Gunn, Presiding

1:00 Introduction .

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


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. Jiménez

4:25 345. Hydrogen Binding and Dissociation in Metal Hydride Clusters. J.T. Lyon
4:50 Concluding Remarks.

Birmingham Jefferson Convention Center
East Ballroom B

Theoretical chemistry: Method development and applications 1

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

1:00 Introduction.

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

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

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

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

2:45 Intermission.

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

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

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

Birmingham Jefferson Convention Center
East Meeting Room C

Methods and strategies for modern organic synthesis

Financi ally supported by Oakwood Chemical, VWR, Auburn University

M. Chen, R. Karimov, Presiding

1:15 Introductory Remarks.

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

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

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

2:55 Intermission.

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

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

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

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

Birmingham Jefferson Convention Center
East Meeting Room J
Small molecule activation at biological or bio-inspired metal centers

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

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

1:15 Introductory Remarks.


1:45 362. 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


3:20 Intermission.


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


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

Birmingham Jefferson Convention Center
East Meeting Room E

Spatially resolved spectroscopy: Applications in Biomedical and Materials Imaging

A. Ghosh, Presiding

1:15 Introduction.


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


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

Birmingham Jefferson Convention Center
East Meeting Room I

Contemporary Fluorine Chemistry in the Southeast 2

Cosponsored by FLUO
M. Etzkorn, Presiding

1:30 Introduction.

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


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

3:05 Concluding Remarks.

Design, Chemistry, and Application of Active, Functional Materials

A. Koh, Presiding

1:30 Introductory Remarks.


2:55 Intermission.


4:05 Intermission.


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

Birmingham Jefferson Convention Center
East Meeting Room G

**Ground truth: bridging knowledge gaps between computational and experimental enzymology**

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

N. J. DeYonker, *Presiding*

1:30 Introductory Remarks.


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\textsuperscript{pro} Antiviral drug development. S. Stoddard

3:10 Intermission.


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

Birmingham Jefferson Convention Center
East Meeting Room A

**New Directions in Metal-Catalyzed Reactions 2**

Financially supported by Organic Reactions, Biocryst, VWR

X. Cui, *Presiding*

1:30 Introduction.

1:35 396. Electronic Structure of RhO\textsuperscript{2+}, Its Ammoniated Complexes (NH\textsubscript{3})\textsubscript{1-5}RhO\textsuperscript{2+}, and Mechanistic Exploration of CH\textsubscript{4} Activation by Them. N. Khan, E. Miliordos
2:05 397. Development of a Ni-catalyzed Larock Annulation. D. Wilger


3:05 Intermission.


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

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

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

Birmingham Jefferson Convention Center
East Meeting Room L

Electrocatalysts, Solar cell and Electrochemical methods part 2

S. Pan, Presiding

1:30 Introduction.


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


3:20 Intermission.

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


Birmingham Jefferson Convention Center
East Meeting Room O

**Polymer Assemblies: from Fundamental to Applications 2**

Financially supported by the National Science Foundation

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

1:30 Introduction.


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**


3:05 Intermission.


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


4:30 Concluding Remarks.

Birmingham Jefferson Convention Center  
East Meeting Room B

**Small Molecules for the Disruption of Bacterial Processes 2**

Financially supported by Clemson University

D. C. Whitehead, *Presiding*

1:30 Introductory Remarks.

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.


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


Birmingham Jefferson Convention Center
East Meeting Room N

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

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

2:30 Introduction.

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

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

3:30 427. A Cuban Campesino in Chemistry’s Academic Court. R. Hernandez
3:55 428. DEIR in Teaching and Research: Some personal Experiences, Challenges, and Opportunities. D. Rabinovich

4:20 Panel Discussion.

Birmingham Jefferson Convention Center
East Meeting Room K

Chemical Education

The Plant Hunter

C. Quave, Organizer

3:00 Introduction.


4:00 Discussion and Questions.

Birmingham Jefferson Convention Center
East Exhibit Hall 1

Inorganic

Poster session

J. E. Ritchie, Organizer

3:00 - 5:00

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

432. Gas-phase Oxidative Coupling of Alcohols and Amines over Bimetallic Solid Catalysts. A. Minne, J.W. Harris


435. One-electron Oxidation of Methanesulfinic Acid (MSA) by Hexachloroiridate(IV). Y. Yang


438. Pyrrophens and Pyrropyridines: Hexadentate Coordination systems for Uranyl UO$_2^{2+}$. J. Ducilon, A.E. Gorden

439. Syntheses and Characterization of Valence Tautomeric Cobalt Complexes with Magnetic Transition at Room Temperature. P. Wang, M. Shatruk


442. Synthesis and Metalation of Two Redox-active Ligands Functionalized with a Terminal Alkyne for Applications in Flow Chemistry. A. Yu, J. Bacsa, C.E. MacBeth

443. Magnetic Structure of Chain Antiferromagnets MBi$_4$S$_7$ (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


449. To activate or not to activate? Experimental and computational studies of small molecule activation by copper- and zinc-based frustrated Lewis pairs. K. Bledsoe, L.K. Bennett, K.M. Clark

