

**The 68th Southeastern Regional
Meeting of the American Chemical Society
October 23-26, 2016
Columbia, SC**

S. Goode, *Program Chair*

UPDATED as of 4:30 PM

SUNDAY MORNING

High School Chemistry: New Approaches to Catalyze Change for YOU!!!

Columbia Metropolitan Convention Center
Congaree A/B

Cosponsored by CHED and SOCED[‡]
R. Goode, L. E. Slocum, *Organizers, Presiding*

8:00 Registration.

8:30 Introductory Remarks.

8:35 4. Using modeling activities in the high school chemistry classroom. **V.B. Steinbock**

9:30 2. Inquiry in the high school chemistry laboratory: Content, conversion, and concerns. **E.E. Smith**

10:30 Intermission.

10:40 3. Ready to use activities from JCE and ChemEd X. **D. Cullen**

11:35 1. A natural history of Chernobyl. **R. Mancke**

SUNDAY AFTERNOON

Biological Chemistry - Enzymology

Hilton Columbia Center
Breakout 1/2

H. Zur Loye, *Organizer*
F. Outten, *Presiding*

12:30 5. New mechanistic insights of protein arginine methylation. **Y. Zheng**

1:00 6. Retroviral proteases: Correlating substrate recognition with both acquired and native inhibitor resistance. **G.S. Laco**

1:30 7. Bicipin oxalate oxidase product inhibition. **J. Goodwin**, H. Rana, G. Chakrabarti, E.W. Moomaw

2:00 8. Oligomerization-dependent changes to the heme pocket of globin coupled sensors. **S. Rivera**, E.E. Weinert

2:30 9. Mechanistic studies of substituted guaiacols as new substrates for dehaloperoxidase from *Amphitrite ornata*. **A.H. McGuire**, R.A. Ghiladi

Asymmetric Chemistry throughout the Southeast

Columbia Metropolitan Convention Center
Lexington A

K. S. Petersen, S. L. Wiskur, *Organizers*
S. Wiskur, *Presiding*

1:00 Introductory Remarks.

1:05 10. StackPhos: From structural curiosity to enantioselective catalysis. **A. Aponick**

1:35 11. Enantioselective organocatalytic alpha-sulfamidation of aldehydes: Scope and limitations. **T.C. Coombs**

2:05 12. New reactions and reagents to molecularly edit therapeutics and natural products with fluorine. **J.N. Johnston**, B.A. Vara, S.V. Tsukanov, K.S. Schwieter, A.B. Doody

2:35 13. Novel Brønsted acid catalyzed methods for the synthesis of enantioenriched small molecules. **K.S. Petersen**

3:05 Intermission.

3:20 14. Chiral alkylmetals in organic synthesis and enantioselective catalysis. **S. Meek**

3:50 15. Metal-catalyzed alkyne activation: Cyclizations and cycloisomerizations. **E. Ferreira**

Dynamics of Molecular Processes: Theory, Simulations and Insight

Columbia Metropolitan Convention Center
Lexington B

Cosponsored by PHYS
S. Garashchuk, V. Rassolov, *Organizers*
J. Jakowski, *Presiding*

1:00 Introductory Remarks.

1:10 16. Novel therapeutic enzymes designed from high-performance supercomputing. F. Zheng, C. Zhan

1:40 17. Theoretical study of the reaction mechanism of nerve-agent hydrolysis with advanced catalysts. D. Troya, R.C. Chapleski, J.R. Morris

2:10 18. Uncertainty quantification of the water-gas shift reaction over Pt-based catalysts. A. Heyden

2:40 Intermission.

3:00 19. Electronic excited states from pairing matrix fluctuations and particle-particle random phase approximation. W. Yang

3:30 20. Analytic gradients and excitation energies from v2RDM-driven CASSCF. A.E. DePrince

4:00 21. Electronic stopping in condensed matter: Ab Initio understanding of electronic excitation dynamics under proton irradiation and beyond. Y. Kanai

4:30 22. Isotope substitution, electronic structure and dynamics in conducting polymers. J. Jakowski, J. Huang, S. Garashchuk, J.K. Keum, K. Hong, B. Sumpter

Finding Solutions to Environmental Challenges in Agriculture

Columbia Metropolitan Convention Center
Richland A

Cosponsored by ENVR
L. L. McConnell, J. Wang, *Organizers, Presiding*

1:00 23. Pyrolysis for livestock waste-to-energy. K. Ro

1:30 24. Insights into reptile dermal contaminant exposure: Reptile skin permeability to pesticides. **S. Weir**

2:00 25. Environmental toxicology and ecological risk assessment for plant protection products in regulatory compliance. **J. Wang**

2:30 26. Advancing innovations in agriculture to minimize environmental impacts. **L.L. McConnell**, I.D. Kelly, R. Jones

3:00 27. Phosphate adsorption ability of Mg-Al impregnated high surface area biochar. **G. Burk**, T. Mlsna

3:30 Discussion.

Inorganic Chemistry - Organometallic

Hilton Columbia Center
Banquet 2

H. Zur Loye, *Organizer*
G. Elpitya, *Presiding*

1:00 28. Entropy driven bis-macrocycle effect. **M. Invernici**, L. Fabbri, M. Licchelli, M. Bonizzoni

1:30 29. Scope, opportunities and experiences of continuing education in organometallic chemistry. **A. Rahman**, W.D. Jones

2:00 30. Small molecule activation by platinum complexes containing bulky tin groups. **B. Captain**, A. Koppaka, M. Gamage, C.D. Hoff

2:30 31. Coordination complexes of methimazole with copper: Controlling redox reactions and sulfur extrusion. **J.M. Murphy**, C. McMillen, J.L. Brumaghim

3:00 32. Mechanistic study of iron catalyzed Kumada coupling reactions. **L. Freeman**, D. Elorriaga, R. Bedford, T.A. Nile, A.G. Glenn

3:15 Intermission.

3:30 33. Biologically-relevant redox catalysis by a ruthenium-hydride intermediate. **A.G. Tennyson**

4:00 34. Mechanochemical and solvent effects on ligand lability in $Cp_mMX_n(OR)_{4-(m+n)}$ (M = Ti, Zr, Hf)(X = Cl, Br) species. **N.C. Boyde**, T.P. Hanusa

4:30 35. Reactivity of N-polydentate copper(II)-alkylperoxo complexes. **B. Pella**

Interdisciplinary Chemistry

Columbia Metropolitan Convention Center
Hall of Fame

H. Zur Loye, *Organizer*
L. Grabowski, *Presiding*

1:00 36. Development of a pH sensor for non-invasive in vivo detection and imaging of implant associated infection. **U. Uzair**, J.N. Anker, D. Benza, F. Wang, Y. Raval, T.J. Tzeng

1:30 37. Effect of media physicochemical properties on aggregation kinetics of citrate-coated silver nanomaterials. **K. Afshinnia**, M. Baalousha

2:00 38. Self-organization of biomimetic polycrystalline silica-carbonate microstructures. **P. Knoll**, E. Nakouzi, O. Steinbock

2:30 39. Tube formation in precipitation reactions under controlled hydrostatic pressures. **M. Bentley**, B.C. Batista, O. Steinbock

2:45 Intermission.

3:00 40. Using quantitative proteomics to profile changes in individual immune cell types after an AS03-adjuvanted H5N1 vaccine. **A.C. Galassie**, J. Goll, P. Samir, T. Jensen, K.L. Hoek, L. Howard, T.M. Allos, X. Niu, L.E. Gordy, C.B. Creech, H. Hill, S. Joyce, K.M. Edwards, A. Link

3:30 41. An updated look at the safety policies of chemical journals. **L. Grabowski**, S.R. Goode

4:00 42. Oil separation from water under environmentally relevant conditions using polymer-coated magnetic nanoparticles. **S. Mirshahghassemi**, J. Lead

Organic Chemistry - Synthetic Methodology

Hilton Columbia Center
Banquet 1

H. Zur Loye, *Organizer*
L. Cai, *Presiding*

1:00 43. Facile two-component synthesis of acacetin. Y. Zhao, **L. Cai**, Q. Gao

1:30 44. Progress toward development of an *in situ* click chemistry approach for discovery of cystic fibrosis transmembrane conductance regulator (CFTR) modulators. **M.L. Turlington**, S. Aller, S. Rowe, D. Alligood, A. Carter, S. Jordan, N. Thacker, L. Tang

2:00 45. Finding a general and tunable method for the reduction of esters to ethers via *in situ* React IR. **A. Hart**, J.A. Pigza

2:30 Intermission.

3:00 46. A new convergent synthesis of 1,3,4-oxadiazoles from acyl hydrazides. **K. Tokumaru**, J.N. Johnston

3:30 47. Alpha substitution of nitriles mediated by trimethylsilyl trifluoromethanesulfonate. **C.W. Downey**

4:00 48. Calcium catalyzed Friedel-Craft and Mukaiyama-Mannich reactions. **K.A. Nolin**

4:30 49. Construction of spiro[4.5]cyclohexadienones via intramolecular phenolic allylation for natural product synthesis. **M.G. Donahue**, N.G. Jentsch, E. Realini

Polymer Chemistry - Synthesis

Columbia Metropolitan Convention Center
Richland B

H. Zur Loye, *Organizer*
L. Yuan, *Presiding*

1:00 50. Ring opening polymerization of lactone rings using metal catalysts to form cross-linkable biodegradable polyesters. **N. Payne**, P. Binda

1:30 51. Polymer-grafted silica nanoparticles towards hybrid assemblies in one step. **Y. Zheng**

2:00 52. Synthesis of bottlebrush polymers using ring-opening metathesis polymerization. **S. Radzinski**, J. Foster, R.C. Chapleski, K. Arrington, D. Troya, J.B. Matson

2:30 53. Linear poly(ethyleneimine) synthesized by living anionic polymerization. **L. Reisman**, C.P. Mbarushimana, S.J. Cassidy, E. Rowe, P. Rugar

3:00 54. Synthesis, characterization, and comparison of polyborafluorene and polyborafluorene copolymers. **I.A. Adams**, P. Rugar

High School Chemistry: New Approaches to Catalyze Change for YOU!!!

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1:30 55. A forensic DNA case study: The disappearance of Brooke Wilberger. **R. Craig**

2:30 56. Collaborative chemistry: Engaging students in small group learning experiences. **J. Enlow**

3:30 Intermission.

3:40 57. Workshop to introduce the guidelines for chemical laboratory safety in secondary schools. **W.H. Breazeale**

Biological Chemistry - Enzymology & Microbiology

Hilton Columbia Center
Breakout 1/2

H. Zur Loye, *Organizer*
S. L. Witcher, *Presiding*

3:15 58. Importance of an active-site histidine in directing decarboxylation by P450 OleT. **J. Grant**, T.M. Makris

3:45 59. Molecular recognition and regulation of a nonribosomal peptide synthetase-modifying P450. **C.E. Wise**, T.M. Makris

4:15 60. *Saccharomyces cerevisiae* Hsp104 is a non-processive polypeptide translocase. **C. Weaver**, M. Jackrel, J. Lin, K.L. Mack, E.A. Sweeney, L. Castellano, J. Shorter, A.L. Lucius

4:45 61. Examination of *E. coli* ClpA self-assembly and linkage to nucleotide binding. **E.C. Duran**, A.L. Lucius

SUNDAY EVENING

Analytical Chemistry Posters

Columbia Metropolitan Convention Center
Exhibit Hall

H. Zur Loye, *Organizer*

5:00 - 7:00

62. Implementation of picoSpin™ benchtop NMRs into organic chemistry teaching laboratories through spectral analysis of Fischer esterification products. **K.L. Yearty**, J.T. Sharp, E.K. Meehan, D.R. Wallace, D. Jackson, R.W. Morrison
64. Development of a microfluidic system for monitoring glucagon secretion from islets of Langerhans. **W. Leng**, B. Bandak, L. Yi, K. Evans, M.G. Roper
65. Development of analytical methods to measure residues of a commercial fungicide and a tannic acid biopesticide. **B. Bien**
66. Analysis of phytoestrogens found in the symbiotic relationship between sea anemone and algae using HPLC UV-VIS and MS. **S.K. Mowery**, A.M. Roark, N.J. Kuklinski
67. Boron-containing conjugated materials with ultrahigh Stokes shift. **J. Cassidy**, I.A. Adams, M.F. Smith, M. Bautista, P. Rugar, D.A. Dixon, L.E. McNamara, N. Hammer
68. Developing a fluorescence anisotropy immunoassay for real-time profiling of islet of Langerhans secretions. **J. Adablah**
69. Towards noninvasive imaging of implant strain and localised pH on implanted medical device surfaces coated with radioluminescent particles via a focused X-ray beam. **D. Benza**, F. Wang, U. Uzair, Y. Raval, J.N. Anker
70. Qualitative analysis of silicone contamination in market pulp using multi-temperature pyrolysis GC-MS. **T. Cotter**
71. Toward imaging radiolabeled antibiotics near radioluminescent phosphor films coated on biomedical implant surfaces. **G. Schober**, D. Benza, Y. Raval, U. Uzair, T.J. Tzeng, J.N. Anker
72. Classification of pre-dyed textile fibers exposed to weathering and photodegradation by non-destructive excitation-emission fluorescence spectroscopy paired with linear discriminant analysis. **N. Mujumdar**, A. Munoz de la Pena, A.D. Campiglia
73. Microfluidic bioreactor for testing the effect of glucose and insulin on glucose output from HepG2 cells. **A.G. Adams**, M.G. Roper
74. Nanospray desorption electrospray ionization mass spectrometry of intact bacterial cells. **A. Uwakweh**, D. Todd, Z. Jia, N. Chiu
75. Cyclic voltammetry: Determination of ferrocyanide concentration through the use of two standard addition equations. M. Barnhill, **M. McCrimmon**, K. Varazo
76. Comparison of aroma profiles between gluten-free and gluten-containing beers using SPME in combination with GCMS. **N. Stafford**, D. Budner
77. Study of the thermal behavior of select alkaline earth carbonates. **E. Miller**, C.M. Earnest

- 78.** Layer-by-layer, xerogel-based 1st generation amperometric biosensors for uric acid with nanoparticle network incorporation to enhance sensitivity. G.E. Conway, M.J. Pannell, M.A. Schwarzmann, M.B. Wayu, **M.C. Leopold**
- 79.** Development of microfluidic paper based analytical devices for detection of γ -hydroxybutyric acid. **B. Liyana Pathirannahel**, S.W. Huffman
- 80.** Detection of uric acid using hydrothermally synthesized ZnO nanoparticles tethered to multiwalled carbon nanotubes. **S. Chapagain**, C.C. Chusuei
- 81.** Quantifying the cooling effect on molecular ions resulted from passing through the ion mobility cell in an ion mobility mass spectrometer. **J. Mwangi**
- 82.** Identification of volatile organic compounds present in cigarette smoke via purge and trap coupled with GC/MS. **P. Skersick**, C.H. Lisse
- 83.** Collision-induced dissociation mass spectrometry of model deprotonated peptides and peptide amides. **C. Cui**, C.J. Cassady, D.A. Dixon
- 85.** Fabrication and characterization of metal organic framework thin films. **J. Shankwitz**
- 86.** HPLC-ELSD used to check silicone emulsions during their manufacture, shelf life, and in the field. **D.K. Griffith**
- 87.** Detection of antioxidants in black, green, and oolong teas. **K. Jones**, A.C. Suroviec
- 88.** Comparative study of two different methods for the determination of ochratoxin A in grape pomace. N. Mikiashvili, **J. Yu**, I. Smith
- 89.** Characterization of noise sources in inductively coupled plasma: Optical emission spectroscopy. **L. Grabowski**, S.R. Goode
- 90.** The effectiveness of buffer composition on fly-brain chromatograms. **K.D. Kumar**, M.H. Stodghill, N.J. Kuklinski

Chemical Education Posters

Columbia Metropolitan Convention Center
Exhibit Hall

H. Zur Loye, *Organizer*

5:00 - 7:00

- 63.** Promoting scientific competence through metacognitive skills in forensic chemistry. R. Bowen, **S. Verberne-Sutton**, C. Brame

- 91.** The microwave synthesis of phenylalanine: A two-step synthesis in the organic teaching laboratory using acetone as solvent. **M. Veers**, C. Thurman, S. Brady, C. Coca, J.R. Boone, **C. Clinger**
- 92.** Talk to an NSF Program Officer! **T.B. Higgins**
- 93.** Enhancing student success rates in general chemistry through the use of active learning strategies and course redesign. **K. Senevirathne**, M.D. Edington, L. Johnson, D. Stephens
- 94.** Scholarship program in science and mathematics at Kennesaw State University: Supporting the academic achievements of disadvantaged students. **D. Tapu**, A. Croicu
- 95.** Chemisthenics: A literal VSEPR exercise. **C. Rezsnyak**
- 96.** Evaluation of the procedure used for production of Canine Accelerant Detection training materials. **D.W. Carpenetti**, S. Giammona
- 97.** Conceptual and calculation based experiments used to improve student understanding of equilibrium. **A. Cook**
- 98.** Determining the antioxidant potential of *Hedera helix* extracts: Chemistry education through the Scots Science Scholars program. **E. Burnham**, A.D. Gibson, M. Siopsis
- 99.** L.A.D.I.E.S.: An after-school program to encourage an increased persistence of women in STEM. **E.E. Hardy**, M.M. West, C.D. Tutson, A.E. Gorden
- 100.** Meso-tetrakis(2-chloro-3-quinoly)porphyrin and its water-soluble derivative, meso-tetrakis(2-chloro-4-sulfonato-3-quinoly)porphyrin. **A. Adeyemo**
- 101.** The synthesis and characterization of a new photosensitizer and its metal derivatives: Potential anticancer drugs. **A. Adeyemo**
- 102.** The development of teaching and learning materials for cognition accelerating science classes for lower elementary students (I). **K. Young Tae**
- 103.** Examining web-based peer review in 2373 general chemistry students: Improving cognitive, interpersonal, and intrapersonal competencies. **L. Anderson**, J. Moxley, **U. Kulatunga**, **J. Figueroa**, **C. Vetromile**