450. Dimethyl zinc complexes supported by TBAM ligands: Exploration of ligand exchange thermodynamics and the mechanism of protonolysis. L.K. Bennett, K.M. Clark

451. Magnetic and optical properties of NaLnS$_2$ (Ln = La, Ce, Pr, Eu, Er, Yb, Lu). F.I. Danladi


455. Effect of Tethered, Axially Coordinated Ligands (TACLs) on Rh(II)-Catalyzed Cyclopropanation: A Linear Free Energy Relationship Study. C. Zavala, A. Darko


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


460. Dynamically and Statically Tailoring the Properties of Metal-Organic Frameworks. C.R. Martin, N.B. Shustova

461. A Novel Magnetic Drug Screening Nanoplatform Based on Immobilized Transmembrane Proteins on Magnetic Superparticles. S. Mansur, J. Horne, S.E. Velu, Y. Bao


463. Unprecedented Ag Doping and the Crystal Structure of Au_{30-x}Ag_x(S-tBu)_{18}. K.H. Wijesinghe, N. Sakthivel, T.C. Jones, A. Antonysamy

464. Short-range Ordered 2D Phases and their Electronic Properties in Nb_xV_{1-x}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


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

Birmingham Jefferson Convention Center
East Exhibit Hall 1
Multidentate Ligands in Inorganic Chemistry

Poster session

W. E. Lynch, Organizer

3:00 - 5:00

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


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


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


THURSDAY EVENING

Birmingham Jefferson Convention Center
East Ballroom B

Plenary

D. A. Dixon, Presiding

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

Birmingham Jefferson Convention Center
East Meeting Room G

Research in Practice 1

Financially supported by Wilson Dam Local Section of the ACS

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

8:00 Introductory Remarks.

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

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

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

9:05 Intermission.

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

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

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

10:20 493. “I Felt Like I was Losing Like, an Hour of my Time”: Examining the
Experiences of Pregnant and/or Parenting Women in STEM Doctoral Programs. C.
Wright
10:40 Discussion.

11:00 Concluding Remarks.

Birmingham Jefferson Convention Center
East Meeting Room I

**Classroom Chemistry: Innovations in Practice**

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

8:00 Introductory Remarks.

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

8:35 **495.** Psi4Education: Free and Open-Source Programing 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. Yezierski

9:40 Intermission.

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

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

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

11:20 Concluding Remarks.

Birmingham Jefferson Convention Center  
East Meeting Room F

**f-Element Chemistry and Applications**

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

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

8:00 Introduction.


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


10:05 Intermission.


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**


Birmingham Jefferson Convention Center
East Meeting Room D

**Frontiers in Organic Synthesis and Catalysis 1**

Cosponsored by ORGN
W. Santos, *Presiding*

8:00 Introductory Remarks.


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

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

9:15 516. Heterogeneous acid- and base-catalyzed Conversion of Unprotected Aldose Sugars to Furan Derivatives via the Garcia Gonzalez Reaction. **S.A. France**
9:40 Intermission.

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

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

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

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

Birmingham Jefferson Convention Center
East Meeting Room L

Main Group Chemistry and Inorganic Materials

P. Rupar, Presiding

8:00 Introductory Remarks.

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


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. Rupar

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

10:05 Intermission.


Birmingham Jefferson Convention Center
East Meeting Room K

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

W. E. Lynch, Presiding

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

8:00 Introductory Remarks.

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

8:55 534. 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**


9:45 Intermission.


10:30 537. New hydroxy substituted Salen-type Pd and Pt complexes: Spectroscopical properties, Structural characterization, DFT calculations, and CO$_2$ reduction. **D.M. Pinero Cruz**, J.O. Rivera


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

Birmingham Jefferson Convention Center
East Meeting Room E

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

B. Beckingham, *Presiding*

Financially supported by Polymers

8:00 Introductory Remarks.
8:05 540. Tethered Electrolyte Active-layer Membranes (TEAMs): Expanding the Avenues for Polyelectrolyte Membranes. **C. Porter**, R. DuChanois, E. MacDonald, S. Kilpatrick, M. Zhong, M. Elimelech

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

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

9:20 Intermission.

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


10:45 Intermission.


11:40 Concluding Remarks.

Birmingham Jefferson Convention Center
East Ballroom B

**Theoretical chemistry: Method development and applications 2**
Financially supported by Auburn University
E. Miliordos, Organizer
K. D. Vogiatzis, Presiding

8:00 Introduction.

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

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


9:45 Intermission.

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


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


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

Birmingham Jefferson Convention Center
East Meeting Room J

Women in Chemistry: Advances and Experiences in the Field A
Financially supported by ACS Women Chemists Committee

S. K. Hamilton, Organizer
X. Jiang, Presiding

8:00 Introduction.

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

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

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

9:35 Panel Discussion.

Birmingham Jefferson Convention Center
East Meeting Room A

STEM Education in K-12

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

STEM K-12 1

E. Menard, C. Willingham, Organizers

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

10:00 Intermission.

11:10 Intermission.

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

1:40 Intermission.

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

2:50 Intermission.

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

Birmingham Jefferson Convention Center
East Meeting Room B

**STEM Education in K-12**

**STEM K-12 2**

E. Menard, C. Willingham, *Organizers*

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

10:00 Intermission.

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

11:10 Intermission.

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

1:40 Intermission.
1:50 568. Proportional Reasoning to Describe (Qualitatively and Quantitatively) gas Behavior using Modeling Instruction. C. Manor

2:50 Intermission.

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

Birmingham Jefferson Convention Center
East Meeting Room C

STEM Education in K-12

STEM K-12 3

E. Menard, C. Willingham, Organizers

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

10:00 Intermission.

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

11:10 Intermission.

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

1:40 Intermission.

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

2:50 Intermission.

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

Birmingham Jefferson Convention Center
East Exhibit Hall 1
Energy and Fuels

10:00 - 12:00

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


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


Birmingham Jefferson Convention Center
East Exhibition Hall 1

Undergraduate Research 2

Poster Session Undergraduate Research 2

J. A. Nikles, Organizer

10:00 - 12:00


585. Expression and Characterization of Lanthipeptide Components from the Marine Bacteria Salinispora arenicola. A. Deen Sesay, D. Ellis, E. Limbrick


596. Quantification of Heavy Metals in Commercial Tuna. M. McCormack, J.D. Leyba


598. One-pot Synthesis of Furans from 3-(trimethylsilyl)propargyl Carboxylates. A.V. Helbling, D. Sklar, C.W. Downey


601. Synthesis of 2,3-Dihydroisoxazoles from Ketones and N-benzyl Nitrones. R.M. Goodner, C.W. Downey


603. Withdrawn

604. Withdrawn


606. Correlating the Regioselectivity of Bromohydrin Formation from Unsymmetrical Alkenes with Bromonium ion C-Br Bond Lengths. N. Johansen, B. Tutkowski


609. Ampicillin-induced Biophysical Changes of *Escherichia coli* Cells Over Multiple Generations. **A. Carranza-Parras, K. Dungey**


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**


615. Colorimetric and Fluorometric Dual Sensor for the Detection of Copper and Aluminum Ions. **A. Foret, E. Fasusi, S. Westervelt, D. Ghosh**


619. Preparation and Analysis of Vanadium–Amoxicillin Complexes. **R. Overend, J.A. Dabrowski**

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

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

**Selenium heterocycles and the enzymatic inhibition of SARS-CoV-2’s Mprotease.**
**R.E. Panella**, M. Donahue, J. Kessl, F. Bai

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

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

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


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

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


Birmingham Jefferson Convention Center
East Meeting Room J

**Women in Chemistry: Advances and Experiences in the Field B**

Financially supported by **ACS Women Chemists Committee**

S. K. Hamilton, **Organizer**
J. M. Murphy, **Presiding**
10:00 Introduction.


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

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

11:40 Panel Discussion.

FRIDAY AFTERNOON

Birmingham Jefferson Convention Center
East Meeting Room G

Research in Practice 2

Financially supported by Wilson Dam Local Section of the ACS

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

1:00 Introductory Remarks.

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


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

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.

Birmingham Jefferson Convention Center
East Exhibition Hall 1

**COMP**

**Poster session**

T. P. Hamilton, **Organizer**

1:00 - 3:00

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

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

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

**643.** Computational Study of Hydrated H$_2$SO$_4$-NH$_3$-(H2O)$_n$ Clusters. **V. Fowler**, T. Odbadrakh, 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


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


650. \( \sigma \)-Hole Flexibility in Chalcogen Bond Donors. K.A. French, T.L. Ellington, K.L. Shuford


652. QM/MM studies of Xanthine Oxidase Inhibitors. Y. Maghsoud, C. Dong, G.A. Cisneros


Birmingham Jefferson Convention Center
East Exhibition Hall 1

Physical Chemistry

Poster session

T. P. Hamilton, Organizer

1:00 - 3:00

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

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

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


668. QM-cluster Modeling of Chorismate Mutase Based on Sampling MD Simulation. D.A. Agbaglo, T.J. Summers, Q. Cheng, N.J. DeYonker


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


674. Pro-drug Encapsulation by Cyclodextrin in a Model Biomimetic System. S.E. Westervelt, K.S. Aiken, S.M. Landge, D. Ghosh


676. The Ideal Gas Thermodynamic Properties of PtC. L. Biolsi

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**


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**


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

Birmingham Jefferson Convention Center
East Exhibition Hall 1

**Polymer Chemistry**

**Poster session**

V. Thomas, *Organizer*

**1:00 - 3:00**

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

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 Ionenes in Ionic Liquids using Dynamic Light Scattering. C. Patton, J.E. Bara, K.E. O'Harra, G. Thompson


695. General Access to Allene-containing Polymers using the Skattebøl Rearrangement. N. Galan, J.N. Brantley


Birmingham Jefferson Convention Center
East Exhibition Hall 1

Polymer Materials Science and Engineering

Poster session
V. Thomas, Organizer

1:00 - 3:00


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


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


707. Electrospinning Parameters and Chemical Additives in Fabricating PVA Electrospray 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**


713. Effect of Nanoparticle Size on Internalization and Transport Across the Corneal Barrier. **M. Azadi**, A.E. David


Birmingham Jefferson Convention Center
East Meeting Room J

**Women in Chemistry: Advances and Experiences in the Field**

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

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

**1:00** Introduction.

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

**1:35 716.** Equity in Parental Leave? or You Have a Baby...In a Pandemic!. **S. Zingales**
2:05 717. Changing the Academic Culture as a Woman in STEM. J.L. Brumaghim

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


3:05 Panel Discussion.