Computation Chemistry Posters

H. Zur Loye, *Organizer*

Columbia Metropolitan Convention Center
Exhibit Hall

5:00 - 7:00

- 104.** Hartree-Fock and density functional theory calculations of DMPO and DMPO-OH - water clusters. P. Campbell, **S.J. Kirkby**
- 105.** Improving the light harvesting capability of Ru(II)-polypyridine dyes for dye-sensitized solar cells. **J. Brannock**
- 106.** Analytic gradients for variational two-electron reduced-density-matrix (ν 2RDM)-complete active space self-consistent field (CASSCF) methods. **E. Maradzike**
- 107.** Identification of experimentally observed intermediates along the prebiotic formation of nucleobases. **B. Ross**, Y.A. Jeilani
- 108.** Comparison of several computational methods for amine-imine tautomer prediction in biofilm inhibitors. **R.T. Fallows**, J.J. Pajski
- 109.** Hartree-Fock and density functional theory calculations of nitrile ligated dirhodium complexes. **Y. Asiri**, S.J. Kirkby
- 110.** The sensitivity of halogen bonds to the bonding environment. **S.K. Jaini**
- 111.** Weak interactions as diagnostic tools for inductive effects in organic compounds: Influence of benzene substituents on halogen bonds. **P. Ravichandran**, K. Donald
- 112.** Density functional theory studies of the prebiotic routes for the formation of RNA nucleosides. **P. Williams**
- 113.** Antagonistic effects of green tea on cancer chemotherapy: Computational and experimental investigation of epigallocatechin-3-gallate/sunitinib interactions. **B. Horswell**, K. Flatt, L. Shade, M.J. Vergne, M.V. Voehler, **A.J. Privett**
- 114.** Linear absorption spectra from explicitly time-dependent equation-of-motion coupled-cluster theory. **D.R. Nascimento**, A.E. DePrince
- 115.** Time dependent density functional theory (TDDFT) studies of Eu(III) thenoyltrifluoroacetone complexes with dipyrrophenazine ligand derivatives. **C. Jensen**, C.R. De Silva
- 116.** Hartree-Fock and density functional theory calculations of glucan building blocks. U.P. Patel, **S.J. Kirkby**
- 117.** Dynamical studies on liver receptor homolog-1 bound to small molecule effectors. **B. Scott**, **I.N. Ivanov**
- 118.** Top-down vs. bottom-up formation mechanism for fullerenes and endohedral metallofullerenes. **H. Bell**, B. Amofah, A. Lambert, T.J. Fuhrer

119. Predicting the properties of high oxidation state AnF_x complexes. **Z. Lee**, M. Vasiliu, D.A. Dixon

120. Molecular structures and energetics of small gold and copper clusters. **R. Persaud**, Z. Fang, M. Chen, D.A. Dixon

121. Withdrawn

122. Propionaldehyde gas phase oxidation pathways. **C. Odom**, T.D. Jordanov, A. Masunov, S.S. Vasu

123. Benchmarking the many-body expansion. **M. Zott**, R. Richard, C.D. Sherrill

124. Influence of π -conjugated donors on electronic properties of $[Fe(tpy)_2]^{2+}$. **D. Torres**, S. Mukherjee, E. Jakubikova

125. Calculated bond dissociation energies for use in analyzing collision induced dissociation processes for small amino acids. **A.S. McNeill**, S. Miller, M. Stover, C.J. Cassady, D.A. Dixon

126. Estimation of nuclear quantum effects of large molecular systems. **N. Ekanayake**, B. Gu, S. Garashchuk

127. Molecular modeling of the binding modes and affinities of sulfonamide interactions with glycolytic enzymes and target receptors. **N.Y. Forlemu**, R. Babalola

MONDAY MORNING

Plenary Session

Columbia Metropolitan Convention Center
Ballroom A/B

J. H. Dawson, *Organizer, Presiding*

8:00 128. Metal-oxos in chemistry and biology. **H.B. Gray**

Advances in Forensics Chemistry

Columbia Metropolitan Convention Center
Carolina A

S. L. Morgan, *Organizer, Presiding*

9:15 129. Determination of Am-241 in weapons grade plutonium for chronometry applications. M.D. Yoho, **D.R. Porterfield**, J.H. Rim, D.J. Klundt

9:45 130. Applications of steam thermography to the detection of forensic evidence. **R. Belliveau**, S. DeJong, B. Cassidy, Z. Lu, S.L. Morgan, M. Myrick

10:15 131. Novel psychoactive substances (NPS) and their impact on forensic science providers. **R.M. Sears**

10:45 132. Forensic characterization of environmentally weathered textile fibers by liquid chromatography with UV/visible detection. **M.R. Burnip**, S.L. Morgan

11:15 133. Meeting the opportunities of a forensic science career. **W. Bell**

Analytical Chemistry - Spectroscopy

Columbia Metropolitan Convention Center
Ballroom C

H. Zur Loye, *Organizer*
J. McCutcheon, *Presiding*

9:15 134. IR-MALDESI mass spectrometry imaging: Visualization of molecular distributions. **M. Bokhart**, M. Nazari, K. Garrard, D.C. Muddiman

9:45 135. Discrimination of metal cation mixtures in aqueous solution using a cross-reactive sensor array. **M. Ihde**, M. Bonizzoni

10:15 136. Study of negative mode electron-based dissociation tandem mass spectrometry techniques with acidic peptides on a FT-ICR mass spectrometer. **C. McMillen**, C.J. Cassady

10:45 137. Mass spectrometry fragmentation of derivatized and non-derivatized metal-adducted oligosaccharides. **R. Schaller-Duke**, C.J. Cassady

11:15 138. Electron transfer dissociation mass spectrometry of trivalent metal cationized acidic phosphorylated peptides. **J. Commodore**, C.J. Cassady

Asymmetric Chemistry throughout the Southeast

Columbia Metropolitan Convention Center
Congaree A

S. L. Wiskur, *Organizer*
K. S. Petersen, *Organizer, Presiding*

9:15 139. Synthesis of chiral sulfoxides and sulfinamides utilizing benzoxathiazine-2-oxide derivatives. Z.S. Han, C.H. Senanayake, **G. Wang**

9:45 140. Understanding internal chirality induction of asymmetric silylation via circular dichroism. **L. Wang**, T. Zhang, B.K. Redden, C.I. Sheppard, R. Clark, M.D. Smith, S.L. Wiskur

10:15 141. Human milk as a defense against group B *Streptococcus*. D.L. Ackerman, R.S. Doster, J.A. Gaddy, **S.D. Townsend**

10:45 142. Atom-transfer processes mediated by earth abundant metal complexes. **J.L. Roizen**

11:15 143. Novel synthesis routes for prostaglandins and prostaglandin intermediates using metathesis. **G. Yiannikouros**

11:45 Concluding Remarks.

Chemical Education

Columbia Metropolitan Convention Center
Richland C

H. Zur Loye, *Organizer*
W. Cory, *Presiding*

9:15 144. NSF programs in the Division of Undergraduate Education. **T.B. Higgins**

9:45 145. Investigation into which questions promote deep learning in general chemistry. **C. Shuniak**, S.E. Lewis

10:15 146. Flipping the general chemistry classroom: Less lecture, more learning. **W. Case**

10:45 147. Variation of dimensional analysis to enhance problem solving for nursing chemistry students. **D.P. Pursell**, N.Y. Forlemu, L.E. Anagho

11:15 148. Nursing chemistry course scheduling and student performance: Implications for administrators and students. **N.Y. Forlemu**, D.P. Pursell, L.E. Anagho

Cutting Edge of Biological Inorganic Chemistry

Columbia Metropolitan Convention Center
Richland A

A. Rogers, *Organizer*
J. H. Dawson, *Organizer, Presiding*

9:15 149. Catalysis of C-H bond cleavage by heme proteins and metalloporphyrins. **J.T. Groves**

9:45 150. Cytochrome P450 oxidations: A controlled burn of inert organic compounds. **M. Green**

10:15 151. Light-driven P450 enzymes. **L.E. Cheruzel**

10:45 152. Tuning P450 metal-oxo reactivity for the biosynthesis of fungible fuels. **T.M. Makris**

11:15 153. P450 catalyzing chemical changes: Mechanisms of carbon-carbon bond cleavage. **S.G. Sligar**, J.R. Kincaid, M.C. Gregory, P. Mak, I.G. Denisov, R. Duggal

Dynamics of Molecular Processes: Theory, Simulations and Insight

Columbia Metropolitan Convention Center
Richland B

Cosponsored by PHYS
V. Rassolov, *Organizer*
S. Garashchuk, *Organizer, Presiding*

9:15 154. Light harvesting and delivery at the molecular scale: Oscillator strength focusing and Dexter coupling pathways. **D.N. Beratan**

10:00 155. σ Interfacial electron transfer in $[\text{Fe}(\text{CNC})_2]^{2+}$ -TiO₂ assemblies: The role of photoactive state lifetime in increasing the electron injection yield. **S. Mukherjee**, E. Jakubikova

10:15 156. Impact of the dye conformation on interfacial electron transfer in dye-TiO₂ assemblies. **E. Jakubikova**, C. Liu

10:45 157. Unusual properties of chiral amphiphiles. **P.L. Polavarapu**

11:15 158. Solvation and spectroscopy of hydrogen atom dopants in solid parahydrogen: Quantum Monte Carlo studies. **R.J. Hinde**

Inorganic Chemistry - Organometallic

Columbia Metropolitan Convention Center
Ballroom B

H. Zur Loye, *Organizer*
D. Swinton *Presider*

9:15 159. Examining the construction of potential coordination polymers with mercury(II) and aromatic N-oxides. W.E. Lynch, **M. Tran**, C.W. Padgett

9:45 160. Trinuclear nickel cluster-fulleride superatomic solids. **J.L. Shott**, M.B. Freeman, N. Saleh, D.S. Jones, C. Bejger

10:15 161. Metal-ligand cooperativity in carborane-based metal complexes. **D.V. Peryshkov**

10:45 162. Pyridine containing Schiff base donor ligands and corresponding uranyl complexes. **E.E. Hardy**, M. Eddy, K.M. Wyss, A.E. Gorden

11:15 163. Environmental uranium sensing using metal complexation of salphenazine ligands. **M. Eddy**, E.E. Hardy, A.E. Gorden

11:30 164. Group 12 metal halide clusters: A search for the cause and location of a structural transition in mercury (II) fluoride. **Z. Shafi**, K. Donald

Materials Chemistry

Columbia Metropolitan Convention Center
Hall of Fame

H. Zur Loye, *Organizer*
D. S. Boucher, *Presiding*

9:15 165. Highly fluorescent and electrochromic thiazolo[5,4-d]thiazole viologens. **A. Woodward**, J. Kolesar, S. Hall, **M.G. Walter**

9:45 166. Optical and dielectric properties of methacrylate polymers with pendant carbazole moieties for use as memristors. **T. McFarlane**, S.H. Foulger, I. Bandera, B.V. Zdyrko

10:15 167. Surface modification of conducting polymer films using ATRP. **L. Pendleton**, T.W. Hanks

10:45 168. Synthesis and photophysical characterization of novel porphyrin donor acceptor materials. **D.M. Marin**, K. Ren, M. Kaushal, J. Kolsar, S. Hall, D. Marin, B. Miller, K. Gebreyowhance, M.G. Walter

11:15 169. Understanding effects of heating in long alkyl chain carboalkoxyphenyl porphyrins in porphyrin-fullerene bilayer solar cells. **M. Kaushal**, P. Srinivasamurthy, M.G. Walter

New Chemistry Toward Functional Polymeric Materials

Columbia Metropolitan Convention Center
Lexington A

Cosponsored by PMSE and POLY
Financially supported by NSF, Ingevity
C. Tang, *Organizer, Presiding*

9:15 170. New functional polymeric materials based on organoboron building blocks. F. Guo, X. Yin, N. Baser-Kirazli, P. Chen, F. Cheng, W. Wan, **F. Jaekle**

9:45 171. Polydiacetylene-containing sensing systems. **T.W. Hanks**

10:15 172. Dual-functional antifogging/antimicrobial polymer coating. J. Zhao, **W. Ming**

10:45 173. Creating complex interfaces using surface-initiated polymerization and post-polymerization modification. **J.J. Locklin**

11:15 174. Oil-soluble hairy nanoparticles as lubricant additives. **B. Zhao**

Organic Chemistry - Natural Product Synthesis

Columbia Metropolitan Convention Center
Congaree B

H. Zur Loye, *Organizer*
E. Adogla, *Presiding*

9:15 175. Carbonyl sulfide: An enzyme-promoted route to H₂S. **C. Powell**, J. Foster, B. Okyere, M. Theus, J. Matson

9:45 176. Natural dibenz[b,f]oxepin as a potential novel antibacterial agent: Progress towards the synthesis and optimization of Empetroxepin A and B. **E.C. Young**, A.L. Wolfe

10:00 177. Synthesis and antibiotic evaluation of heterocyclic A and C ring depsidone analogs. **J.S. Katz**, A.L. Wolfe

10:15 178. Synthesis and antibiotic evaluation of simplified pestalone analogs. **R. Taylor**, **A.L. Wolfe**

10:30 179. Asymmetric synthesis of propargylamines for the construction of chiral aza-heterocycles. **D. Penk**, N. Robinson, H. Hill, M.L. Turlington

10:45 180. Enantioselective synthesis of dioxanones. **A. Kelley**

Scattering Measurements of Polymers & Nanomaterials

Columbia Metropolitan Convention Center
Carolina B

M. Stefik, *Organizer, Presiding*

9:15 181. From nanometer to devices: X-ray and neutron scattering insight into macromolecular behavior. **D. Perahia**

10:05 Intermission.

10:15 182. Elucidating polymer structures and dynamics by scattering techniques. **K. Hong**

10:45 183. Evaluation of the growth of substituted ferrites for magnetically modulated energy delivery (MagMED) via SAXS. **O.T. Mefford**, B. Fellows, J. Livingston, B. Wright, K. Lantz, M. Stefik

11:15 184. Small-angle X-ray scattering for quantum dot sizing and film characterization. **A.B. Greytak**

Supramolecular Assemblies & Metal-Organic Frameworks

Hilton Columbia Center
Banquet 1

N. B. Shustova, *Organizer, Presiding*

9:15 185. Coordination polymers with electroactive pincer complexes as metalloligands. **J.R. Gardinier**

9:45 186. Supramolecular MOFs organized by flexible and robust π - π stacking interactions: Metal complexes with unusual structures and properties. **D.L. Reger**

10:15 187. New developments in the chemistry of covalent organic frameworks. **W. Dichtel**

10:45 188. Towards free MONTs: Controlling intermolecular interactions between tubes. K.M. Vailonis, H.J. Martin, T. Etampawala, D.L. Mull, C. Murdock, M.D. Dadmun, **D.M. Jenkins**

11:15 189. Post-synthetic modification of metal organic frameworks for catalysis; a computational study. **S.L. Pellizzeri**, I. Jones, R. Getman

Women Chemists in the Southeast

Hilton Columbia Center
Breakout 1/2

J. M. Iriarte-Gross, *Organizer*
T. Faulks, *Organizer, Presiding*

9:15 190. Mentoring women in STEM disciplines: A women's college perspective. **A. Oxley**

9:45 191. To postdoc, or not to postdoc; that is the question. **E. Draganova**

10:15 192. Leading the way for women chemists of color: First steps needed in undergraduate chemistry education. **T. Faulks**

10:45 193. Introduction to a woman starting her chemical education and career. **J. Albertson**

11:15 194. Rockin' Raider Robots are increasing middle school girls' interests in STEM. **L. Anderkin**, J. Earls, J.M. Iriarte-Gross

11:45 Concluding Remarks.

MONDAY AFTERNOON

Advances in Forensics Chemistry

Columbia Metropolitan Convention Center
Carolina A

S. L. Morgan, *Organizer, Presiding*

1:00 195. New psychoactive substances (NPS) and the death investigation: A case study. **D. Garvin**

1:30 196. Fast, simple method for the analysis of benzodiazepines in meconium and an interlaboratory method comparison. **K.R. Mastrianni**, W.E. Brewer, S.L. Morgan, S.J. Marin, G. McMillin

2:00 197. Classification of magnetic audio tape degradation for various tape chemistries using spectroscopy and chemometrics. **A. Abraham**, N. Fuenffinger, B. Cassidy, N. Ratnasena, T. Burdette, A. Singleton, M. Myrick, E. Breitung, S.L. Morgan

2:30 198. An overview of FBI TEDAC: Terrorist explosive device analytical center. **R. Craig**, J.G. Kelley

3:00 Intermission.

3:20 199. Multivariate classification model transfer of UV/visible spectral data from acrylic fibers without standards. N. Fuenffinger, J.V. Goodpaster, E.G. Bartick, **S.L. Morgan**

Analytical Chemistry - Electrochemical Instrumentation

Columbia Metropolitan Convention Center
Ballroom C
H. Zur Loye, *Organizer*
A. Abdalla, *Presiding*

1:00 200. Chemically modified amorphous carbon electrodes: New chemistries and applications. **M.R. Lockett**

1:30 201. Ultra-sensitive electrochemical detection of Cr (VI) using double polymer membrane. **A. Izadyar**

2:00 202. Fast scan cyclic voltammetry analysis of serotonin: Does thimerosal alter neurotransmitters at a fundamental level? **A. West**, A. Abdalla, P. Hashemi

2:30 203. A novel micro-electrochemical cell for PEM fuel cell catalysts screening. **S. Bukola**, S.E. Creager

3:00 Intermission.

3:20 204. Characterization of ionophore-grafted carbon fiber microelectrodes. **J.A. Holmes**, P. Pathirathna, T. Siriwardhane, P. Hashemi

3:50 205. Role of nanoparticles in voltammetric signal enhancement exhibited by layer-by-layer gold nanoparticle-modified screen-printed carbon electrodes. **B. Ahiadu**, J. Smith, J. Patterson, G.W. Bishop

4:20 206. Organo-soluble Au₁₀₂(SPh)₄₄ nanomolecules. **M. Rambukwella**, A. Dass

Chemical Education

Columbia Metropolitan Convention Center
Richland C

H. Zur Loye, *Organizer*
W. Cory, *Presiding*

1:00 207. Can they succeed? Exploring at-risk students' study habits in college general chemistry. **L. Ye**, S.E. Lewis

1:30 208. Classroom strategy for promoting understanding of chemistry among underrepresented minority students. **P.I. Binda**

2:00 209. Fire size as a function of solvent volume. **J.W. Hall**, M.T. Griffin, A.N. Manzewitsch, K.S. Kroeger, S.K. Hutchison, J. Coleman, T. Stegall

2:30 210. Electrochemical determination of a solubility product constant: A tested laboratory experiment. **L. Grabowski**, S.R. Goode

3:00 Intermission.

3:20 211. Advancing 9-12 Educator knowledge using a new polymer semiconductor education kit. J. Enlow, D.M. Marin, **M.G. Walter**

3:50 212. Catching criminals with chemistry: A general elective course in forensic science. **W. Case**

4:20 213. Going digital: Revamping traditional lab reports in an honors general chemistry lab. **C.R. Simmons**, A.M. Sanders

Cutting Edge of Biological Inorganic Chemistry

Columbia Metropolitan Convention Center
Richland A

J. H. Dawson, A. Rogers, *Organizers*
L. Lebioda, *Presiding*

1:00 214. Mechanism of nitrogen fixation by nitrogenase. **B.M. Hoffman**

1:30 215. Probing low frequency vibrational excitations and their effect on electron, proton, and group transport in proteins. **P.M. Champion**

2:00 216. Conformational dynamics in cytochrome c redox reactions. **E.V. Pletneva**

2:30 217. Paradigm shift in heme degradation in pathogenic bacteria. T. Matsui, H. Fujii, **M. Ikeda-Saito**

Electronic Structure: Concepts & Applications

Columbia Metropolitan Convention Center
Richland B

Cosponsored by PHYS
S. Garashchuk, *Organizer*
V. Rassolov, *Organizer, Presiding*

1:00 218. Transport across lipid bilayer membranes near a phase transition temperature: Effects of interfacial line tension on permeability. **J. Kindt**, L. Yang

1:30 219. Reformulating classical molecular dynamics simulations in the microcanonical and isothermal-isobaric ensembles to match rigorous results for small systems. **M. Uline**

2:00 220. The role of charge transfer excitons in high-mobility polymers. **H. Jaeger**

2:30 221. In silico determination of gas permeabilities in porous polymeric materials. **C.M. Colina**

3:00 Intermission.

3:20 222. Fragment based ab initio molecular dynamics: “On-the-fly” dynamics with coupled cluster accuracy. **S.S. Iyengar**

3:50 223. Including nuclear quantum effects into simulations of large molecular systems. **S. Garashchuk**

4:20 224. Twisting motions in $[\text{Fe}(\text{bpy})_3]^{2+}$ and other tris-chelate polypyridyl complexes. **D.C. Ashley**, E. Jakubikova

4:35 225. Applying the finite-temperature string method to DNA base eversion. **T.W. Dodd**, B. Kossmann, I.N. Ivanov

Inorganic Chemistry - Organometallic

Columbia Metropolitan Convention Center
Ballroom B

H. Zur Loye, *Organizer*
M. Raja, *Presiding*

1:00 226. Synthesis and coordination chemistry of saturated N-heterocyclic chalcogenones. **J. Patterson, D. Rabinovich**

1:30 227. Synthesis and reactivity of N-heterocyclic thione (NHT) and selone (NHSe) derivatives of caffeine. **M. Styron, D. Rabinovich**

2:00 228. Synthesis and reactivity of six-membered N-heterocyclic chalcogenones. **J.J. Flanagan, D. Rabinovich**

2:30 229. Coordination chemistry of new sterically-demanding N-heterocyclic chalcogenones. **M. Kocherga, D. Rabinovich**

3:00 Intermission.

3:20 230. Synthesis and characterization of novel antimony(III) oxo bridged complexes with aromatic N-oxide ligands. **W.E. Lynch, C.W. Padgett, M. Tran, M. Raymundo**

3:50 231. Stabilization of the parent monochlorosilylene (HSiCl). **H. Hickox, Y. Wang, G.H. Robinson**

New Chemistry Toward Functional Polymeric Materials

Columbia Metropolitan Convention Center
Lexington A

Cosponsored by PMSE and POLY
Financially supported by NSF, Ingevity
C. Tang, *Organizer*
G. Liu, M. Stefik, *Presiding*

1:00 232. Interplay between molecular design and materials processing: Impact on devices. N. Kleinhenz, N. Persson, P. Chu, Z. Yuan, **E. Reichmanis**

1:30 233. Molecular and nanostructure engineering of polymer semiconductors for electronics and optoelectronics. **E. Egap**

2:00 234. Electrolyte chemistries with responsive polymers for thermal safety in Li-ion batteries. **M.E. Roberts**

2:30 235. Block copolymers and plasmonic metal nanoparticles for energy and sensing applications. **G. Liu**

3:00 Intermission.

3:20 236. Precision functional materials derived from block copolymers. **M. Stefik**

3:50 237. Synthesis of a bio and photodegradable thermal plastic elastomer. **K. Arrington, J. Waugh, J. Matson**

Organic Chemistry - Synthetic Methodology

Columbia Metropolitan Convention Center
Congaree A

H. Zur Loye, *Organizer*
E. Adogla, *Presiding*

1:00 238. Size-dependent diastereoselective Grignard reactions of macrocyclic 1,4-diketones. **K.F. Johnson, N. Saha, B.L. Merner**

1:30 239. Macrocyclization and aromatization protocols for accessing highly strained arene-bridged systems. **N. Mitra, B.L. Merner**

2:00 240. Syntheses, structures and chemistry of selected isoindene dimers. **M. Etzkorn, J. Franklin, V. Wait, A.D. Mills**

2:30 241. Long-range donor-acceptor effects in constrained heterocyclic 8-membered rings: Structural analysis and Perlin effects. **P. Wiget**

3:00 Intermission.

3:20 242. Ab initio and DFT calculations related to conformations and NMR spectral calculations for pyranose sugar peracetates. **J.C. Hubbs**

3:50 243. Syntheses and binding studies of novel trisamine-based thiosemicarbazide receptors for anions. **C. Johnson, K.E. Kawamura, A. Hossain**

4:20 244. Development of a calibration system for hydrocarbons emitted from biomass burning. **A. Lynn, J. de Gouw, A. Koss**

Polymer Chemistry - Synthesis

Columbia Metropolitan Convention Center
Congaree B

H. Zur Loye, *Organizer*
M. Lamm, *Presiding*

1:00 245. Aqueous ROMP: Finally fast and controlled. **A. Ashcraft**, H.J. Schanz

1:30 246. Advances and challenges in functional poly(ϵ -caprolactone) synthesis. **B.A. Van Horn**, A.M. Esper, E.P. Bailey, V.O. Bailey, E.E. Burry

2:00 247. Synthesis and characterization of high melting temperature polysulfones via ADMET polymerization. **M.H. Bell**, H. Hester, T.W. Gaines, K.B. Wagener, K.I. Winey, E. Trigg

2:30 248. Next-generation plant oil-based polymers: Emerging chemistry and applications. **L. Yuan**, Z. Wang, M. Lamm, X. Zhang, C. Tang

3:00 Intermission.

3:20 249. Solution polymerization of polybenzimidazole. **A.T. Pingitore**, K. Fishel, A. Gullede, J. Hoffman, W.P. Steckle, B.C. Benicewicz

3:50 250. Influence of crosslinking agents on *in vitro* chondrogenesis and osteogenesis of mesenchymal stem cell in thiol-ene “click” hyaluronic acid hydrogels. **P. Maturavongsadit**, Q. Wang, B. Xiangdong, T. Gado

Realities of the Chemical Industry: Career Opportunities & Paths

Columbia Metropolitan Convention Center
Hall of Fame

Cosponsored by I&EC
Financially supported by Eastman Chemical Company
M. K. Engelman, *Organizer, Presiding*

1:00 251. David McCollam forensic chemist explosives unit FBI laboratory Part 1. **D. McCollam**

1:30 252. David McCollam forensic chemist explosives unit FBI laboratory Part 2. **D. McCollam**

2:00 253. David McCollam forensic chemist explosives unit FBI laboratory Part 3. **D. McCollam**

2:30 254. Technician career paths in process innovation, Eastman Chemical Company. **J.R. Clarkson**

3:00 Intermission.

3:20 255. From laboratory technician to director, Robin Minga. **R. Minga**

3:50 256. Discovering chemistry outside the lab. **S. Large**

4:20 257. From working the lab to saving the lab. **T. Joshua**

Scattering Measurements of Polymers & Nanomaterials

Columbia Metropolitan Convention Center
Carolina B

M. Stefik, *Organizer, Presiding*

1:00 258. Widely tunable morphologies in block copolymer thin films through solvent vapor annealing using mixtures of selective solvents. **M. Chavis**, D. Smilgies, U.B. Wiesner, C.K. Ober

1:30 259. Living on the edge: Chemistry at the interfaces. **M. Dolgos**

2:00 260. Diffraction measurements on 2D materials and their assemblies. **S.C. Warren**

2:30 261. Using machine learning to map phase diagrams and discover new hypothesis in old data sets. **J. Hattrick-Simpers**, J. Bunn, B. Ruiz-Yi

3:00 Intermission.

3:20 262. P3HT/graphene composites synthesized *via in-situ* GRIM methods. D. Presto, **D.S. Boucher**

Structure-Property-Relationship of Nanoscale Materials - Advances in Nanomaterial Characterization and Properties

Hilton Columbia Center
Banquet 2

D. A. Chen, A. B. Greytak, T. Vogt, *Organizers*
H. Wang, *Organizer, Presiding*

1:00 263. Tuning localized surface plasmon resonance in metal oxide nanocrystals. **D.J. Milliron**, A. Agrawal, J. Kim, E. Runnerstrom

1:30 264. Linking the forward and reverse vapor-liquid-solid mechanisms in metal oxide nanostructures. B.M. Hudak, L. Yu, Y. Chang, M.E. Park, **B.S. Guiton**

2:00 265. Utilizing electron microscopy to determine the growth mechanism of nanoparticles. **A.D. Dukes**

2:30 266. *In Situ* super-resolution imaging of catalytic reaction and molecular transport on single nanocatalysts. **N. Fang**, B. Dong

3:00 Intermission.

3:20 267. Mechanically modifying nanoparticle shape. F. Ameer, S. Varahagiri, D. Benza, D.R. Willett, Y. Wen, G. Chumanov, **J.N. Anker**

3:50 268. Plasmonic enhancement of chromophores using hybrid gold nanoparticles. **A.K. Tobias**, M. Jones, M.G. Walter, R. Johnston

4:05 269. Probing magnetic exchange limits in core@shell magnetic nanoparticles. **D. Carnevale**, M. Shatruk, G.F. Strouse

Supramolecular Assemblies & Metal-Organic Frameworks

Hilton Columbia Center
Banquet 1

N. B. Shustova, *Organizer, Presiding*

1:00 270. Stimuli-responsive metal–organic frameworks. **S. Saha**

1:30 271. Atomic layer deposition for nucleation and synthesis of metal organic framework thin films. **G. Parsons**, J. Zhao, D. Lee, H. Barton, C.J. Oldham, H.J. Walls, G. Peterson

2:00 272. Nanospace within metal-organic frameworks: Plenty of opportunities for heterogeneous catalysis. **S. Ma**

2:30 273. Assessing the role of structure quality and internal flexibility on computational screening of MOFs for adsorption applications. **D. Sholl**, D. Nazarian, J. Camp, D. Tang

3:00 Intermission.

3:20 274. Ru(II)tris(2,2'-bipyridine) templated metal organic frameworks- structure and photophysics. **R.W. Larsen**

3:50 275. Photophysics of metal-organic frameworks. **N.B. Shustova**

Undergraduate Research Posters - Biological, Nano, & Interdisciplinary Chemistry

Columbia Metropolitan Convention Center
Exhibit Hall

H. Zur Loye, *Organizer*

1:00 - 2:30

276. Stability studies of a mutated protein causing cystic fibrosis. **K. Nilsson**

277. Thermodynamic binding characterization of Cr(III) diimine complexes and DNA utilizing isothermal titration calorimetry, spectrophotometric titration and equilibrium dialysis. **D.E. Monteith**, D.A. Watts, N.A. Kane-Maguire, S. Wheeler, S.R. Goudy, J.A. Wheeler, J.F. Wheeler

278. Investigating the DNA binding behavior of tris(diimine) Cr(III) systems capable of inducing DNA photooxidation. **S. Wheeler**, N.A. Kane-Maguire, D.A. Watts, M.M. Sprinkle, J.F. Wheeler

279. Chalcones as anti-cancer therapeutics. **M. Wallace**, S. Zingales

280. Click inhibition of HMGA binding. **D. Mesa Sanchez**, H. Stubbs, L. Rabenold, K.L. Buchmueller

281. HMGA binding disruption through selective modification of DNA. **H. Stubbs**, D. Mesa Sanchez, L. Rabenold, K.L. Buchmueller

282. Affinity and structural characterization of biological AT hook motif variants. **K. Dobbins**, K.L. Buchmueller

283. Introduction of fluoroaromatics in proteins via S_NAr . **J. Derryberry**, **D. Linklore**, M. Forconi

284. Characterization of the N^5 -methyl-formamidopyrimidine-deoxyguanosine lesion. **H. Pan**, S. Bamberger, C.K. Malik, T.L. Johnson-Salyard, C.J. Rizzo, M.P. Stone

285. Biochemical characterization of MEMO1 protein. **M. Newkirk**, T. Tran, J.A. Pollock

286. Selective estrogen receptor modulators as inhibitors of lung cancer proliferation. J.A. Pollock, **J.P. Henry**, K.A. Gunn

288. Fluorescence and colorimetric response of polydiacetylene liposomes to amphiphiles. **H.R. Holmes**, I. Miller, T.W. Hanks

289. Improving xylose metabolism in engineered strains of *Yarrowia lipolytica*. **L. Gambill**, G.M. Rodriguez, M.A. Blenner

290. Spectroscopic characterization of flutamide-polymer (PVP) interaction: Improving bioavailability of drug molecules. **H. Nickson**

291. Structure-function relationships in psychrophilic, mesophilic and thermophilic bacterial topoisomerases. **J. Bonsutto**, **L. DeSousa**, **R. Koch**, A. Schoeffler

- 292.** Nature of the proposed anti-hyperglycemic chromium(III) malate. **M. Smart**, S. Brown, J.B. Vincent
- 293.** Effects of the glycation of transferrin on chromium binding and the transport and distribution of chromium *in vivo*. **S. Dyroff**, G. Deng, J.B. Vincent
- 294.** Vitamins and steroids: Bioanalysis of the *in-vivo* synthesis by Coccinellidae *septumpunctata*. **R.G. Kropp**, Y. Kajita, M.F. Santiago
- 295.** Sequence, structure and function of small opioid peptides. **A.C. Schwartz**, M.W. Giuliano
- 296.** Routine HPLC ESI-MS method to screen drug effectiveness in inhibition of amyloid-beta peptide aggregation. **M. Herbert**, P.A. Martino
- 297.** Interrogation of activator-SAGA complex interactions. **M.E. Davis**, C.M. Joiner, A.K. Mapp
- 298.** Synthesis and biological evaluation of triazole-containing VX-809 analogs for in situ click chemistry with cystic fibrosis transmembrane conductance regulator (CFTR). **A. Carter**, **N. Thacker**, L. Tang, S. Rowe, S. Aller, M.L. Turlington
- 299.** Synthesis and characterization of three isomeric porphyrins for photodynamic therapy of tumor (PDT). **A. Adeyemo**
- 300.** Progress towards evaluation of 1,2,3-triazole as an amide bioisostere in a VX-809 analog. **S. Jordan**, L. Tang, S. Rowe, S. Aller, M.L. Turlington
- 301.** Determining the role of MKNK1 in RET-dependent cancer growth. **M. Murray**, M. Sonoshita, R. Cagan
- 302.** PEGylated DNA: A platform for screening encoded biochemical libraries in organic solvents. **J. Chambers**
- 303.** Conformational control of dipeptide mimetics through targeted modification of side chain and backbone functional groups. **J. Hohl**, A. Johnson, R. Lavrich
- 304.** The antimicrobial properties of *Kalmia latifolia* L. **J. Herring**, V. Avanzato, J.O. Hauptfleisch
- 305.** Analysis of the methods by which Mitochondria-targeted antioxidants prime adipocyte differentiation through qPCR analysis of relative expression of genes related to adipocyte differentiation. **K. Tavares**, B.E. Christian
- 306.** Analysis of SdsA1 and Bds1 sulfhydrolase activity by NMR and GC-MS. **C.R. Gilmer**, J.S. Reveral, G.L. Waddell

- 307.** Identification of new quorum sensing peptide from *Staphylococcus caprae*. **N. Chung**, D. Todd, A. Horswill, N.B. Cech
- 308.** Inhibition of Cytochrome P450's using undecylenic aldehyde. **P.S. Boyd**, S.P. Puckett, G.M. Raner
- 309.** Synthesis and characterization of opioid peptides containing dual pharmacophores for the delta and kappa opioid receptors. **S. Ballard**, S. Sedberry, A. Varadi, E.J. Williamson, S. Majumdar, K.R. Wilson
- 310.** Inhibition of microtubule affinity-regulating kinase-2 in regards to the hyperphosphorylation of the Tau protein. **J. Reed**, P.A. Martino
- 311.** Silver clusters and DNA ligands. **J.T. Petty**, **Y. Wang**
- 312.** Modification of fabric surfaces to prevent biofouling. **S. Douglas**, G. Mbah, T.W. Hanks
- 313.** Enzymatic synthesis of sequence-defined synthetic nucleic acid polymers with diverse functional groups. **W. Yeung**
- 314.** Silver cation interactions with DNA. J.T. Petty, **M. Gillan**
- 315.** Dehydrogenative coupling of a polysiloxane and dodecanethiol by way of the Piers-Rubinsztajn reaction. **A. Abdul-Haqq**, G. Mbah, T.W. Hanks
- 316.** Antibacterial effects of metallic nanoparticles-doped MOFs on James River. **J. Walker**, K.T. Jackson, K. Couser, N.H. Le
- 317.** DMSO mediated cellular uptake of phenol red. **H.I. Udo**, K.K. Griffin, J.M. Meyers
- 318.** Controlled drug delivery utilizing thermo-responsive nanoporous membrane. **J. Taylor**, S. Trull, J. Wu
- 319.** Investigating antimicrobial properties of human galectin-9. **J. Van Riper**, N. Kamili, C. Gerner- Smidt, C. Arthur, S. Stowell, A. Blenda
- 320.** De novo synthesis of 4TM proteins. **A.I. Noras**, A. Meletiou, P. Curnow, A.G. Glenn, T.A. Nile
- 321.** Molecular inhibition of oligomer formation and A β aggregation. **D. Higgins**, P.A. Martino
- 322.** Aldo-keto reductase YDL124w: Preliminary crystallization experiments. **A. Neely**, L. Lovelace, M. Weiland
- 323.** Protonation enhancement of peptides using metals in matrix assisted laser desorption ionization mass spectrometry. **S. Puckett**, R. Duke, R. Persaud, C.J. Cassady