3:35 Concluding Remarks.

Birmingham Jefferson Convention Center
East Meeting Room F

Women in STEM

Undergraduate Discussions: Women in STEM

Financially supported by UAB Department of Chemistry, UAB Educational Foundation

J. M. Meyers, Presiding

1:00 Introduction.

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

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

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

2:25 Intermission.

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

3:05 724. Biomolecules do amazing things and I get to work with amazing people. J.M. Heemstra
3:30 Panel Discussion.

Birmingham Jefferson Convention Center
East Meeting Room I

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

M. S. Reeves, Presiding

1:15 Introductory Remarks.


1:45 726. 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


3:00 Intermission.

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

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

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

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

4:55 Concluding Remarks.
Birmingham Jefferson Convention Center  
East Meeting Room E  

**Optoelectronic Materials**  
Financially supported by Mississippi EPSCoR  
C. N. Scott, *Presiding*  

1:15 Introduction.  


1:45 **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*  


2:45 Intermission.  

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


4:10 Intermission.


Birmingham Jefferson Convention Center
East Ballroom B

**Theoretical chemistry: Method development and applications 3**

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

1:15 Introduction.


3:00 Intermission.

3:50 749. Electronic spectroscopy of the \(^1\)A\(^e\)\(-\)X transitions of jet-cooled calcium methoxide (CaOCH\(_3\)) and calcium ethoxide (CaOC\(_2\)H\(_5\)) 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


4:50 Concluding Remarks.

Birmingham Jefferson Convention Center
East Meeting Room D

Frontiers in Organic Synthesis and Catalysis 2

Cosponsored by ORGN
W. Santos, Presiding

1:30 Introduction.

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

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


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

3:10 Intermission.


3:50 757. Carbohydrate Derived Macrocycles in Catalysis. G. Wang
Forging Dissonant Functional Group Pairs through Cu-catalyzed
Asymmetric Reductive Coupling Reactions of N-Substituted Allenes. J.D. Sieber

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

Birmingham Jefferson Convention Center
East Meeting Room K

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

W. E. Lynch, Presiding

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

1:30 Introduction .

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

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

2:25 762. Copper-based Redox Shuttles Featuring Preorganized Polydentate Ligands

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

3:15 Intermission.

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


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

Birmingham Jefferson Convention Center
East Meeting Room L

Risk Management in Teaching and Research Settings

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

Financially supported by ACS Division of Chemical Health & Safety

1:30 Introductory Remarks.

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

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


3:05 Intermission.

3:20 Discussion.

4:05 Concluding Remarks.
Birmingham Jefferson Convention Center  
East Meeting Room M

**Intellectual Property Basics**

A. Hoeher, *Presiding*

2:30 Introduction.


3:15 Discussion and Questions.

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Birmingham Jefferson Convention Center  
East Exhibit Hall 1

**Chemical Education**

**Poster Session**

3:00 - 5:00

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

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

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

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

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


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

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

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

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

Birmingham Jefferson Convention Center
East Exhibit Hall 1

Undergraduate Research 3

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

3:00 - 5:00

786. Withdrawn. Expression, Purification, and Assay Development to Study STK1, a Kinase Implicated in Antibiotic Resistance. M. Callender, M.S. Blackledge, H.B. Miller, J.A. Pollock


792. Removal of Cobalt(II) Aqueous Ions via Hydrogel Formation of Sodium Alginate in Synthetic Waters of Varying Harnesses. P.N. Smith, J.L. Hawk

793. Using Sodium Alginate Hydrogels to Remove Cu^{2+} Contaminants from Various Aqueous Solutions. K. Spalding, J.L. Hawk

794. Optimization and Characterization of Phosphonium Salts. B. Wicker, M.B. Miller


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


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


809. Effect of CMPO Ligand Scaffold Variation on Lanthanide Extraction and Luminescence Properties. B. Lake, W. Larrinaga, S.M. Biros, E.J. Werner


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
Efforts Towards the Design and Synthesis of a New Aminotroponiminate Supported Zinc Complex for Hydroamination. E.J. DiBlasio, R.J. Harris


Computational Study of the Structure, Vibrational Spectra, and Hydrogen Bonding of $\text{H}_2\text{O}_2^+$ and its Methylated Derivatives. S. Sprouse, D. Herbert, B. Freeman, M. Kaledin

Synthesis of Hyperbranched Polymers via Metal-free Self-condensing ring-opening metathesis polymerization. G. Dinges, M.D. Schulz, H. Almuzaini

Development of a Protecting Group Scheme for the Synthesis of Modified Deep-Cavity Cavitands. T. Nsubuga, M. Meadows

Optimization of Synthesis and Spectroscopic Analysis of Vanadium–tetracycline Complexes. S. Eastman

Effects of Pdr1 Phosphorylation Variants on Azole Resistance in *Saccharomyces cerevisiae*. C.S. Burdette, M.E. Breen

Mapping Pho85-Pho80 Phosphosites in the *Saccharomyces Cerevisiae* transcription factor Pdr1. R.E. Singer, M.E. Breen

Investigation of the Phosphorylation Status of the *Candida Glabrata* Pdr1 Transcription Factor. J.R. McCallum, M.E. Breen

Detection of Nicotine Vapor through Photoacoustic Spectroscopy. B. Freeman, H. Park

Development of Field Test for Identification of Cocaine with TLC. E. Schrider, J.O. Boles

Predicting Protein Function in *Pythium Insidiosum* using Computational Techniques. R.H. Gray, S. Johnson

Anion Effect on Octaethyltetrphenylporphyrin Protonation. M. Swanson, M. Ballester, V. Castro


836. Hofmeister Anion Interactions with Coumarin. **O. Mumma**, Y. Zhang


838. Investigation of Quinolines as HIV-integrase Inhibitors. **J. Patterson**, M. Donahue


842. Investigation of Pomalidomide-Derived Halo PROTAC 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


Birmingham Jefferson Convention Center
East Ballroom A

Undergraduate Research 4

J. A. Nikles, Organizer

3:15 - 5:15


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
Towards the Synthesis of a Simple Alkyl-substituted meta-poly(arylene ethynylene). **C. Bontempo, J. Faircloth, P. Lundin**


Facile Chitosan Isolation for Heavy Metal Remediation. **R. Tikkala, B. Corbett**

Investigating the C–H Arylation of Furan using a Carbazole Derivative as a Photocatalyst. **K. Ribeiro, A.R. Longstreet**

A Carbazole Derivative as a Photocatalyst in the C–H Arylation of N-Methylpyrrole. **N.A. Reece, A.R. Longstreet**

Storage of Carbon Dioxide in Basalt: An In-Depth Study of the Reaction Kinetics and Products of Enstatite Carbonation. **L.J. Hardee, B. Aguila**

Experimental analysis of double-stranded DNA cleavers on bacterial cells. **T. Fraley, J. Heath, W. Yang**

Small molecules stabilizing the secondary structure of CCG repeat expansion. **L. Wise, W. Yang**

Effect of Initiator Structure on Poly(3-hexylthiophene) Polymerization and Aggregation Properties. **O.J. Armendarez, P. Lundin**


Fabrication of Structures on Surfaces: From the Macro to the Molecular Scale. **P. Perdikis, B.H. Augustine**


Evaluation of Polymer Surface Modification as an Inhibitor of Methicillin-resistant Staphylococcus aureus (MRSA) Biofilm Formation **M. Mauer, A. L. Akers, A. Copeland, M. S. Blackledge, P. Lundin**
863. Determination of Metal Binding Specificity and Stoichiometry to a Monooxygenase Involved in Sulfur Cycling. K. Zammit, Z. Adamson, M. Culpepper

864. Comparing Correlation Energy Approximations Derived from TDDFT within the Asymmetric Hubbard Dimer. L. Everhart, J.E. Bates

865. Withdrawn. Fabrication of Microfluidic Devices Used for Electrophoretic Separations. A. Wohlwend, P. Lundin, K. Fogarty

866. Withdrawn

867. Time-resolved Protein-protein Interactions of Coronavirus nsp2 Constructs using a Trifunctional Small-molecule Probe. M. Sullivan, C. Cameron, L. Plate


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


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


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

FRIDAY EVENING

Birmingham Jefferson Convention Center
East Ballroom B

Plenary

A. E. Gorden, Presiding

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

McWane Science Center

Student Chemistry Chapter Activities During Covid19 Poster Session at the McWane

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

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

7:00 - 9:00

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

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


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

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

McWane Science Center

Undergraduate Research 1

Undergraduate Research at the McWane Center

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

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

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

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


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

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

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


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**


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

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


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


SATURDAY MORNING

Birmingham Jefferson Convention Center
East Meeting Room G

Analytical Chemistry

Advanced materials and Surfaces for Analytical Chemistry

A. Ghosh, *Presiding*

8:00 Introduction.

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

8:30 908. Transparent Ultramicroelectrodes for Studying Interfacial Charge Transfer Kinetics of Photoelectrochemical Water Oxidation at TiO$_2$ Nanorods with Scanning Electrochemical Microscopy. **X. Li**, S. Pan


9:30 Intermission.

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


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

Birmingham Jefferson Convention Center
East Meeting Room O

Biochemistry

General Session Biochemistry 1

J. Zhang, Presiding

8:00 Introduction.


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

9:05 918. Utilizing Multi-scale Simulation to Reveal Mechanisms of Molecular Motors’ Motility. L. Li
9:25 Intermission.