- 324.** Identification of a membrane interacting region with human perforin: A chimeric approach. **W. Hiester**, A. Neely, M. Weiland
- 325.** Studying DNA polymorphisms via thermodynamic measurements. **M. Fuenmayor Llanos**, J. Obliosca, T. Yeh, J.T. Petty
- 326.** Synthesis of sphingosine kinase inhibitor 1 with modifications of zone 2. **T.C. Grattan**, A. Nemeth
- 327.** Synthesis of novel inhibitors of human sphingosine kinase 1 and investigation of their efficacy as antimicrobial agents. C. Cridland, J.C. Hurlbert, **T.C. Grattan**
- 328.** Withdrawn
- 329.** Understanding the rules of responsive hybrid promoters. **S. Smith**
- 330.** Characterizing the lipid binding of Nox1. **K.N. Threatt**, M. Thomas, M. Huynh, N. Davis
- 331.** Chalcones as potential anti-fungal agents. **M. Kelly**, S. Gremillion, S. Zingales
- 332.** Overexpression of manganese superoxide dismutase in mice liver leads to defects in oxidative phosphorylation. **S. Steyl**
- 333.** Evaluation of biphenyltetrols as aggregation inhibitors for Alzheimer's amyloid- β peptide. **M.J. Hurtt**, **W.J. Schreiber**, J.M. Hanna, R.K. Lammi
- 334.** Effects of chemotherapy treatment on cell-free telomeric DNA of AML cell lines through qPCR analysis. **M. Habash**, K. Stoltz, K. Harris, K. Hayden
- 335.** Cloning, expression, and purification of histone methyltransferases for inhibition studies. A.C. Spencer, **A. Jahan**, **Z. Shaikh**
- 336.** Antibacterial studies of *Mentha spicata* from leaf extracts: A medicinal plant. A.W. Peters, **K. Boyd**, A. Kalsum
- 337.** Identification of the pharmacophore of VX-809 for the development of new correctors for the cystic fibrosis transmembrane conductance regulator. **D.M. Alligood**, L. Tang, S. Rowe, S. Aller, M.L. Turlington
- 338.** Enhancement of FasL-induced cytotoxicity by activation of tumor-specific cytotoxic T lymphocytes with novel ceramide analogs. I. Lovett, A. Plotkin, J. Calkins, S. Bataille, R. Land, T. Albers, **I. Lebedyeva**
- 339.** Interaction of SH2 domain proteins with Net1A in breast cancer cells. **M. Jones**, A. Ulu, J. Frost

- 340.** Effects of ethanol on adipose inflammation and markers of insulin signaling in obesity-prone and resistant rats. **P. MgBodile**, S. Primeaux
- 341.** C-terminus function in LptB. **A. Mestre**, B. Simpson, R. Natividad
- 342.** Nanostructures based on perpendicular arrangements of carbon nanotubes and molecular linkers: Nano-hashtag. C.W. Frye, **T.R. Rybolt**
- 343.** More efficient and faster photocatalytic water purification materials. **J.D. Glover**, J.E. Boyd
- 344.** Quantification of adsorption of organic compounds by silver nanoparticles. **S. Goines**, K.M. Mullaugh
- 345.** Sulfidation of silver nanoparticles. **N. Fletcher**, K.M. Mullaugh
- 346.** Synthesis, functionalization, and testing of SERs-active silver-rhodium nanoparticles. **J.L. Bass**, S. Hunyadi Murph, K. Coopersmith
- 347.** Evaluation of the aromatic stacking interaction between pyrene and 1,8-naphthalic imides. **J. Morgan**, S.M. Strickland
- 348.** Energy and sustainability through the usage of energy operation dashboard and innovative analytical concepts at Virginia Union University. **N.H. Le**, K.T. Jackson, D.N. Eseonu
- 349.** Effects of sea level rise on carbon and nitrogen turnover in coastal forested wetlands of South Carolina. H. Robinson, A. Acoasta, D. Miller, A.M. Ruecker, W.H. Conner, **A.T. Chow**
- 350.** Celebrating 30 years of our ACS student chapter at Francis Marion University. M. McCrimmon, C. Witt, **J.G. Kelley**
- 351.** Using digital documentaries to encourage student reflection after international service learning experiences. **M. Chavez**, **C.M. Will**, C.P. Moore, A.M. Kiefer
- 352.** Surface-functionalization of magnetite nanoparticles for potential cellular imaging. **A. Lipchak**, C.R. De Silva
- 632.** Urine as an alternative nitrogen source for growing *Yarrowia lipolytica*. **M.R. Brabender**, G. Rodriguez, M.A. Blenner

Women Chemists in the Southeast

Hilton Columbia Center
Breakout 1/2

J. M. Iriarte-Gross, *Organizer*
T. Faulks, *Organizer, Presiding*

1:00 353. Unlocking the secrets of a successful technical career. **D.G. Schmidt**

1:30 354. Women chemists in the ACS: Initiatives, programs and how you can be involved. **L.S. Sremaniak**

2:00 355. I go to work to color. **C. Holdaway**

2:30 356. Volunteerism: Jumping in feet-first. **S. Verberne-Sutton**, L. Hiatt, J.R. McKenzie

3:00 Intermission.

3:20 357. Green Girls: Renewable energy activities that focus on science and civic engagement. **J.M. Iriarte-Gross**

3:50 358. Why diversity matters: Solutions to generate excellence through gender equity. **D. Stallings**, S. Iyer, R. Hernandez

4:20 359. A 5 year persistency study of chemistry undergraduate women within the University of North Carolina system. **G.P. Redd**, E.C. Gravely, T.C. Redd

4:50 360. Planning one's career. **D.J. Nelson**

5:20 Concluding Remarks.

Undergraduate Research Posters - Organic & Physical Chemistry

Columbia Metropolitan Convention Center
Exhibit Hall

H. Zur Loye, *Organizer*

2:45 - 4:15

361. PEGMA grafted SiO₂ nanoparticles as an antibiotic delivery vehicle. **R.B. Fletcher**, J.G. Pribyl, B.C. Benicewicz

362. Synthesis of a conjugated styrene-alt-maleic thioanhydride copolymer via post-polymerization modification. **N.M. Sikes**, D.W. Holley

363. Calcium catalyzed Friedel-Crafts reactions of donor-accepter cyclopropanes. K.A. Nolin, **P. Maloney**

364. Calcium catalyzed 1,3-dipolar cycloadditions of nitrones. K.A. Nolin, **C. Brieva**

365. Synthesis and *in silico* conformational analysis of 1,1-difluorosilolepane (1,1-difluoro-1-silacycloheptane). **T.J. Carrigan-Broda**, J. Bunn, D.V. Hickman, C.R. Metz, G.A. Guirgis

- 366.** Self-assembly with diacetylene alcohols on mica. **E. Garcia**, A. Francuz, M. Gonzalez, J. Klecker, **L.L. Wright**
- 367.** Synthesis and characterization of boronic ester estrogens. **H. Park**, J.A. Pollock
- 368.** Aldol condensations mediated by trimethylsilyl trifluoromethanesulfonate. C.W. Downey, **A. Takashima**, H. Glist
- 369.** Alkylation of ketones and thioesters with propargyl and allyl carboxylates. C.W. Downey, **Y. Liu**, X. Lin, D. Confair
- 370.** Friedel-Crafts additions of indoles to nitrones. C.W. Downey, **C. Poff**
- 371.** Structural and luminescent properties of co-crystals of pyridyl bis-urea macrocycle and naphthalene disulfonic acid salts. **J. Shue**, B. Som, M. Smith, L.S. Shimizu
- 372.** Thin film deposition and polymerization of 10,12-tricosadiynoic acid on PMMA. **Y. Ni**, R. Jelinek, T.W. Hanks
- 373.** Photocatalytic degradation of tetracycline using floating PMMA-TiO₂ microspheres. **A.C. Hartley**, J.D. Glover, J.E. Boyd
- 374.** Activation by reduction of KP1019. **J. Guyton**, J.D. Martin, M. Dunbar, L.K. Stultz
- 375.** White light from hybrid water soluble Au (I) phosphor systems for OLED applications. **C. Williams**, S.B. Marpu, M.A. Omary
- 376.** Toward the synthesis of a new anionic N-heterocyclic carbene and its corresponding metal complexes. A. Carter, **M. Baker**, **A. Mason**, D. Bettler, A. Chagas, D. Tapu
- 377.** Adsorption and reaction of dimethyl methylphosphonate (DMMP) on zirconium hydroxide (Zr(OH)₄). **J. Canty**, C. Gottschau, J. Kollar, M.B. Mitchell
- 378.** Employing a flexible tritopic linker to construct metal-organic frameworks. **C.R. Martin**, G.J. McManus
- 379.** General and enantioselective approach to functionalized piperidines via nucleophilic alkynes. **N. Robinson**, **H. Hill**, D. Penk, M.L. Turlington
- 380.** Synthesis and in vitro characterization of opioid tetrapeptides containing a benzophenone functionality for photoaffinity crosslinking the μ -opioid receptor. **E. Pruitt**, C. Cook, S. Ballard, G.F. Marrone, S. Majumdar, K.R. Wilson
- 381.** Isotopic dependence of the hydrogen-transfer-triggered methyl-group rotation in 5-methyltropolone. **A. Johnson**, J. Hohl, R. Lavrich

- 382.** Withdrawn.
- 383.** Synthesis of TOSUO-containing polyesters using organocatalysts. **A.M. Esper**, B.A. Van Horn
- 384.** Synthesis and characterization of functionalized magnetic iron oxide nanoparticles for shape-memory polymers in epoxy telescope mirrors. R. Cubillan, **K.L. Brodhacker**
- 385.** Intramolecular proton transfer dynamics in malonaldehyde based on Hamilton-Jacobi equation. **S. Shaw**, B.K. Dey
- 386.** Metal-organic frameworks based upon a flexible ligand. **A.J. Soares**, G.J. McManus
- 387.** Complications and opportunities in organocatalytic polymer synthesis: Alkyl-functionalized poly(ϵ -caprolactones). **E.P. Bailey**, B.A. Van Horn
- 388.** Progress toward the total synthesis of speradine E. **K. Weeks**, M. Nakhla, J.L. Wood
- 389.** Concise total synthesis of khusiol. **K.R. Rutkowski**, G.R. Boyce
- 390.** Synthesis of 4'-substituted amino derivatives of pyridoxine. **B.L. Jimenez**, G.R. Boyce
- 391.** Favorskii-type green synthesis of acrylates from cyclopropenones. **S.A. Coury**, J.A. Yazarians, G.R. Boyce
- 392.** Hydrophosphination of styrene using different iron (III)- μ -oxo precatalysts. **E. Minerali**, R. Webster, A.G. Glenn, T.A. Nile
- 393.** Exploiting iron catalyzed hydroboration for the hydrogenation of unsaturated primary aminoalkene substrates. **R. Huntwork**, M. Espinal, R. Webster, A.G. Glenn, T.A. Nile
- 394.** Synthesis of allylic isocyanates. **L.P. Jay**, T.J. Barker
- 395.** Copper-catalyzed radical cascade trifluoromethylation reaction. **J.L. Biaco**, T.J. Barker
- 396.** Synthesis of small molecules for inhibiting aggregation of Alzheimer's amyloid- β peptide. **B.P. Hernandez**, J.A. Roberts, J.M. Hanna, R.K. Lammi
- 397.** Synthesis of substituted urazole radicals. **K.S. Aktepe**
- 398.** Synthesis and antibacterial properties of chalcones. **M. Nguyen**, S. Zingales
- 399.** Synthesis of a pure, dually activated α,β -unsaturated lactam using NaIO₄. **B.A. Miller**, J.M. Plummer

- 400.** Synthetic method to increase the elasticity of boronate-ester linked polymers. **D.A. Free**, S.D. West
- 401.** Synthesis of linear, high molecular weight poly-dicyclopentadiene (PDCPD) via controlled ring opening metathesis polymerization (ROMP). **N. Steese**, H.J. Schanz
- 402.** Synthesis and characterization of heterogeneous carbon supported catalysts by thermally programmed oxidation and reduction. **A. Risner**, T. Kotbagi, M.G. Bakker, F. Sayler
- 403.** Complexation of boronic acids with ditopic Lewis bases. **W.R. Archer**, **E.F. Pounds**, R.D. Pike, W.R. Kwochka
- 404.** Metal-organic frameworks from targeted degradation products. J.F. Eubank, **J. Garcia**, E. Alonso
- 405.** Flipping pre-labs for organic chemistry. **T. Edwards**, T.R. Hayden
- 406.** Trifluorotoluenesulfonyl as a new nitrogen protecting group. **A. North**, M.M. Sibley, M. Wasilewski, M. Wetzler
- 407.** Visible light-promoted additions of potassium organotrifluoroborates to carbonyl compounds. **D.P. Plasko**, J.M. Hanna
- 408.** Visible light-promoted addition of potassium organotrifluoroborates to imines. **C.J. Jordan**, J.M. Hanna
- 409.** Functionalization of silicon substrates with small organic molecules. **M. Carter**
- 410.** Facile synthesis of PEGylated vasopressin, lypressin, and oxytocin analogs. **V. Haberman**, P. Hamilton, M. Wetzler
- 411.** Synthesis of a septanoside from D-ribose. **K. Woolard**, J.A. Hurtak, F.E. McDonald
- 412.** Synthesis of room temperature ionic liquids. **O. Alquzah**, T.R. Hayden
- 413.** Synthesis of pyrrole analogs of combretastatin A-4 from chalcones. H. Holt, **M. Navarez**
- 414.** Phenstatin analogues with non-aromatic attachments in place of the B-ring. H. Holt, **A. Oswald**
- 415.** Withdrawn
- 416.** Fluorinated derivatives of *cis*-stilbene and their anti-cancer potential. H. Holt, **L. Breiner**
- 417.** Growth and structural characterization of mixed self-assembled monolayers (SAMs): 11-Mercaptoundecanoic acid and dodecanethiol. **J. Watkins**, M.R. Martin

- 418.** Refinement of production grade biodiesel. K.C. McGill, **Z. Huffman**, A. Jackson, C. Axt, C. Barret, E. Cronan, J. Williams, T. Wilhoit
- 419.** Halogen-directed Co-catalyzed hydroacylation. **P. Chavis**, D. Wilger
- 420.** A proposed abiotic synthesis of 1-deoxy-d-xylulose-5-phosphate: A potential precursor in the self-catalytic prebiotic synthesis of thiamine pyrophosphate. **M. Syed**, G.G. Springsteen
- 421.** Photo-initiated modification in the hydrophobic nature of a PMMA copolymer. **A. Arndt**, **M. Whitfield**, D. Thompson
- 422.** Factors affecting the electrocatalytic activity of Fe-doped NiO core-shell nanoparticles as catalysts for the oxygen evolution reaction. **E. Lucas**, V. Augustyn, B. Lynch, J.B. Tracy
- 423.** Microwave spectrum of the of 2,3-difluoropyridine-CO₂ complex. **S. Gaster**, C. Funderburk, G.G. Brown
- 424.** Indirect determination of enzyme kinetics using capillary electrophoresis with chemiluminescence detection. **B. Seaton**
- 425.** Jet-cooled high resolution infrared spectroscopy of small van der Waals SF₆ clusters. **A. Turner**, Y. Berger, V. Boudon, L. Bruel, M. Gaveau, M. Mons, A. Potapov, P. Asselin
- 426.** Extraction and microwave spectrum of eugenol. **C. Funderburk**, S. Gaster, G.G. Brown
- 427.** Photoacoustic effect of ethylene: Sound generation due to optically thick plant hormone gases. **D. Ide**, H. Park
- 428.** Atomic force microscopy of polydiacetylene films deposited on poly(methyl methacrylate). **C. Frabitore**, T.W. Hanks, L.L. Wright
- 429.** Halogen bond strength analysis from crystallographic data using quantum mechanical calculations and Hirshfeld surface analysis. **K. Liu**, A.M. Siegfried, C. McMillen, W.T. Pennington, T.W. Hanks
- 430.** Preliminary study on the rate of decay of the chemiluminescent reaction found in glow sticks. C. Baumgardner, D.A. Free, **C.E. Dahm**
- 431.** Calculations of UV-Vis spectra of organic dyes with time-dependent density functional theory. **D. Marshburn**, C. Liu, D.C. Ashley, E. Jakubikova
- 432.** Investigation of periodic trends in catalytic activity for O-H and C-H bond cleavage of ethanol by periodic density functional theory. **M. Schueneman**, S.A. Wasileski
- 433.** Single molecule approach to thin film thickness and its effect on surface dielectric properties. **R. Haley**

434. The rovibronic spectrum of *cis*- and *trans*-HCOH⁺. **R.A. Theis**, R.C. Fortenberry
435. Structural analysis of vanadium and peptide complexes. **A. Brechbill**
436. Withdrawn
437. Metal binding by shell powder of acorns from different *Quercus* species. **M. Bamisile**, B.F. Lasseter
438. Conformational studies of 1-fluoro-1-methylsilacyclohexane. **D.V. Hickman**, T.J. Carrigan-Broda, R.A. Peebles, S.A. Peebles, G.A. Guirgis
439. Multidentate polymer ligands for biocompatible quantum dots: Does sequence matter? **A.F. Loszko**, A.B. Greytak
440. Fuel cell catalyst formation by simultaneous reduction of platinum and graphene oxide. **T. Kusumadjaja**, W. Zhou
441. Kinetic study of ligand exchange by a copper(II) Schiff-base complex. **S. Maxwell**, B. Rose, J.A. Krause, J.J. Stace
442. Studying the physical properties of copper(II) complexes with various counter ions. **P. Kumar**, C. Williams, J.A. Krause, J.J. Stace
443. Increasing nanorod concentration by using a laser during synthesis. **T. Santaloci**, **M. Melvin**
444. Conformational studies of 1,3,5-trisilapentane. **W. Tonks**, D.V. Hickman, T.J. Carrigan-Broda, G.A. Guirgis
445. Stabilization and reaction of small molecules on TiO₂/Au(111) inverse model catalysts. **J. Wilke**, A. Baber
446. The Use of Fluorescence Anisotropy to Study Ligand Binding Events. **C. Donaghy**, M. Paolino, J. Perry Cecile, B.C. Hester
447. Crowding and the activation free energy of protein folding and unfolding. **G.M. Perez Goncalves**, A.H. Gorenssek, A.E. Smith, G.J. Pielak
448. Withdrawn
449. Atoms-in-molecules consideration of the electron density properties of ionic, covalent and metallic bonds. **M.B. Young**, D.A. Clabo
450. Atoms-in-molecules consideration of the electron density properties of inter- and intramolecular hydrogen-bonded molecules. **T.E. Broach**, D.A. Clabo

451. Microwave synthesis of silver nanoparticles using different pentose carbohydrates as reducing agents. **D. Kim, J. Lee, J. Ko, B. Hwang, G. Paniconi**

845. Passive acoustic flow meter. K.C. McGill, **A. Shue**, A. Savage, A. Burleson, C. Gantt, J. Moore

863. Determining the activation energy of the rate-limiting step of the Fenton reaction. **L.A. Ligon**, P. Tumlin, T. Cohen, T. Spence

905. Determination of polycyclic aromatic hydrocarbons from decorative candles and incense. **C. Erb**, T. Ragsdale, K. Williams

941. Probing candidates for the active transport of neurotherapeutic agents. **K. Russell**, D.J. Schedler

942. Synthesis of broad spectrum glycosidase inhibitors through Diels-Alder cycloaddition. **J. Mason**, D.J. Schedler

Cutting Edge of Biological Inorganic Chemistry

Columbia Metropolitan Convention Center
Richland A

J. H. Dawson, A. Rogers, *Organizers*
T. Bryson, *Presiding*

3:20 452. Unravelling the complexity in the multi-protein heme shuttle pathway in *Staphylococcus aureus*: LSD cog-wheel kinetics from electrospray ionization mass spectrometry. **M.J. Stillman**, M. Tiedemann

3:50 453. Synthesis and spectroscopic properties of P(V) phthalocyanines and tetraazaporphyrins. **N. Kobayashi**