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


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

Birmingham Jefferson Convention Center
East Meeting Room K

Chemical Education Oral Presentations 1

J. March, Organizer

8:00 Introduction.

8:10 926. Teaching Design of Experiments for Method Development in Analytical Chemistry. R. Thompson, R. Saylor
8:30 927. Supporting the Motivation of Engineering Students with Design Challenges in General Chemistry Laboratory. M. Korolev, K. Crippen, L. Imperial, C. Payne, B. Phil, C. Wu

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

9:10 Intermission.

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

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

10:10 Concluding Remarks.

Birmingham Jefferson Convention Center
East Meeting Room B

Engineering Solutions for Social Challenges: Renewable Materials and Resources 1

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

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

8:00 Introductory Remarks.

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


9:55 Intermission.

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


Birmingham Jefferson Convention Center
East Meeting Room J

**Inorganic**

**General Session Inorganic 1 - Ligands and Metals in Catalysis**

J. E. Ritchie, *Presiding*

8:00 Introduction.

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

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


9:40 Intermission.

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


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


Birmingham Jefferson Convention Center
East Ballroom B

Machine Learning in Computational Chemistry

S. Irle, Presiding

8:00 Introduction.

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

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

9:20 Intermission.


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


11:30 Panel Discussion.

Birmingham Jefferson Convention Center
East Meeting Room A

Nanomaterials 1

S. Street, *Presiding*

8:00 Introduction .


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

9:30 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


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


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

Birmingham Jefferson Convention Center
East Meeting Room E

Organic

Natural Products/Biological Applications of Organic Synthesis/Heterocycles

L. Yet, Organizer

8:00 Introduction .

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


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


9:50 Intermission.


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


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**

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

Birmingham Jefferson Convention Center
East Meeting Room I

Physical Chemistry

General Session Physical Chemistry 1

M. G. Bakker, Presiding

8:00 Introduction .

8:05 980. Long-lived 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


10:05 Intermission.


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

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

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

Birmingham Jefferson Convention Center
East Meeting Room C

Polymer Materials Science and Engineering

General Session Polymer Materials 1 - Polymeric materials and composites

D. Dean, Presiding

8:00 Introduction.

8:00 991. Withdrawn.


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

9:15 Intermission.


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

Birmingham Jefferson Convention Center
East Meeting Room F

**Synthesis of Fluorescent Probes and Their Applications from Sensing to Imaging**

M. Henary, *Presiding*

Financially supported by Molecules, De Gruyter

8:00 Introductory Remarks.

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

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

9:40 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


11:20 Concluding Remarks.

Birmingham Jefferson Convention Center
East Meeting Room D

Project SEED

A. Mallia, D. Masterson, Presiding

8:30 Introductory Remarks.

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

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


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

10:45 Panel Discussion.

11:45 Concluding Remarks.

Birmingham Jefferson Convention Center
East Exhibit Hall 1

Undergraduate Research 1

Poster Session

J. A. Nikles, Organizer

10:00 - 12:00


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


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
Analysis of Different Types of Alcohol using gas Chromatography. A.C. Gaquere, **A. Cormier**, A. Watson

Theoretical Studies of Benzoquinone Reactivity in Acidic and Basic Environments. **N. Majoras**

Role of the Cation in Ionic Liquid-Facilitated Transdermal Transport. **A.N. Hunter**, E.E. Tanner

Synthesis of Nano Carbon Microspheres (nCMS) from Natural Materials for the Removal of Water Pollutants. **E. Banks**, M.M. Moyer


Improved LC-MS Methodology for Determination of Endocrine-disrupting Chemicals (EDCs) in Southwest Florida Waterways. **M. Sciancalepore**, D. Paull, N. Demers


Incorporating a Collagen Analog and a Bioengineered Protein into Modern Wound Dressings. **J. Spiva**, S.K. Hamilton

Towards the Study of Flow and Mass Transport of Species in a Two-phase Flow Inside a Microreactor using Computational Fluid Dynamics. **O. Ayeni**


Regioselective Asymmetric Akynylation and Arylation of Pyridiniums. **A. Subhit**, T.A. Grigolo

Optimizing Rhodamine B Encapsulation in ZIF-8 Metal Organic Frameworks. **E. Stravolo**


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


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


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


1048. Designing an undergraduate forensic chemistry experiment on the levels of amphetamine in urine using two different methods. M. Teigen, M. Popkin, W. Medawala

1049. Developing a Synthetic Strategy Toward β-ketoalkynes. K. Glorioso, R. Francis, B.D. Feske

1050. Withdrawn. Computational contributions to the design of new metal-organic framework materials (MOFs) with improved opto-electronic properties. C. Crawford, D.A. Clabo


1055. Investigation of Ni(£lPDI)²⁺ as a Catalyst for Light-driven Hydrogen Production. R.G. Musicante, L.M. Rhodes, W.T. Eckenhoff


1058. Using Extended DLVO Theory to Characterize Primary Colonization of Bacteria. N. Pathak, T.B. Cavitt


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. Cojocaru, T.W. Majors


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


1066. Withdrawn. Uncovering Determinants of Temperature Specificity in Extremophilic Bacterial Type II Topoisomerases. A. Schoeffler, T. Littleton, A. Byrd

1067. Design and Synthesis of Fluoroquinolone Conjugates as Potential Antimicrobial Agents. A. Rocque, S.S. Panda

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

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

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

SATURDAY AFTERNOON

Birmingham Jefferson Convention Center
East Meeting Room J

**Inorganic**

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

J. E. Ritchie, *Presiding*

1:00 Introduction.