4:20 454. Investigating cytochrome P450, peroxidases and other heme iron enzymes. **J.H. Dawson**

Undergraduate Research Posters - Analytical & Inorganic Chemistry

Columbia Metropolitan Convention Center
Exhibit Hall

H. Zur Loye, *Organizer*

4:30 - 6:00

- 84.** The analysis of EDTA in dried bloodstains using DRIFTS and ATR to determine limits of detection with chemometrics. **C.O. Granger, C.E. Witt, J. McCutcheon**
- 455.** Redox dopamine sensing with chitosan-catechol modified electrodes. **B. McDowell, H. Ben-Yoav, N. Peixoto, A. Silue**
- 456.** Using cotton plant waste to remove cadmium from aqueous solutions. **A. Rizzuti, K. Mouzone**
- 457.** Photoacoustic microscopy with carbon black: Sound generation by pure elemental carbon. **A. Korshun, H. Park**
- 458.** UPLC-MS characterization of membrane phospholipids from *Vibrio* species following exposure to exogenous fatty acids. **D. Anderson, Z.J. Avello, S. Symes, D. Giles**
- 459.** HPLC method development for separation of methanol extracts from yellowstriped oakworm. **J. Howell, M. Melnychuk, J. Ellenburg, P.B. Nolibos, A. Thomas**
- 460.** Atomic absorption analysis of electrolyte content in sports drinks and food products utilized by athletes for muscle cramp relief. **K. Dowlatshahi, S.E. Hooper**
- 461.** Elemental analysis of cigarette butt leachates in seawater. **M. DeMaily, G.E. Potts**
- 462.** Development of an inexpensive atomic emission spectrometer for the detection of easily ionizable elements. **D.A. Free, J.P. Troutman, C.E. Dahm**
- 463.** GC-MS analysis of commercially available food products containing mint flavoring. **V.R. Griffin, C.E. Dahm**
- 464.** A first-generation amperometric galactose biosensor. **C. Steele, T. Munoz, S. Borum, W. Case, M.C. Leopold**
- 465.** Carboxylic acid multi-walled carbon nanotubes modified with β -cyclodextrin for the detection of uric acid on an electrochemical sensor. **M.A. Schwarzmans, S.D. Gillespie, M.B. Wayu, M.C. Leopold**
- 466.** Carboxylic acid functionalized carbon nanotubes covalently modified with β -cyclodextrin for the electrochemical detection of uric acid. **S.D. Gillespie, M.A. Schwarzmans, A. Kane, C. Bowles, M. Trawick, M.B. Wayu, M.C. Leopold**
- 467.** Fluorescence studies of aromatic and polycyclic aromatic compounds. **N. Dos Santos, H.V. Clontz**
- 468.** Optimization of sarcosine oxidase production for use in amperometric biosensors. **E. Doll, N. Labban, M.J. Pannell, J.A. Pollock, M.C. Leopold**

- 469.** Effects of solvent on electrochemistry of biogenic amines in non-mammalian systems. **S.M. Wright**, N.J. Kuklinski
- 470.** Characterization of two different laser dyes using spectral characteristics and mass spectrometry. **L. Hochman**, K.W. Davies
- 471.** Solvatochromism in complexes with Fe(II) to Ti(IV) charge transfer. E.S. Carlton, A. Myers, M. Turlington, J. Pienkos, **P.S. Wagenknecht**
- 472.** Effect of the dispersant Corexit 9500A on the vertical movement of oil spill material through Alabama beach sand. **K. Hobbs**, K. Livermore, A.C. Nichols, D. Steffy
- 473.** Testing 7,000 year old hair for cocaine and plasticizers. **E. Fairchild**, N.M. Sikes, J.M. Meyers
- 474.** Defensive and attractive chemicals isolated and identified from predatory lady beetles. **A. Hixson**, Y. Kajita, M.F. Santiago
- 475.** Column chromatographic comparison of methanol extracts derived from yellowstriped oakworm and oak leaves. **J. Ellenburg**, J. Howell, E. Vences, S. Dauda, P.B. Nolibos, A. Thomas
- 476.** Boat drone: Progress towards continuous autonomous environmental monitoring of Savannah River Site water bodies. **T. Whiteside**, N.A. Moya, D. Nasol
- 477.** Cesium-133 column chromatography separation via ammonium molybdophosphate polyacrylonitrile resin. **A.M. Owen**, Y. Tsai, J. Steeb
- 478.** Bronze supported gold nanostructures for zinc radioisotope capture. **D.S. Meeker**, S. Hunyadi Murph
- 479.** Antioxidant activity of plant extracts derived from *Hedera helix*. **E. Burnham**, N. Duncan, A.D. Gibson
- 480.** *Dracaena braunii* as a phytoremediation agent for toxic heavy metal contamination from soil and water. **K. Allaire**, C.E. MacGowan, T.J. Hizer
- 481.** Analysis of heavy metal concentrations in the Conasauga, Oostanaula, and Coosa Rivers utilizing a PerkinElmer NexION 350D ICP-MS. **C. Fernandes**, **W. Jones**, D. Jones, K. Zimmermann
- 482.** FRET-based fluorescence assay for microRNA detection. **R.D. Croxton**, C.L. Colyer
- 483.** Profiling over the counter remedies commonly used to treat arthritis-related disorders. **H.Z. Msimanga**

- 484.** Evaluation of the effects of tetracycline on the growth of freshwater algae. **R.R. Reiter**, N. Nelsen, A. Mina
- 485.** Incorporating aerogels into electrochemical glucose biosensors. **N.D. Kosciuszek**, L. Sheard, M.C. Leopold, A.S. Harper-Leatherman
- 486.** Synthesis and preliminary hydrolytic degradation of monoiodo and triiodo PCL materials. **V.O. Bailey**, E.E. Burry, B.A. Van Horn
- 487.** Identifying conjugated molecules from mixtures by mass spectrometry with selective excitation. **R. Ford**, R.B. Grubbs
- 488.** Analysis of SdsA1 and Bds1 sulfohydrolase activity by liquid chromatography-mass spectrometry. **G.L. Waddell**, J.S. Reveral, C.R. Gilmer, M. Forconi, J.L. Fox
- 489.** Determination of oxy and met Mb in cow tissue. **A. DeBusk**, A.C. Suroviec
- 490.** Effect of molecular oxygen on T1 relaxation times and interproton distance determinations by NOE. **S. Ge**, J. Bame, C. Butts, A.G. Glenn, T.A. Nile
- 491.** Ultra performance liquid chromatography mass spectrometry of ribonucleosides. **J.H. Simpson**, D. Todd, B. Tannous, N. Chiu
- 492.** Quantitative determination of oxalic acid and caffeine in tea using gas chromatography-mass spectrometry. **J.A. Kroeger**, K.S. Kroeger
- 493.** The inclusion of benchtop NMR technology in the analysis of products from the separation of a three component mixture via acid/base extraction. **C.E. Glessner**, S.M. Deimling, K.L. Yearty, R.W. Morrison
- 494.** Binding studies of Monensin A methyl ester with alkyl amines. D. Downes, K. Bacon, N. Blair, A. Bass, A. Sennett, M. Fujita, **F.A. Khan**
- 495.** Identifying impurities in TBAF. **A. Andreen**, P. Rugar, I.A. Adams
- 496.** Progress toward the development of an X-ray fluorescence method for the detection of mercury vapor. **A.C. Westmoreland**, R.E. Bachman
- 497.** Determination of zinc, copper, and iron in multivitamin/multimineral tablets. **S.S. Stephenson**, S.C. Willis, R. Fietkau
- 498.** Kinetics of crystal violet color fading experiment via a small footprint diode array spectrometer. **P.E. Lott**, R. Fietkau
- 499.** Determination of oxalate levels in common tea brands. **R.A. Crane**, R. Fietkau

- 500.** Visible spectra of various colored ballpoint inks. **R.C. Pendley**, R. Fietkau
- 501.** Kinetics of bromophenol blue color fading experiment via a small footprint diode array spectrometer. **Z. Popovic**, R. Fietkau
- 502.** Catalytic ability of platinum overgrown on various geometries of gold nanostructures for water splitting. **K. Hoang**
- 503.** Room temperature ionic liquids as a greener alternative for the extraction of acetaminophen. **V. Harris**, T.R. Hayden
- 504.** Withdrawn
- 505.** Quantification of aspartame via solid phase extraction and high performance liquid chromatography. **C. Hamilton**
- 506.** Investigating the pH dependent Fe(III/II) redox behavior using a novel tridentate ligand. **M. Haggard**, A. Hand, P.S. Ray, S.J. Slattery
- 507.** Effect of golf course on water quality. A. Walton, **S.A. Myers**
- 508.** Molecular dynamics investigation of factors influencing self-assembly of detergent micelles. **B. Bonnett**, C. Scaggs, L. Freeze, A. Hoffmaster, S.F. Ganjabad, B. Mertz, E.L. Harvey
- 509.** Investigation and optimization of a calcium carbonate precipitation experiment. **K. Manaley**, J. Cooper
- 510.** Bovine rumen bacteria application to improve electricity production from cellulose by dairy digester in microbial fuel cells. **S. Chung, C. Kim, R. Chung, D. Moon**
- 511.** Effect of *Ruminococcus albus* addition into microbial fuel cells constructed with dairy digester microorganisms. **S. Chung, T. Kong, J. Kim**
- 512.** Identification of chromium reducing bacterial isolates from a wastewater treatment plant. **A. Dacres**, R.H. Harris
- 513.** Characterization of chromium reducing bacteria from a wastewater treatment plant. **C. Duscent**, J. Ewan, C. Hawkins, S. Bradley, R.H. Harris
- 514.** Synthesis and characterization of ruthenium(II) complexes involving electron-rich arene ligands and cyclononane-based ligands. **P. Zdunek**, J.P. Lee
- 515.** Synthesis and characterization of cyclopentadienyl- and pentamethylcyclopentadienyl-Co(III) complexes containing chiral bidentate amine ligands. **J.A. Money**, J.P. Lee

- 516.** Synthesis and characterization of Co(III) phosphite and phosphine complexes supported with pentamethylcyclopentadienyl. **P.A. Dean**, J.P. Lee
- 517.** Designing alkynyl bridged Fe^{II}-Ti^{IV} complexes that are inert to oxidative decomposition. **D. Agakidou**, J. Pienkos, P.S. Wagenknecht
- 518.** Synthetic strategies for anchoring Fe^{II} – Ti^{IV} dyes onto TiO₂ for use in dye-sensitized solar cells. **A. Myers**, J. Pienkos, M. Turlington, P.S. Wagenknecht
- 519.** Transition metal carbide nanoparticles coated with noble metal monolayers for CO-tolerant catalysis. **A.T. Barth**, M. Milina, Y. Roman-Leshkov
- 520.** Synthesis of metal fluoride complexes relevant to catalysis. D. Wilger, **J. Willis**
- 521.** New annulated thiones and their transition metal complexes. **D. Bettler**, **A. Changas**, D. Tapu
- 522.** New transition-metal complexes of polycyclic thioureas. **R. Hooper**, **O. Kuykendall**, D. Tapu
- 523.** Novel thione based ligands: Synthesis and complexation. **P. Jean**, **B. Hunt**, D. Tapu
- 524.** Preparation and characterization of new schiff base ligands and their complexes with Cu(II) and Ni(II). **R. Davis**, A. Garcia, P.H. Mueller, N. Deifel
- 525.** Iron polypyridyl complexes for photocatalytic hydrogen generation. **R.J. DiRisio**, C.L. Hartley, M.E. Screen, W. McNamara
- 526.** Hydrogen evolution catalyzed by a cobalt complex containing an asymmetric Schiff-Base ligand. **J.E. Armstrong**, P.M. Crossland, M.A. Frank, W. McNamara
- 527.** Hybrid organic-inorganic epoxy/polyhedral oligomeric silsesquioxane nanocomposites reinforced with functionalized multi-walled carbon nanotubes for epoxy telescope mirrors. L. Smith, **K.L. Brodhacker**
- 528.** Understanding the formation of copper (II) oxide through solid-state metathesis. **D.T. Boyle**, A.J. Martinolich, J.R. Neilson
- 529.** Development of electrodes of hydrated and solvated transition metal oxides for energy storage. **A. Costine**, R. Wang, W. Lo, V. Augustyn
- 530.** Effect of hydroxylation on anthocyanin-based dye sensitized solar cells. **J. Wilson**, D. Mathews, B. Thurman, B. Kirkwood
- 531.** Microwave synthesis of silicon nanoparticles for high capacity Li-ion battery anodes. **R. Bujol**, R. Quirino, J. Wu

532. Withdrawn

533. Synthesis of a novel iminophosphorane ligand. **N. Chung**, A. Buchard, A.G. Glenn, T.A. Nile

534. Characterizing iron oxide nanoparticles with Mossbauer spectroscopy in a nontraditional matrix: An application of Mossbauer spectroscopy to bioinorganic nanoscience. **M. Vidmar**

535. Evaluation of coated gold nanorods on zebrafish embryos. **M. Braselton, J. Smith**

536. Synthesis and characterization of platinum indazole complexes with potential anti-cancer activity. **K.W. Barwick**, A.J. Bachman, K.A. Wheeler, R.E. Bachman

537. Peculiar properties of quantum dots: Cadmium sulfide and zinc sulfide nanoparticles. **K. Parson**, K.T. Jackson

538. Symmetry breaking in nanorod synthesis using metal salts. **S. Cannavino**, D. Ferrara

539. Structure and biophysical study of human galanin truncation peptide hGal(2-11). **S.E. Clinkscales**, M.W. Giuliano

540. Synthesis and characterization of some new halometallates. L. Peterson, J.G. Kelley, **M. Barnhill**

541. Synthesis of “Trithiopod”, a potential mercury chelator. **J. Liles, S. Keaney**, J. Hugdahl, A.M. Kiefer

542. Synthesis of new unsymmetric, bidentate pyridyl-n-heterocyclic carbene ligands and their cationic silver and ruthenium complexes. **K.D. Leibfried**, H.J. Schanz

543. Complexation of borinic acid derivatives with Lewis bases. **N.J. Wiebelhaus**, R.D. Pike, W.R. Kwochka

544. Studies on water sorption by metal saccharinate compounds. L. Peterson, A. Guy, **J. Blackwell**

545. Characterization of hierarchically porous palladium on carbon catalysts in vapor-phase continuous hydrogenation reactions. **B. Lummus**, T. Kotbagi, M.G. Bakker

546. Transition-metal catalyzed nitrene transfer reactions of olefins using PhINTs in the presence of an ionic liquid. **K. Riley**, H.U. Valle, J.P. Emerson

547. Synthesis, characterization, and antimicrobial studies of chemically modified textile materials using zinc oxide nanoparticles for potential prevention of healthcare-associated infections. **M.D. Reece**, C.R. De Silva, N.A. Dragan, H.N. Kline, S. Printz, C.L. Huffman, I. Bose

548. Synthesis of vinyl phosphonates using organocopper reagents. **T. Gerschick**, S. Mize, C.W. Alexander

549. Investigation of zirconium-based metal organic frameworks for photocatalytic applications. **K. Westendorff**

550. Novel nanoparticle conjugates for prevention of oxidative damage. **J. Rodriguez Gonzalez**, D. Gil, V. Reukov

551. Electrocatalytic activity of metal-organic framework PCN-223 in the oxygen reduction reaction. **B. Huffman**, P. Usov, A.J. Morris

552. Enhancement of iodine hopping in dye-sensitized solar cells: Tetralkylammonium triiodide oranoiodide cocrystals. **A. Miller**, A. Siegfried, T.W. Hanks, W.T. Pennington

553. Swelling properties of microgel/polycation polyelectrolyte complexes. **G. Hwang**, **J. Woo**, **J. Park**, **J. Kim**

1048. Towards the synthesis of azobenzene dicarboxylic acid derivatives for the preparation of novel microporous metal organic frameworks. **S. Avant**, P.J. Rosado

TUESDAY MORNING

Plenary Session

Columbia Metropolitan Convention Center
Ballroom A/B

A. W. Peters, *Organizer, Presiding*

8:00 554. GFP: Lighting up life. **M. Chalfie**

Analytical Chemistry - Neuro- & Electrochemistry

Columbia Metropolitan Convention Center
Ballroom B

H. Zur Loye, *Organizer*
P. Hashemi, *Presiding*

9:15 555. Coregulation of serotonin and histamine in the context of neurodegeneration. **S.A. Samaranayake**, R.F. Roscoe, A. Abdalla, R. Robke, H. Nijhout, M. Reed, J. Best, R. Booze, P. Hashemi

9:45 556. Serotonin neurotransmission in different brain regions: A combined voltammetry, microscopy and mathematical study. **A. Abdalla**, P.U. Pathirathna, S.A. Samaranyake, Y. Jin, C. Atcherley, M. Heien, M. Reed, H. Nijhout, J. Best, D. Linden, P. Hashemi

10:15 557. Amphetamine's influence on cortical serotonin neurotransmission in mice: A voltammetric analysis. **R. Robke**, P. Hashemi

10:45 558. Voltammetric and behavioral characterization of the involvement of serotonin in depression. **R.A. Saylor**, P. Hashemi

11:15 559. Monitoring neurotransmitter release *in vivo* via fast-scan cyclic voltammetry following pesticide exposure. **S. Berger**, P. Hashemi

Biological Chemistry - Structural Biology

Columbia Metropolitan Convention Center
Richland C

H. Zur Loye, *Organizer*
C. Washington, *Presiding*

9:15 560. Solid state NMR structure determination of membrane proteins in phospholipid bilayers: New developments and applications. **B.B. Das**, F.D. Doty

9:45 561. A transition state "Trapped": Using the QM cluster model to examine the energetics of constrained biphenyl dihedral rotation within a modified threonyl-transfer RNA synthetase. **N.J. Deyonker**, T.J. Summers

10:15 562. Role of sodium ions in peptide and protein structures. **A.L. Stewart**, A. Lorts, H. Parmer, R.L. Lewis, E.L. Seal, R.C. Fortenberry

10:45 563. Synthetic biology approach to natural product diversification. **G.J. Williams**

11:15 564. Peptoid library agar diffusion assay to identify antimicrobial peptoids. **K. Bicker**, K. Fisher, A. Corson, J. Turkett, S. Armstrong

Chemical Education

Columbia Metropolitan Convention Center
Carolina A

H. Zur Loye, *Organizer*
C. R. Dockery, *Presiding*

9:15 565. Why are students so scared of organic chemistry? **S. Zingales**

9:45 566. Electronic cigarettes: Teaching students to be instrumental in analysis. **L. Hiatt, M. Mann**

10:15 567. Development of an organometallic course: Preparing students for graduate work. **K. McWilliams**

10:45 568. Open source instruments for environmental monitoring and science education. **J.S. Summers, B. Hickman, T. Stack**

11:15 569. A story of continuing education in chemistry. **A. Rahman**

Cope Symposium: Molecules to Functional Supramolecular Materials

Hilton Columbia Center
Banquet 1

Cosponsored by ORGN
L. S. Shimizu, *Organizer*
K. Shimizu, *Organizer, Presiding*

9:15 570. Designing singlet fission materials. **L.M. Campos**

10:05 Discussion.

10:15 571. Withdrawn

11:05 Discussion.

Cutting Edge of Biological Inorganic Chemistry

Columbia Metropolitan Convention Center
Richland A

J. H. Dawson, A. Rogers, *Organizers*
D. P. Ballou, *Presiding*

9:15 572. Biological and biomimetic oxidation of lignin. **A. Butler, S. Springer**

9:45 573. Defining the cellular iron pools used for stress-resistant metallocofactor biogenesis. **F. Outten**

10:15 574. N₂ase & H₂ase vibrational spectroscopy with NRVS & FT-IR. **S.P. Cramer**

10:45 575. Nucleotide-resolution structural maps of DNA and RNA. **T.D. Tullius**

11:15 576. Novel Fe-S cluster binding partners in *E. coli*: Biochemical characterization of the Grx4-IbaG interaction. A. Dlouhy, H. Li, A. Albetel, B. Zhang, D. Mapolelo, S. Randeniya, A. Holland, M. Johnson, **C.E. Outten**

Electronic Structure: Concepts & Applications

Columbia Metropolitan Convention Center
Congaree B

Cosponsored by PHYS
S. Garashchuk, V. Rassolov, *Organizers*
D. A. Clabo, *Presiding*

9:15 577. Sculpting at the nanoscale. **B. Sumpter**, L. Liang, J. Jakowski

10:00 578. A computational workflow for designing silicon donor qubits: From electronic structure to device modeling. **F.A. Mohiyaddin**, J. Jakowski, J. Huang, B. Sumpter, T. Humble

10:15 579. Ab initio condensed-phase chemistry. **S. Hirata**

10:45 580. Implicit models for short-range contributions to solvation energies from exchange repulsion, dispersion attraction, and hydrogen bonding. **D. Chipman**

11:15 581. *Ab initio* propagator studies of P-N cluster, superhalogen and double-Rydberg anions. **J.V. Ortiz**

Emerging Environmental Contaminants

Columbia Metropolitan Convention Center
Congaree A

Cosponsored by ENVR
Financially supported by LECO Corp
S. D. Richardson, *Organizer, Presiding*

9:15 582. Emerging per- and polyfluorinated compounds in environmental media. **M. Strynar**, S. Newton, R. McMahan, L. McMillan, A. Lindstrom

9:45 583. 1,4-Dioxane: A surface water contaminant with important implications for drinking water quality. **D. Knappe**, C. Lopez-Velandia

10:15 584. Using granulated activated carbon in the control of emerging disinfection by-products in drinking water disinfection plants. **A. Cuthbertson**, S.D. Richardson, S.Y. Kimura, D. Knappe, B.D. Stanford, E. Dickenson, R.S. Summers

10:45 585. Exploring environmental chemical space through HR/AM mass spectrometry and cheminformatics: The example of wastewater-derived organic micropollutants. **L. Ferguson**, G.J. Getzinger

11:15 586. Photochemical release of sediment bound brevetoxin (PbTx-2) from resuspended sediments. **R.N. Mead**, W. Mickler, G.B. Avery, S.A. Skrabal, R.J. Fiber, J.D. Felix

Materials Chemistry - Nanoparticles

Columbia Metropolitan Convention Center
Carolina B

H. Zur Loye, *Organizer*
V. A. Villareal, *Presiding*

9:15 587. Incorporation of transition metal complexes into polymers and their conversion to metal nanoparticles supported on hierarchically porous carbons. **M.G. Bakker**, T. Kotbagi, K.H. Shaughnessy, C. LeDoux, H. Cho, J. van Zee

9:45 588. Withdrawn

10:15 589. Multipod nickel nanostructures: Synthesis, characterization and applications. **P. Vakil**, B. Ashley, G.F. Strouse

New Chemistry Toward Functional Polymeric Materials

Columbia Metropolitan Convention Center
Lexington A

Cosponsored by PMSE and POLY
Financially supported by NSF, Ingevity
C. Tang, *Organizer*
B. C. Benicewicz, *Presiding*

9:15 590. Covalent mechanochemistry for functional polymers. **S. Craig**

9:45 591. Photoinitiated, living, cationic polymerization of 4-methoxystyrene. **W. You**

10:15 592. Cancer cell-selective killing polymer/copper combination. **P. Xu**

10:45 593. Polymer grafted nanoparticles as functional hybrid materials. **B.C. Benicewicz**

11:15 594. Melt processable precursors for carbon fiber production. **G.C. Miller**, J.S. Riffle

11:45 Concluding Remarks.

Physical Chemistry - Theory/Computation

Columbia Metropolitan Convention Center
Ballroom A

H. Zur Loye, *Organizer*
Z. S. Davis, *Presiding*

9:15 595. Evolution of chemical reaction fronts based on a modified Hamilton-Jacobi equation and computing reaction paths. **B.K. Dey**

9:45 596. Investigation of the mechanism of fullerene and carbon nanotube formation by molecular dynamics simulation. **T.J. Fuhrer**, B. Amofah

10:15 597. Improving ab initio absorption intensities for HNO. **H. Dhah**, R.J. Hinde

10:45 598. Understanding superfluid helium droplets using nuclear density functional theory. **M. Dutra**, R.J. Hinde

11:15 599. Ab initio calculations of CO₂ polarizabilities and hyperpolarizabilities using a finite field approach. **R. Beil**, R.J. Hinde

Structure-Property-Relationship of Nanoscale Materials - Spectroscopy, Surfaces & Catalysis

Hilton Columbia Center
Banquet 2

A. B. Greytak, T. Vogt, H. Wang, *Organizers*
D. A. Chen, *Organizer, Presiding*

9:15 600. Exciton dynamics and light-driven H₂ generation in multicomponent semiconductor-metal colloidal nanorod heterostructures. **T. Lian**

9:45 601. Unraveling trap state fluorescence in colloidal quantum dots. D.L. Woodall, A.K. Tobias, **M. Jones**

10:15 602. Bimetallic nanocrystals: A unique probe for monitoring the catalytic reactions by surface-enhanced Raman scattering. **D. Qin**, Y. Wu, J. Li

10:45 603. Direct visualization of atomic-scale model catalyst features from ultrahigh vacuum to near-ambient pressures. **A. Baber**

11:15 604. Chemical activity of single-site transition metal centers in metal-organic coordination complexes at surfaces. **S.L. Tait**

Synthesis & Application of Biofunctional Nanomaterials

Columbia Metropolitan Convention Center
Richland B

Cosponsored by COLL
Q. Wang, *Organizer*
Q. Wang, *Presiding*

9:15 605. Coupling vascularization and osteogenesis by timed and localized delivery of growth factors with self-assembled nanogels. **E. Jabbari**

9:45 606. Quantifying oxygen's role in modulating cellular proliferation, invasion, and drug resistance in 3D paper-based cultures. **M.R. Lockett**

10:15 607. Biological membrane manipulation through use of a biocompatible ferrofluid. **E. Freeman**

10:45 608. Effect of nanotopography created by plant virus nanoparticles on osteogenic differentiation of bone derived mesenchymal stem cells. **K. Metavarayuth**, P. Sitasuwan, J. Luckanagul, Q. Wang

11:15 609. Polymeric implants for the treatment of diet induced obesity and glucose intolerance. **M. Gower**

Biological Chemistry Posters

Columbia Metropolitan Convention Center
Exhibit Hall

H. Zur Loye, *Organizer*

10:15 - 11:45

287. Tat-specific factor 1's role in HIV RNA stability. **A.P. Goodwin**, H.B. Miller

610. Withdrawn

611. Novel application of TEC-disulfide replacement showcased in the synthesis of SFTI-1. **J. Barbaretta**

612. Statistical thermodynamic modeling of early A β oligomer formation: Incorporation of solvation in a self-consistent field framework. **N. van der Munnik**, T. Wei, M. Moss, M. Uline

613. High-throughput screens of drug-induced cytochrome P450 inhibition. **J. McIntosh**, N.A. Whitman, M.R. Lockett

- 614.** Structural analysis of gluten exorphin B5 by NMR and computational methods. **S. Hemmerly**, B. Horswell, S.M. Damo, M.V. Voehler, R. Bowen, W.A. Tallon, A.J. Privett, J. Beale, **C. Clinger**
- 615.** Designing synthetic lectins to investigate metastatic potential in colon and prostate cancers. **T. Hundal**, R. Huang, D.J. Gordon, E.E. Gatrone, K. O'Connell, A.A. Veldkamp, J. Lavigne
- 616.** Regulation of gene expression via peptide mimics. **O. Perdue**, A.L. Stewart
- 617.** The structure of the biofilm-controlling response regulator BfmR from *Acinetobacter baumannii* reveals details of its DNA-binding mechanism. **G.L. Draughn**, E. Feldmann, B. Bobay, B. Roth, A. Olson, R. Thompson, M. Milton, L. Actis, C. Davies, J. Cavanagh
- 618.** Ionic interactions that stabilize and denature protein and peptide structures. **A. Lorts**, A.L. Stewart
- 619.** Pyrazinamide conjugates as possible potential anti-tubercular agents. **D.D. Buchanan**, **B. Torkian**, K. Bathala, Z.L. Corley, S. Panda
- 620.** Curcumin conjugates as potential pharmacophores. **S.J. Thomas**, **J. Capito**, K. Bathala, S. Panda
- 621.** Structure-based design of dimer interface peptides of B-Raf which block paradoxical signaling induced by Vemurafenib. C.M. Beneker, **C. McInnes**
- 622.** Cellular uptake of curcumin by yeast. **J. James**
- 623.** Structural and biophysical investigation of the antiviral molecule BST-2 interactions with ligands. **C. Keutcha**, D. Kober, T. Brett
- 624.** Phytochemical profiles, antioxidant, and anti-diabetic properties of two Pigeon pea varieties. R.J. Syed, L. Wang, **Y. Wu**
- 625.** Identifying the roles of individual phosphate groups in multiply phosphorylated binding motifs in DNA repair. **K. Kim**, L. Pedersen, E.F. Derose, T.W. Kirby, R. London
- 626.** Kinetic and mechanistic study of tetrahydrodipicolinate *N*-succinyltransferase from *Serratia marcescens*. **S. Graham**, C.M. Johnson
- 627.** Laccase-catalyzed oxidation products of phenolic pollutants and product identification using mass spectrometry. **C. Rae**, C.M. Johnson
- 628.** Kinetic analysis of pyruvate kinase from *Cryptosporidium parvum* and the effects of a novel disulfide bridge. **E.A. Ballew**, K.L. Hayden, D. Chattopadhyay

- 629.** Elucidation of the efficacy of the antitumor quinone, beta-lapachone in *BRCA1* mutant breast cancer cells expressing elevated NQO1 levels. **K.E. Brokaw**, L. Palmquist, M. Srougi
- 630.** Sequence and structure in human neuropeptides. **M.W. Giuliano**, S.E. Clinkscales, E.A. Mendoza, A.C. Schwartz
- 631.** Expression, purification and characterization of allergen Cuc m 2. **A.B. Kapingidza**, C. Schlachter, M. Chruszcz
- 633.** Expression and purification of a globin-coupled sensor diguanylate cyclase from *Shewanella* sp. strain ANA-3. **J.A. Walker**, E.E. Weinert
- 634.** Hydrogenation of 3-methyl- and 4-methoxy-biopterin to their corresponding tetrahydro derivatives for crystallographic studies of nitric oxide synthase. **J. Boscia IV**, A. Rogers, C. Davies
- 635.** Isolation and characterization of antibiotic compounds produced by two strains of Gram-negative bacteria. **D. Beals**, A.L. Wolfe
- 636.** Purification and characterization of adenosine aminohydrolases from *Pisum sativum*. **L. Thicklin**, P. Kline
- 637.** Increased accuracy and resolved positive bias in HPLC analysis of vitamins B₁ and B₆ in whole blood/serum. **T. Wright**
- 638.** The use of choline and its derivatives to retain viable cells of the probiotic bacteria *Lactobacillus reuteri*. **T. Zimmerman**, S. Walston, R. Gyawali, N. Nwamaioha, S. Ibrahim
- 639.** 4-Hydroxy tetrahydropicolinate reductase from lysine biosynthesis pathway as target for development of antimicrobial compounds. **S. Pote**, T. Sheahan, K. Datar, M. Chruszcz
- 640.** Isolation and extraction of pseudopyronine B, an antibacterial compound, from a *pseudomonas* strain RG/RF B10. **L. Bouthillette**, A.L. Wolfe
- 641.** Antibiotic activity of natural products produced by bacteria isolated in Western North Carolina. **A.M. Thurman**, S.C. Seaton, A.L. Wolfe
- 642.** Eukaryotic heme *a* synthase: Importance of oligomerization. **N.J. Harris**, N.G. Taylor, O. Khalimonchuk, J.L. Fox
- 643.** Characterization of SufS-SufE interaction during Fe-S cluster assembly in *Escherichia coli*. **G. Dong**, F. Outten
- 644.** Synergistic effect of *LactoBacillus paracasei* 441 and inulin to improve the viability of bifidobacteria in fermented milk. **D. Gad El-Rab**, A. Ayad, T. Zimmerman, S. Ibrahim

- 645.** Date palm (*Phoenix dactylifera*) extract has inhibitory effect against *Escherichia coli* O157:H7. **D. Gad El-Rab**, A. Ayad, T. Zimmerman, S. Ibrahim
- 646.** Preliminary expression and purification of a putative flavin reductase from *Hyphomicrobium sulfonivorans*. **E. Featherston**, M. Culpepper, M.B. Culpepper
- 647.** Evolutionary conservation of binding of hemoglobins to haptoglobins across species. **O.A. Vanderpuye**, K. Troutman, N. Kellam, C. Dunn
- 648.** Development of new antimicrobials by a novel fusion method. O. Bagasra, **A.T. Perez-Johnson**
- 649.** Activation of protein tyrosine kinase by environmental toxicants. **Y. Beni**, S. Guha
- 650.** Effects of sodium ions on collagen structure. **H. Parmer**, A. Stewart
- 651.** Quantifying laccase activity and degradation of 17 α -ethinylestradiol using *Lentinula edodes* and *Phanerochaete chrysosporium*. **A. Milliken**, C.M. Johnson
- 652.** Structural and biochemical analysis of Bat-CoV HKU9 C nonstructural protein 3 domain. **R. Hammond**, M. Chan, N. Tan, M.A. Johnson
- 653.** Facets of weak preferential interactions between folate and betaine. P. Bhojane, **M.R. Duff**, K. Bafna, G. Rimmer, P.K. Agarwal, E.E. Howell
- 654.** Chemoselectivity in OleT(JE): Substrate constriction sets the tone . **J.A. Amaya**, C. Rutland, N. Leschinsky, T.M. Makris
- 655.** Investigating mutagenic forms of cytochrome P450 BS β for biofuel application. **C. Rutland**, J.A. Amaya, T.M. Makris
- 656.** Characterization of the SufR transcriptional regulator in the regulation of the exclusive iron-sulfur cluster assembly pathway in pathogenic *Mycobacterium* species. **S.L. Witcher**, F. Outten, A. Gutierrez, O. Manley
- 657.** Improvements to microbial biodiesel production through dynamic regulation. **E. Arvay**, A. Yaguchi, G. Rodriguez, M.A. Blenner
- 658.** Molecular mechanism for polypeptide translocation catalyzed by domain I & II of ClpA. **N. Scull**, A.L. Lucius
- 659.** Heme uptake via the HtaB surface-anchored protein in *Corynebacterium diphtheriae*. **B.L. Ferrell**, R.C. Uluisik, B. Adobaw, M.P. Schmitt, D.W. Dixon
- 660.** Role of ferritins in iron donation to Suf Fe-S cluster assembly in *Escherichia coli*. **N. Bolaji**, P.A. Lindahl, F. Outten

- 661.** Autoreduction studies of ShrNEAT2 domain in *Streptococcus pyogenes*. **S.S. Thompson**, E. Draganova, Y. Cao, M. Ouattara, Z. Eichenbaum, G.S. Lukat-Rodgers, K.R. Rodgers, D.W. Dixon
- 662.** Cellular uptake of polyphenols in a bacterial protein expression system. **B. Griffin**
- 663.** Isothermal titration calorimetry studies on the binding of 4-methoxy-tetrahydrobiopterin to endothelial nitric oxide synthase. **L. Tran**, J.H. Pinner, J. Boscia IV, J. Barton-Souza, J. Tucker, A. Rogers
- 664.** Eukaryotic heme *a* synthase: Roles of conserved amino acid residues. **N.G. Taylor**, N.J. Harris, O. Khalimonchuk, J.L. Fox
- 665.** Effect of mitochondrial reactive oxygen species on pre-adipocyte differentiation. **C.M. Matzie**
- 666.** The effects of aspirin on the growth, functionality, and protein expression profile of the beneficial gut bacterium *Lactobacillus rhamnosus* (ATCC 53103). **S. Ibrahim**, T. Obanla, S. Adjei-Fremah, R. Gyawali, T. Zimmerman, M. Worku
- 667.** Impact of hydrocolloids on the production of acid whey in Greek yogurt. **R. Gyawali**, S. Walston, T. Obanla, N. Idris, N. Nwamaioha, T. Zimmerman, S. Ibrahim
- 668.** Synthesis and characterization of meso-tetrakis(2-fluoro-4-methoxyphenyl)porphyrin. **A. Adeyemo**
- 669.** Fluorescence and UV-VIS studies of quinone-induced protein modifications. **C. Thomas**, M. Booker, T.V. Albu, J. Kim
- 670.** Characterization of the DNA binding activity of bacterial response regulator BfmR from *Acinetobacter baumannii*. **M. Milton**, G. Draughn, R. Thompson, J. Cavanagh
- 671.** Sulfated diflavonoids are potent, selective, and allosteric inhibitors of human plasmin. **D.K. Afosah**, R. Al-Horani, N. Sankaranarayanan, U.R. Desai
- 672.** Comparison of structure and function of 2-methylcitrate synthase (*mcsA*) from *Aspergillus fumigatus* and citrate synthase (HCS) from *Homo sapiens*. **C. Schlachter**, M. Chruszcz
- 673.** Lipophilic optimization of peptoid library design. **J. Turkett**, K. Fisher, K. Bicker
- 674.** Biomolecular interaction determination and quantification by microscale thermophoresis. **E. Lee**, A. Lazic, S. Duhr, D. Breiersprecher
- 675.** Characterization of the monooxygenase subunit of dimethylsulfide monooxygenase from *Hypomicrobium sulfonivorans*. **J. Gordon**, B.D. Johnson, M.B. Culpepper, M. Culpepper