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

1:35 1074. Physical and Electrochemical Properties of Synthetically Optimized p-type CuCrO$_2$. **A. Chown, B.H. Farnum**

1:50 1075. Fabrication and Application of Zinc Oxide Modified Cellulose Networks as Gas Separation Membranes. **A. Kinnebrew, C. Rhoades, M.L. Curry**
**2:05 1076.** Electronic Properties and Thermodynamics Investigation of Heterometallic Actinide-Based Metal–Organic Frameworks with Retrievable-Structure. **J. Yu, N. Shustova**

**2:25** Intermission.

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

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


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

Birmingham Jefferson Convention Center
East Meeting Room F

**Synthesis of Fluorescent Probes and Their Applications from Sensing to Imaging 2**

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

**1:00** Introductory Remarks.

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

**1:35 1083.** Chemical Sensing through Fluorescence Modulation in Conjugated Polymers. **M. Bonizzoni**
2:05 1084. Excited State Proton Transfer Dye with an Emission Quantum Yield up to 60% upon Zn$^{2+}$ Coordination. **K. Hanson**, S. Ayad, E.S. Knorr


3:05 Intermission.


4:55 Concluding Remarks.

Birmingham Jefferson Convention Center
East Meeting Room E

Organic

Organic Probes/Methodology/General

L. Yet, **Organizer**

1:15 Introduction.


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


2:50 1095. Withdrawn. Molecularly Imprinted Polymer Based Real-time Sensor for PFOA. S.T. Hobson

3:05 Intermission.


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


Birmingham Jefferson Convention Center  
East Meeting Room G

**Analytical Chemistry**

**Advanced Analytical Chemistry Studies of Biomolecule and Tissue Systems**

A. Ghosh, S. Pan, *Presiding*

1:30 Introduction.


2:00 1104. Analysis of Microplastics (MPs) and Perfluoroalkyl Substances (PFAS) in Marine Animal Tissues. **C. Navarathna**


3:00 Intermission.


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

4:45 Concluding Remarks.

Birmingham Jefferson Convention Center
East Meeting Room O

Biochemistry

General Session Biochemistry 2

J. Zhang, Presiding

1:30 Introductory Remarks.


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.


4:15 1118. Withdrawn. Targeting a Conserved Structural Element from the SARS-CoV-2 Genome Using Mirror Image Aptamers. J. Li, J.T. Sczepanski


Birmingham Jefferson Convention Center
East Meeting Room K

Chemical Education

J. March, Organizer

Chemical Education Oral Presentations 2

1:30 Introduction.

1:40 1120. Improving Student Attitudes Towards General Chemistry I Laboratory as an Effect of Switching Lab Partners. L. Smith, D. Mlsna, T. Wei

2:00 1121. Measuring Internalized Stereotype Threat in Introductory Chemistry Courses Using a Customized Implicit Association Test (IAT). T. Blue, T.L. McGill

2:20 1122. Emerging Stronger through Resources Developed During the Pandemic. B. Casselman

2:40 Intermission.

3:00 1123. Pre-COVID and during-COVID: A comparison of general chemistry instruction at the University of Florida. M.T. Sumner, S. Benjamin, S. Harris, S. Lopez, M. Veige

3:20 1124. Effects of a Preparatory Adaptive Module on Student Performance in General Chemistry I at University of Florida. S. Benjamin, S. Harris, S. Lopez, M.T. Sumner, M. Veige
3:40 Concluding Remarks.

Birmingham Jefferson Convention Center
East Meeting Room B

Engineering Solutions for Social Challenges: Renewable Materials and Resources 2

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

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

1:30 Introductory Remarks.


2:20 1126. Cellulose Nanofiber-based Hydrogels for Rapid Removal of Methyl Blue dyes in Water. Y. Nan


3:20 Intermission.


4:55 Concluding Remarks.
Industrial Careers in Chemistry

Undergraduate Discussion: Industrial Careers in Chemistry

Financially supported by Refresco
J. A. Nikles, Organizer

1:30 Introduction .

1:40 1130. The Unconventional Career path of a Chemist in Industry. H.L. Davis

2:05 1131. Technical challenges facing the food and beverage industry. D.E. Ragland

2:30 Intermission.

2:40 1132. Chemistry Leads Beyond – Creating Your Career. T. Tice

3:05 1133. From a PhD in Biochemistry to the Director of Marketing: A Look at a Non-Traditional Career for your STEM Degree. K. Sims

3:30 1134. Successful Careers in the STEAM Field. Y. Crawford

3:55 1135. Transitioning from Academic Studies to an Industrial Career. T.R. Totsch

4:20 Panel Discussion.