676. Effects of crowding on the activation enthalpy and entropy of protein folding. **A.H. Gorenssek**, A.E. Smith, G.M. Perez Goncalves, G.J. Pielak

Catalysis & Biocatalysis Posters

Columbia Metropolitan Convention Center
Exhibit Hall

T. M. Makris, *Organizer*

10:15 - 11:45

677. Taming complexity in reverse: "Simplifying" complex natural products. **T.A. Bender**, M.R. Gagne, J.A. Dabrowski

678. Interaction of atomic oxygen with Ag(111) and Ag(110) Surfaces: Oxygen adsorption at surface versus subsurface. **S. Isbill**, S. Roy

679. Methane partial oxidation on nickel carbide. **R. Smoak**, C. Wen, J. Lauterbach

680. Uptake mechanism and binding energetics of the chemical warfare agent simulant 2-CEES within MOF UiO-66. **C.H. Sharp**, J. Abelard, A. Plonka, Q. Wang, A. Frenkel, W. Guo, C.L. Hill, D. Troya, J.R. Morris

681. Selective catalytic behavior of water-soluble Pd and Pd-alloy nanoparticles capped with glutathione for bilayer-hydrogenation/isomerization of allyl alcohols. **S. Bhama**, F.P. Zamborini

682. Single-site ruthenium catalyst for CO₂ hydrogenation. **S. Sanchez**, J. Jimenez, C. Wen, J. Lauterbach

683. Comparison of CO oxidation activity on Pd/ α -Fe₂O₃ nanorods and Pd/ α -Fe_{2-x}Mn_xO₃ nanorods with controlled surface structure and morphology. **E. Freeman**, C. Wang, J. Lauterbach

Frontiers in Nucleic Acid Chemistry Posters

Columbia Metropolitan Convention Center
Exhibit Hall

M. W. Germann, W. Wilson, *Organizers*

10:15 - 11:45

684. Cellular uptake study of fluorescently tagged minor groove binders targeting glucose transporters. **C. Needham**, N. Neill, M. Buchanan, A. Bourdelais, S. Varadarajan

- 685.** Thiophene “sigma-hole” as a concept for preorganized, specific recognition of G•C base pairs in the DNA Minor Groove. **P. Guo**, A. Paul, A. Kumar, A. Farahat, D. Kumar, S. Wang, D.W. Boykin, W. Wilson
- 686.** Understanding electrostatic effects on binding kinetics and affinities of ETS transcription factors and DNA. **T.D. Vo**, S. Wang, G.M. Poon, W. Wilson
- 687.** Progressing development on systematic mixed DNA minor groove binding agents. **A. Paul**, A. Kumar, R.K. Nanjunda, D.W. Boykin, W. Wilson
- 688.** Effects of β -alanine inserts and cationic substituents on polyamide-DNA binding and PU.1 inhibition. **B. Liu**, S. Wang, K. Aston, K. Koeller, J. Bashkin, W. Wilson
- 689.** DNA-methylation characteristics of a DNA minor groove alkylator conjugated to various cancer cell-targeting ligands. **D. Lasch**, C. Mills, S. Varadarajan
- 690.** Structural impact of single ribonucleotides in duplex DNA. **M. Evich**, A. Spring-Connell, M.W. Germann
- 691.** Probing complex formation of DNA and the ETS family transcription factor PU.1 using NMR diffusion. **M. Evich**, S. Esaki, G.M. Poon, M.W. Germann
- 692.** Intermolecular interactions of TIAR with the -3' stem loop of West Nile Virus. **J. Siemer**, J. Zhang, H. Liu, M. Brinton, M.W. Germann
- 693.** Probing the osmotic sensitivity of DNA recognition by ETS-Family proteins. **A.V. Albrecht**, S. Xhani, G.M. Poon
- 694.** Efficient photocleavage of DNA with near-infrared irradiation using a symmetrical quinoline pentamethine cyanine dye. **K. Kiernan**, C. Holder, M. Henary, K.B. Grant
- 695.** Testosterone conjugated DNA methylating agents targeted to prostate cancer cells. **L. Lowder**, M. Powell, E. Elliott, N. Neill, A. Bourdelais, S. Varadarajan
- 696.** Chloride-specific, photo-induced DNA cleavage by a 9-aminomethyl anthracene dye. **M. Safiarian**, K.B. Grant
- 697.** Identification and validation of *Thermus thermophilus* FadR-binding DNA sequences. **M. Lee**, H. Um, M. Van Dyke
- 698.** Directed covalent attachment of peptide nucleic acids to proteins. **J. Gerlach**, N. Shank
- 699.** Synthesizing disulfide monomers to create biologically susceptible linkages in PNA oligomers. N. Shank, **B. Campbell**

- 700.** Statistical thermodynamic study on ssDNA aptamers in varying biological environments. **M. Jahan**, M. Uline
- 701.** Cyano-nilotamide conjugated DNA methylating molecules targeting androgen receptor positive cancer cells. **C. Mills**, M. Powell, E. Elliott, N. Neill, A. Bourdelais, S. Varadarajan
- 702.** DNA interactions and photocleavage by a neutrally charged tri-nuclear Cu(II) hexaazatriphenylene complex. **C. Fischer**, D. Williams, M. Kassai, L. Gude, M. Fernández, A. Lorente, K.B. Grant
- 703.** Identify high-fidelity codon set for incorporating peptide modified oligonucleotides. **C. Guo**
- 704.** Assessing the DNA binding affinities of polyamine anthracene conjugates under high ionic strength conditions. **K.T. Nguyen**, K.T. Schuster, J.J. Archer, O. Phanstiel, K.B. Grant
- 705.** DNA binding interactions and long-wavelength photocleavage by pentamethine-bridged phenanthridinium carbocyanine dyes. **K. Basnet**, E. Soriano, M. Henary, K.B. Grant
- 706.** DNA photocleavage in frozen solutions using meso sulfur-substituted heptamethine cyanine dye and near-infrared light. **A.C. Clay**, X. Ma, M. Henary, K.B. Grant
- 707.** Characterization of silver nanoclusters encapsulated with alternate DNA templates. **I. Rankine**, J.T. Petty, M.W. Germann, B. Bello
- 708.** Fluorescence polarization assays for characterization of chemical modulators of PU.1. **N. Erlitzki**, G.M. Poon
- 709.** Fine structural details of HIV-1 and HTLV-II DNA substrates. **Q. Li**, C.N. Johnson, M.W. Germann
- 710.** Exploring HIV integrase 3'-processing using designed DNA substrates: Importance of the CA step. **Q. Li**, Z. Ferris, M.W. Germann

Inorganic Chemistry - Bonding

Hilton Columbia Center
Carolina Wren

H. Zur Loye, *Organizer*
K. Varazo, *Presiding*

10:45 711. Comparison of nitrogen-iodine halogen bonds and oxygen-iodine halogen bonds. **C.W. Padgett**, G. Guillet, S.N. Bailey, A. Goetz, M. Tran, K. Hillis, D. Adams, W.T. Pennington, W.E. Lynch

11:15 712. Uses of self-consistent field calculated atomic radii. **J.R. Wasson**, J.W. Hall, S.K. Hutchison

TUESDAY AFTERNOON

Analytical Chemistry - Instrumentation

Columbia Metropolitan Convention Center
Ballroom B

H. Zur Loye, *Organizer*
A. Allen, *Presiding*

1:00 713. Ecodyst innovative EcoChyll is revolutionizing the rotary evaporator. **G.M. Adjabeng**

1:30 714. Quantitative identification of volatile organic compounds and free base nicotine present in electronic-cigarette vapor via GC/MS detection. **E. Smith**, C.H. Lisse

1:45 715. Synthesis and quantification of the chemical markers of melanin to enhance early diagnosis of melanoma. **C. Weddle**, K. Glass, K.D. Sienerth

2:00 716. Microfluidic system for simultaneous detection of intracellular [Ca²⁺] and insulin secretion from islets of Langerhans in response to fatty acids. **B. Bandak**, L. Yi, N. Mukhitov, W. Leng, M.G. Roper

2:30 717. Novel and practical alternative to the 'Commercial Instrumentation' paradigm. **S.D. Abbott**

3:00 Intermission.

3:20 718. Monitoring primary amine secretion from islets of Langerhans using micellar electrokinetic chromatography with laser-induced fluorescence detection. **K. Evans**, W. Leng, M.G. Roper

Biological Chemistry - Structural Biology

Columbia Metropolitan Convention Center
Richland C

H. Zur Loye, *Organizer*
M. Blahut, C. Wise, *Presiding*

1:00 719. Scope and utility of promiscuous enzymes for natural product diversification. **S.A. Meiser**, G.J. Williams

1:30 720. Chance or design: What makes a good kemp eliminase? **L.R. Fanning**, M. Forconi, E. Sanchez

1:45 721. Probing the structure-activity relationship of *Escherichia coli* extracellular death factor. **R. Ulrich**, L. Nguyen, M. Blackledge

2:00 722. Translating unnatural amino acids with phenotypically-diverse computationally-engineered EF-Tu variants. **V. Cox**, E.A. Gaucher

2:30 723. The abiotic synthesis of pyrimidine nucleobases. **A. Clay**, G.G. Springsteen

2:45 724. Using non-natural components to probe natural biosynthetic pathways. **K. Almasy**, S.A. Meiser, G.J. Williams

3:00 Intermission.

3:20 725. Crystal structure of endothelial nitric oxide synthase in the presence of L-Arginine and 3-methyl-tetrahydrobiopterin or 4-methoxy-tetrahydrobiopterin. **J.H. Pinner**, J. Boscia IV, L. Tran, J. Barton-Souza, J. Tucker, B. Roth, C. Davies, A. Rogers

3:35 726. Determining the structure-activity relationship of the *Bacillus subtilis* extracellular death factor. **L. Nguyen**, R. Ulrich, M. Blackledge

3:50 727. Molecular modeling of lipid monolayers at air/water interface. **D. Ohadi**, M. Uline

4:20 728. Transport of amyloid- β across the blood-brain barrier by p-glycoprotein. **H. Holt**, E. Moore, M. Faucett, F. Gonzalez, M. Moss

Catalysis & Biocatalysis

Columbia Metropolitan Convention Center
Hall of Fame

T. M. Makris, *Organizer*
C. Wen, *Presiding*

1:00 729. CO₂ hydrogenation on single site heterogeneous cobalt catalyst. **J.D. Jimenez**, C. Wen, J. Hattrick-Simpers, J. Lauterbach

1:30 730. High-throughput investigation of cobalt oxide catalysts for CO oxidation and N₂O decomposition. **K. Mingle**, E. Sasmaz, C. Wen, J. Hattrick-Simpers, J. Lauterbach

2:00 731. Withdrawn

2:30 732. Mercury oxidation over Cu-SSZ-13 catalysts under SCR conditions for power plant applications. **B. Galloway**, B. Padak

3:00 Intermission.

3:20 733. Stabilizing effects of polyoxoniobates on molecular copper-oxo species in alkaline water for water oxidation catalysis. **Q. Yin**, Y. Hu, S. Lauinger, C.L. Hill

3:50 734. Withdrawn

4:20 735. Fast molecular O₂ based hydroxylation of tertiary α -carbonyl compounds using KOH as the base. **M.R. Choudhury**, Y. Zheng, B. Wang

Colloid Chemistry

Hilton Columbia Center
Carolina Wren

H. Zur Loye, *Organizer*
D. Swinton, *Presiding*

1:00 736. Bioenabled synthesis of anisotropic noble metal nanoparticles for surface enhanced Raman spectroscopy and colorimetric sensing. **X. Geng**, T. Zarkovic Grove

1:30 737. Catalytic graphitization of monolithic nanocast carbon by iron, cobalt and nickel nanoparticles. **C. Thambiliyagodage**, P. Araujo, M.G. Bakker

2:00 738. Critical sequence dependence in multicomponent ligand binding to gold nanoparticles. **W.D. Siriwardana**, D. Zhang

2:30 739. Counter-ion effects on electrolyte bindings to gold nanoparticles. **H.S. Perera**, D. Zhang

3:00 Intermission.

3:20 740. Particle-protein-dye system toward activated fluorescence and cancer theranostics. **M. Burdette**, R. Jenkins, I. Bandera, R. Powell, T. Bruce, X. Yang, Y. Wei, S.H. Foulger

3:50 741. Adsorption studies of divalent, dinuclear coordination complexes as molecular spacers on nanostructure carbon materials. **N. Elathram**, J.C. Poler

4:05 742. Silica/Poly(propargyl methacrylate) core/shell nanoparticles with surface attached fluorophores. **D. Hendricks**, M. Burdette, I. Bandera, S.H. Foulger

Cope Symposium: Molecules to Functional Supramolecular Materials

Hilton Columbia Center
Banquet 1

Cosponsored by ORGN
K. Shimizu, *Organizer*
L. S. Shimizu, *Organizer, Presiding*

1:00 743. Dynamic processes in crosslinked polymer networks. **W. Dichtel**

1:50 Discussion.

Cutting Edge of Biological Inorganic Chemistry

Columbia Metropolitan Convention Center
Richland A

J. H. Dawson, A. Rogers, *Organizers*
B. Hawkins, *Presiding*

1:00 744. New heme-Cu-O₂ constructs: Factors leading to O-O reductive cleavage. **K.D. Karlin**

1:30 745. Ligand induced allostery in *Pseudomonas aeruginosa* cytoplasmic heme binding protein (PhuS) drives the protein-protein interaction with heme oxygenase. **A. Wilks, D. Deredge, W. Huang, C. Hui, P. Moenne Loccoz, P. Wintrode**

2:00 746. Heme uptake in pathogenic bacteria: Role of the heme axial ligands. **D.W. Dixon, E. Draganova, R.C. Uluisik, S.S. Thompson, B.L. Ferrell, C.S. Keutcha, N. Akbas, Y. Cao, M. Ouattara, Z. Eichenbaum, M.P. Schmitt, D.P. Collins, J.H. Dawson, G.S. Lukat-Rodgers, K.R. Rodgers**

2:30 747. Functionalization of myoglobin by artificial metalloporphyrinoids. **T. Hayashi**

Electrocatalysis

Hilton Columbia Center
Breakout 1/2

A. K. Vannucci, *Organizer, Presiding*

1:00 748. A miniaturized test platform for research on PEM fuel cell catalysts without liquid electrolyte. J.A. Shetzline, S. Bukola, **S.E. Creager**

1:30 749. Effect of co-sensitizers on boron dipyrromethene–thiophene–triphenylamine-based dyes and carotenoid acid dye-sensitized solar cells. **T.C. Douglas, N. Kaneza, J. Zhang, H. Liu, R.E. Adams, R.H. Schmehl, Y. Liu, T. Snowden, S. Pan**

2:00 750. Au nanoparticle modified indium tin oxide ultramicroelectrode for single particle spectroelectrochemistry and ultrasensitive electrochemistry sensing. **Y. Ma, S. Pan**

2:30 751. Electropolymerization of β -cyclodextrin onto multi-walled carbon nanotubes for enhanced selective detection of uric acid. **M.B. Wayu**, L. DiPasquale, M.A. Schwarzmann, S.D. Gillespie, M.C. Leopold

3:00 Intermission.

3:20 752. Electrochemical dioxygen reduction catalyzed by a (nitro)cobalt(perfluorophthalocyanine) complex and the possibility of a peroxy-nitro complex intermediate. **J.A. Goodwin**, J.K. Agbo, J. Zukzek, A. Samuel, T.H. Aslund, S.E. Creager, J.A. Shetzline

3:50 753. Simultaneous electrocatalytic reduction of CO_2 and photoelectrochemical water splitting: Routes toward efficient and selective electrocatalysts. **N. Kaneza**, X. Peng, N. Liyanage, R. Rodrigues, M. Bhula, J.H. Delcamp, S. Pan

4:20 754. Electrocatalytic and photocatalytic reduction of CO_2 to CO with Re-Pyridyl-NHCs. **N. Liyanage**, H.A. Dulaney, A. Huckaba, J.W. Jurss, J.H. Delcamp

Electronic Structure: Concepts & Applications

Columbia Metropolitan Convention Center
Congaree B

Cosponsored by PHYS
S. Garashchuk, V. Rassolov, *Organizers*
D. Chipman, *Presiding*

1:00 755. Getting down to the fundamentals of hydrogen bonding. **G.S. Tschumper**

1:30 756. Theoretical methods for non-covalent interactions. **C.D. Sherrill**

2:00 757. Weak bonds and strong influences: Halogen bonding, other ‘sigma hole’ interactions and applications. **K. Donald**

2:30 758. Investigation of electron density and bonding by the atoms-in-molecules method of mixed main-group metal hydrides and fluorides M_2AX_4 ($\text{M}=\text{Li}, \text{Na}$; $\text{A}=\text{Be}, \text{Mg}, \text{B}^+, \text{Al}^+$; $\text{X}=\text{H}, \text{F}$) and carbon and silicon hydrides Y_mH_n ($\text{Y}=\text{C}, \text{Si}$; $m, n=2, 3, 4, 6$). **D.A. Clabo**

3:00 Intermission.

3:20 759. Inorganic computational astrochemistry: Electronic structure of metal monoacetylides and other stories. **N.J. Deyonker**, S.D. Dickerson, M. Fioroni

3:50 760. Analysis of transition state stabilization by non-covalent interactions in the Houk–List model of organocatalyzed intermolecular aldol additions using functional-group symmetry-adapted perturbation theory. **B. Bakr**, C.D. Sherrill

4:05 761. Comparison of explicitly correlated methods for computing high-accuracy benchmark energies for noncovalent interactions for Noncovalent Interactions. **D. Sirianni**, L.A. Burns, C.D. Sherrill

4:20 762. Correlated orbital approximations: Semiempirical quantum chemistry beyond the neglect of overlap. **J. Margraf**, R.J. Bartlett

Emerging Environmental Contaminants

Columbia Metropolitan Convention Center
Congaree A

Cosponsored by ENVR
Financially supported by LECO Corp
S. D. Richardson, *Organizer, Presiding*

1:00 763. Nanohybrids for the determination of fundamental aspects of nanoparticle effects on the environment. **J. Lead**

1:30 764. What are you inhaling from that e-cigarette liquid? J. Lackey, N. Wallbillich, J.E. Keating, **G.L. Glish**

2:00 765. The co-oxidation of selected emerging contaminants during the autooxidation of humic materials. M. Smith, **J.L. Ferry**

2:30 766. Metals and organic contaminants in oysters and sediments, southeastern North Carolina. **S.A. Skrabal**, R.N. Mead, H.K. Liberatore, L. Kipp, S. Sherard, M. Steagall

3:00 Intermission.