Birmingham Jefferson Convention Center
East Meeting Room A

Nanomaterials 2

S. Street, Presiding

1:30 Introduction .

2:00  1137.  Ionic Liquids as Antifouling Polymeric Nanoparticle Coatings.  **E.E. Tanner**


3:20  Intermission.


4:00  1142.  Metal-Organic Frameworks: From Bulk to Thin Films.  **A. Bajpai**, D. Speed, G.J. Szulczewski


4:40  1144.  Transport Features of Network Materials Built with Carbon Nanotubes Despite of Chiralities and Other Shape Factors.  **S. Tang**

**Birmingham Jefferson Convention Center**
**East Meeting Room I**

**Physical Chemistry**

**General Session Physical Chemistry 2**
T. P. Hamilton, Organizer


1:50 1146. Computational Analysis of the Spin-trapping Properties of Lipoic Acid and Dihydrolipoic Acid. M. Bonfield, S.J. Kirkby


3:10 Intermission.

3:30 1150. Understanding The Structural And Dynamical Properties Of Lignin Polymer In Dmso And Dmso/water Binary Mixtures. N. Jahan


4:10 1152. Unusual Intramolecular Contacts in 2,3-Epoxycyclopentanols and their Analogs: Theoretical Evidence for Hydrogen Bonding. J.M. Carr, G.S. Tschumper


Birmingham Jefferson Convention Center
East Meeting Room C

Polymer Materials Science and Engineering
General Session Polymer Materials 2 - Polymeric Materials for Biological and Environmental purposes

V. Thomas, Presiding

1:30 Introduction.

1:40 1154. Poly(amino acid)s and PEGylated poly(amino acid)s in Biological Applications. U. David, J. Sanchez, C. Scholz

2:00 1155. Polymeric Tissue Scaffolds that Mimic the Structure, Composition and Function of the Extracellular Matrix. D. Dean, J. Ayariga


2:35 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


Birmingham Jefferson Convention Center  
East Exhibit Hall 1

**Undergraduate Research 5**

J. A. Nikles, *Organizer*

**1:30 - 3:30**


**1165.** Biological Activity of Palladium Thiosemicarbazone. **E. Travers**, E.C. Lsic, 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


**1170.** (Diethylamino)Sulfur Trifluoride (DAST) Mediated Oxidation of Alcohols and Amines to Carbonyl Compounds. **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. Lsic, J.D. Conner, X. Jiang

1174. **Withdrawn.** Construction of an Instrument Capable of Two-color Fluorescence Correlation Spectroscopy. A. Lawrence, K.H. Fogarty


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 Au₂₅(SCH₃)₁₈⁻ and its Activation of O₂ Molecules. J. Pinkerton, S. Havenridge, C. Aikens


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. Jarocha

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. Jarocha


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


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


Boron-mediated diastereoselective aldol reactions of \(N,N\)-dialkylphenylacetamides. B. Peco, A. McCullough, S. Reliford, S.W. Primeaux, D.J. Cambre, P.B. Chanda

Analysis of Electronic Cigarette Liquids. M. Deen, L. Butler, V. Geisler

Influence of Spring Water on Two Rivers in Tampa Bay, Florida. P. Mead, K.A. Deister

Regioselectivity of Acid-catalyzed Epoxide Ring-opening Reactions. B.R. Chastang, D.H. Magers

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

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


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

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

Structural Characterization of a Mutagenic 6-oxo-m1dg Adduct in DNA. C.L. Wessel, Y. Fu, L.J. Marnett, M.P. Stone

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

Spin Trapping Reactive Oxygen Species Produced by X-ray Scintillating Nanoparticles. I. Weaver, E. Zhang, C. Kerpal, S.H. Foulger, L. Jarocha
1210. Synthesis of Silver Phosphate Complexes. T. Hussain, N. Dodd, J.P. Sadighi


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


1216. Nitrile Homoepibatididine Synthesis. N.N. Al-Saadi, S. Slauson


1219. Mechanisms of Linoleic Acid Oxidation by Myeloperoxidase. C. Powell, K.M. Matera


1221. Spartan18 QSAR Analysis of Ebselen-Type Heterocycles for the Inhibition of SARS-CoV2. F. Bai, D. Cooper, M. Donahue, J. Kessel

1222. Resolution of Racemic Alcohol through the use of Mosher's Reagent for use in the Synthesis of Enantiopure Allosteric Inhibitors for HIV-1 Integrase. L. Evans, K. Patel, J. Patterson, J.A. Pigza, M. Donahue, J. Kessl

1223. Effects of Self-assembled Monolayer Structure on Conjugated Polymer Morphology. E. Silver, P. Lundin
SATURDAY EVENING

Birmingham Jefferson Convention Center
East Ballroom B

Plenary

T. P. Hamilton, *Presiding*

5:30 1224. A Career in Science: Expect the Unexpected. **L.J. DeLucas**
First Floor East Meeting Rooms
P6 is the recommended Parking Deck
Meetings are in East Meeting Rooms

Sheraton and Westin Hotels are also circled
Elevated walkway from Sheraton to Third Floor East