3:20 767. Fast scan cyclic voltammetry to study speciation of copper in aqueous solution with carbon fiber microelectrodes. P. Pathirathna, **T. Siriwardhane**, S.L. Morgan, S.P. McElmurry, P. Hashemi

3:50 768. Compound specific-combustion-GC-IRMS determination of ethanol in precipitation: Impact of biofuel. **M. Casas**, R.J. Fiber, R.N. Mead, G.B. Avery, J. Willey, C. Lane, M. Shimizu

4:20 769. Effect of ethanol on production of chromophoric dissolved organic matter (CDOM) in rainwater. **M.A. Taylor**, R.N. Mead, R.J. Fiber, G.B. Avery, J. Willey

4:50 770. Identification and quantification of priority disinfection by-products using high resolution mass spectrometry. **S.Y. Kimura**, A. Cuthbertson, J. Allen, S.D. Richardson

Environmental Chemistry Posters

H. Columbia Metropolitan Convention Center
Exhibit Hall

Zur Loye, *Organizer*

1:00 - 2:30

- 771.** An *in situ* ATR-FTIR investigation of the influence of phosphate on oxytetracycline sorption on kaolinite. **M. Dolui**, J. Mierzwa, S. Rakshit
- 772.** Thermodynamic analysis of the PPCPs using computational simulations. **R. Kyung**
- 773.** Co-oxidation of halides during the autoxidation of Fe(II). **F.J. Wang**, J.L. Ferry
- 774.** Trace measurements of greenhouse gases in ambient air using cavity ring-down spectroscopy. **L.P. Gamage**, W.K. Gichuhi
- 775.** Exploring the presence of microplastics in Salt Creek. **T. Tyler**, T. Janesheski
- 776.** Investigation of NO_x and Hg chemistry in oxy-combustion of coal. **N.N. Choudhury**, B. Padak
- 777.** Adsorption of copper (II) by peanut hulls in a fixed-bed continuous flow column. **T.S. Cook**, C.L. Huffman
- 778.** Heterogeneous strategies to reduce HO scavenging during ozonation. **B. Solomon**, J.L. Ferry
- 779.** Development of a rapid mapping technique for quantitatively assessing mercury concentrations in the atmosphere. **S. Pounds**, **W. Moore**, J. Liles, P.B. Usher, R.D. Brown, A.M. Kiefer
- 780.** Multidisciplinary approach to water quality management in the St. Lawrence River. **C. DeVane**, E. Brahmstedt, C. Lumbrazo
- 781.** Adsorption of antimony onto hematite. **J. Mierzwa**, S. Rakshit
- 782.** Abundance and distribution of microplastic particles in Winyah Bay, South Carolina. **D. King**, G. Boneillo, J. Guentzel
- 783.** Taxonomic classification of phytoplankton with multivariate optical computing: Improvements to instrumental design and image processing methods. **C. Rekully**, S.T. Faulkner, S. Tazik, T. Richardson, T.J. Shaw, M. Myrick

- 784.** Influence of phosphate on tungsten (VI) sorption on hematite: A macroscopic and spectroscopic probe into the mechanism. **B.H. Sallman**, S. Rakshit, J. Mierzwa
- 785.** Quantifying the stoichiometry of hydrogen peroxide and gallic acid during the pH-dependent autooxidation of gallic acid. **M. Smith**, J.L. Ferry
- 786.** Salinity and pH dependence of copper leaching from anti-fouling marine paints. **D.W. Carpenetti**, A.C. Martin, K. Reed

Frontiers in Nucleic Acid Chemistry

Columbia Metropolitan Convention Center
Lexington A

M. W. Germann, W. Wilson, *Organizers*
D. Graves, *Presiding*

1:00 787. Epigenetic modification effects on the i-motif and G-quadruplex forms of single strand DNA. M.M. Molnar, R.K. Morgan, B. Summerford, T.A. Brooks, **R.M. Wadkins**

1:30 788. Biophysical characterization of c-MYC NHE-III 1 models for G-quadruplex and i-Motif constructs flanked by duplex DNA. A. Metz, V.H. Le, S.J. West, **E.A. Lewis**

2:00 789. How POT1 unfolds quadruplex DNA. **J. Chaires**, J. Trent, W. Dean, R. Gray, L. DeLeeuw

2:30 790. Complex kinetics and underlying pathways of nucleic acid structural remodeling chaperoned by retroviral nucleocapsid proteins: A single-molecule spectroscopic study. **H. Wang**

3:00 Intermission.

3:20 791. Chemistry and biology of N^5 -alkyl-Fapy-dG lesions. **M.P. Stone**, M. Egli, R.S. Lloyd, A. Mc Cullough, C.J. Rizzo, R.J. Turesky

3:50 792. Towards understanding protein-DNA binding specificity. **J. Guo**

Inorganic Chemistry - Solid State

Columbia Metropolitan Convention Center
Ballroom C

H. Zur Loye, *Organizer*
K. Varazo, *Presiding*

1:00 793. Highly luminescent molecular wires and coils: Linear complex arrays of up to eight cuprous centers. **M. Stollenz**, J.E. Raymond, L.M. Pérez, J. Wiederkehr, N. Bhuvanesh

1:30 794. New frontiers in photochemistry: Semiconductor nanocrystals as triplet sensitizers. **S. Garakyaraghi**, C. Mongin, F.N. Castellano

2:00 795. Structural and optical studies of $\text{Bi}_{13-x}\text{Sb}_x\text{S}_{18}\text{I}_2$ and $\text{Bi}_{1-x}\text{Sb}_x\text{SI}$. **R.A. Groom**, A. Jacobs, M. Cepada, R. Drummey, S.E. Latturner

2:30 796. Bismuth flux synthesis of a novel intermetallic superconductor -- MgNi_2Bi_4 . **M.B. Hertz**, S.E. Latturner

3:00 Intermission.

3:20 797. Cage opening of the *closo*-carborane ligands: The reaction of *closo-o*- $\text{C}_2\text{B}_{10}\text{H}_{10}$ with triosmium carbonyl cluster complexes. **J. Kiprolich**, R.D. Adams

3:50 798. Organometallic chemistry of ruthenium-gold carbonyl cluster complexes. **J. Tedder**, R. Adams

4:20 799. Studies of the reactivity of unsaturated dirhenium-gold carbene complexes. **P. Dhull**, R. Adams, V. Rassolov

Materials Chemistry Posters

Columbia Metropolitan Convention Center
Exhibit Hall

H. Zur Loye, *Organizer*

1:00 - 2:30

800. Synthesis, characterization and self-assembly of pyridine-modified polymer with beta-glucuronidase with retained activity. **Y. Xu**, J. Yan, J. Yang, X. Zhang, Y. Nie, L. Lee, Q. Wang

801. Assembly of polymer-protein core-shell nanoparticles for enhanced *in vivo* immunogenicity. **X. Zhang**, X. Zhao, J. Luckanagul, J. Yan, Y. Nie, A. Lee, Q. Wang

802. Relationship between nanocrystalline structure and water stability of magnesium oxychloride. **R.F. Gochez**, C.L. Kitchens

803. Investigation of carbon nanotubes & cellulose nanocrystals for potential use in microelectromechanical systems. **M. Jiang**, C.L. Kitchens

804. Protein based dual-functional, water- and electro-responsive, actuators. **N. Carter**, T. Zarkovic Grove

- 805.** *In situ* investigation of the influence of neutral ligands on photoluminescence and shell growth in CdSe-based quantum dots. **M.Y. Gee**
- 806.** Synthesis and optical properties of gold/near IR emitting quantum dot hybrid nanoparticles. **K.M. Dipple**, D. Fontecha, A.K. Tobias, M. Jones
- 807.** DNA functionalized gold nanoparticles for thermometry applications. **A. Baumert**, S. Hunyadi Murph, K. Coopersmith
- 808.** Electrodeposition and electrochemical properties of graphene-cobalt oxide polymorph hybrids: Application as pseudocapacitive electrodes. **S.C. Botero Carrizosa**, S. Gupta
- 809.** Reversible approach for silicon surface modification. **X. Zhang**, V. Hollimon, D. Brodus, R. Peters
- 810.** Photocatalytic properties of novel copper tantalum niobium oxide. **N. Pant**
- 811.** Synthesis and characterization of redox active electrochromic coronene containing polyimides. **S.C. Paul**, V. Cammarata
- 812.** Graphene oxide and reduced graphene oxide modified sand for water purification. **D. Corella**, B. Baruah
- 813.** Microwave-specific heating to achieve melting/dissolution of crystalline species formed in nuclear waste glass. **J.H. Christian**, A.L. Washington, K. Fox
- 814.** Electrospun PbTiO₃ nanofibers: An oxygen generating photocatalyst. **M. Donaldson**, Z. Hood, K. Senevirathne
- 815.** Artificial peptides for improved synthesis and performance of lithium ion battery electrodes. **A. Winton**, M.A. Allen
- 816.** Synthesis of zeolite materials for noble gas separation. **O. Rivera**, R. Achey, M.S. Wellons, C. Klug, D. Hunter
- 817.** Investigation into the air stability of fluorescent InP quantum dots through the use of gel permeation chromatography. **A. Roberge**, Y. Shen, J. Stein, B.M. Cossairt, A.B. Greytak
- 818.** Developing radiation tolerant polymers for nuclear material waste storage. **T. Truong**, J. Christian, J. Teprovich, J. Wilson, M. Kesterson, J. Velten, I. Widenhover, L. Baby, A.L. Washington
- 819.** Nanofiber photocatalysts: The effect of co-catalysts in photocatalytic H₂ generation. **K. Latimer**, Z. Hood, K. Gilroy, Y. Xia, K. Senevirathne
- 820.** Graphene oxide modified macroporous TiO₂-CeO₂ photocatalyst. **D. Corella**, B. Baruah

821. Adsorption of caesium from contaminated waters on phosphotungstic acid embedded in silica matrix. **K. Seaton**, I. Little, C. Tate, A. Vasiliev

822. Kinetic isotope effect on the crystallization process with transition zone theory. **F. Hou**, J.D. Martin, E. Dill, J.C. Folmer, A.A. Josey

823. Effects of oleylamine to oleic acid ratios in the surfactant-assisted synthesis of anisotropic brookite Titanium Dioxide nanoparticles. O. Love, **J. Davis**

824. Asymmetric membranes containing micron-size silicon for high performance lithium ion battery anode. **I. Byrd**

Metal Complexes of Scorpionate & Related Ligands

Columbia Metropolitan Convention Center
Carolina A

D. L. Reger, *Organizer, Presiding*

1:00 825. Pyridylborates as a new type of robust scorpionate ligand: From metal complexes to polymeric materials. C. Cui, G. Pawar, P. Shipman, S. Jeong, J. Sheridan, **F. Jaekle**

1:30 826. Dinuclear metallacycles with single anion bridges: Unusual magnetic and NMR properties. **D.L. Reger**, A.E. Pascui, M.D. Smith, J. Jezierska, A. Ozarowski

2:00 827. *N*-confused scorpionates and their metal complexes. **J.R. Gardinier**

2:30 828. Metal complexes of a new ditopic, bis(pyrazolyl)methane-based heteroscorpionate ligand. **R.F. Semeniuc**, J.B. Coulton, A.C. Smith, K.A. Wheeler

3:00 Intermission.

3:20 829. Proton NMR properties of some heavy metal scorpionate complexes. **J.L. Templeton**, K. Lavoie, R. Beattie

3:50 830. Coordination chemistry of N-heterocyclic chalcogenone ligands: From soft scorpionates to NHC surrogates. **D. Rabinovich**

4:20 831. Undergraduate capstone course focused on writing a research proposal. **D. Garza**

4:35 832. How to increase the size of your department by several fold in 3 easy steps. **S.S. Mason**

Physical Chemistry Posters

Columbia Metropolitan Convention Center
Exhibit Hall

H. Zur Loye, *Organizer*

1:00 - 2:30

833. Functional solubility parameters of organic semiconductors: Poly(3-hexylthiophene) (P3HT) and PCBM. **M. Roesing**, J. Howell, D.S. Boucher

834. Preparation of Pd/Al₂O₃ and Pd/CeO₂ catalysts for the oxidation of methane. **J.M. McGuire**, A.C. Banerjee

835. Investigation into catalytic efficiency of Pd/Al₂O₃ and Pd/CeO₂ for oxidation of carbon monoxide. **J.D. Gary**, A.C. Banerjee

836. Controlled dealloying of alloy nanoparticles toward optimization of electrocatalysis on spongy metallic nanoframes. **G.G. Li**, E. Villarreal, Q. Zhang, H. Wang

837. LFER and kinetic study of Brønsted-acid catalyzed lactonization of α,α -disubstituted- γ -hydroxy esters. **G.T. Wilson**, K.S. Petersen

838. Determination of ligand binding and host-guest interactions in one dimensional micro/nanoscale structures via fluorescence microscopy. **P. Kittikhunnatham**, B. Som, P. Paudel, L.S. Shimizu, A.B. Greytak

839. Strong electrostatic absorption of platinum precursors on a model carbon support. **G. Seuser**, R. Banerjee, D.A. Chen, J.R. Regalbuto

840. Electrospray ionization and collision induced dissociation of ionic liquid cluster EMIM⁺ - [EMIM-DCA]. **M. Norton**, C. Annesley, K. Lemke

841. Understanding methanol oxidation on Pt and Pt-Re bimetallic surfaces. **K. Xie**, A. Duke, J.R. Monnier, D.A. Chen

842. Interaction of Lewis acidic gases and Brønsted acids with MOFs: Potential degradation pathways. **L. Flores**, W.B. Copeland, J.G. Murphy, **D.A. Dixon**

843. Examining the impact of the artificial nucleobase imidazole on the properties of silver(I) clusters. **E.J. Baucum**, J.T. Petty, J. Muller, J.C. Leon

844. Mixed self-assembled monolayers of alkanethiols and their formation on gold substrates. **S. Graham**, M.R. Martin

845. Withdrawn

846. Application of a surimi-based coating on shrimp during storage time. **R. Tahergorabi, A. Sharaf-Eddin, S. Ibrahim**

847. CO₂ Adsorption on MIL-53(Al) crystals formed on anodized aluminum oxide disc. **A. Uprety, C. Pyles, A.M. Massari**

848. In situ DRIFTS study of the reactivity of zirconium hydroxide for the decomposition of dimethyl methylphosphonate (DMMP). **J. Kollar, M.B. Mitchell**

849. Plasmon-enhanced spectroscopic study of adsorption, desorption and exchange of thiol ligands on highly curved gold nanoparticle surfaces. **E. Villarreal, G.G. Li, Q. Zhang, H. Wang**

850. Analyzing phosphorylation of prebiotic molecules by schreibersite with polarization-modulation: Infrared reflection-absorption spectroscopy. **K. Slavicinska, T.J. Beckman, H.L. Abbott-Lyon**

851. Analysis of the decomposition of a nerve agent simulant, dimethyl methylphosphonate (DMMP), by the Lindqvist polyoxometalate: C₈[Nb₆O₁₉]. **C. Gottschau, M.B. Mitchell**

852. The rovibronic spectrum of *c*-C₃H. **M. Bassett, R.C. Fortenberry**

853. Insights on plasmon-driven oxidative coupling of thiophenol-derivates: Evidence on steady-state active oxygen species. **Q. Zhang, H. Wang**

854. Electron spin resonance investigation of solvated electrons in a neon matrix. **X. Liu, J.J. Banisaukas, L.B. Knight**

855. Effect of solution ionic strength on the pK_a of the nitroxide pH EPR probe 2,2,3,4,5,5-hexamethylimidazolidin-1-oxyl. **K. Margita, M.A. Voynov, A.I. Smirnov**

856. Profiling reaction progress using automatic spectrophotometric titrations. **M.J. Keller, J.A. Lynch**

857. Understanding the activity of Pt-Re bimetallic clusters on titania and Pt-Re alloy surfaces in the water gas shift reaction. **T.D. Maddumapatabandi, A. Brandt, K. Xie, A. Duke, D. Chen**

858. Chemical gardens confined to two dimensions. **M. Bentley, O. Steinbock**

Physical Chemistry - General

Columbia Metropolitan Convention Center
Ballroom A

H. Zur Loye, *Organizer*
G. K. Kaufman, *Presiding*

1:00 859. Tracking charge carriers in a conjugated polymer nanoparticle. **Y. Jiang**, T. Nongnual, J. McNeill

1:30 860. Fast tracking of single conjugated polymer nanoparticles with high spatial resolution. **T. Nongnual**, J. McNeill

2:00 861. Effect of sample mass on the thermal decomposition of “simple” systems. **T.C. Devore**

2:30 862. Low temperature adsorption of ethanol on TiO₂/Au(111) inverse model catalysts. **D.T. Boyle**, J.A. Wilke, V.H. Lam, A. Baber

2:45 863. Determining the activation energy of the rate-limiting step of the Fenton reaction. **L.A. Ligon**, P. Tumlin, T. Cohen, T. Spence

3:00 Intermission.

3:20 864. Radical chain reduction of CCl₄ initiated by illumination of SPEEK solutions. **M. Islam**

3:50 865. Investigation of prebiotic molecule adsorption on the meteoritic mineral schreibersite by infrared reflection-absorption spectroscopy. **H.L. Abbott-Lyon**

Reform Pedagogy in Undergraduate Chemistry

Columbia Metropolitan Convention Center
Carolina B

C. R. Dockery, G. E. Potts, *Organizers, Presiding*

1:00 866. Gateway chemistry curricular reform improves diversity in STEM majors. **D.A. Canelas**

1:30 867. Flipped peer-led team learning: A reform pedagogy that preserves content coverage. **S.E. Lewis**, J. Robert, R. Oueini, A. Mapugay

2:00 868. Not all students perform equally: A case in general chemistry. **M.L. Head**

2:30 869. Creative exercises in inorganic chemistry: Working to promote meaningful learning. **J. Shaw**

3:00 Intermission.

3:20 870. Pharmaceutical analysis CURE (Classroom Undergraduate Research Experience) in the general chemistry lab. **W. Cory**

3:50 Panel Discussion.

4:15 Concluding Remarks.

Structure-Property-Relationship of Nanoscale Materials - Emerging Approaches to Synthesis and Patterning

Hilton Columbia Center
Banquet 2

D. A. Chen, T. Vogt, H. Wang, *Organizers*
A. B. Greytak, *Organizer, Presiding*

1:00 871. Graphene based building blocks for electronic devices and sensors: Heterojunctions and functionalized surfaces. **G. Koley**, A. Uddin, T. Vogt

1:30 872. Quantifying ligand exchange reactions of CdSe and PbS nanocrystals. **J.L. Dempsey**, R.R. Knauf, H.E. Starr

2:00 873. Morphologically controlled silica overcoating of gold nanorods and CdSe/CdS core/shell nanorods. W. Wu, L.R. Rowe, B.D. Anderson, B.S. Chapman, **J.B. Tracy**

2:30 874. Understanding the vapor–liquid–solid mechanism of Si nanowire growth and doping to synthetically encode precise nanoscale morphology. **C. Pinion**, J. Christesen, J.R. McBride, J. Cahoon

2:45 875. Control of catalytically active interface between faceted nanoparticles and oxide supports. **C. Wen**, J. Jimenez, A. Bird, J. Lauterbach

3:00 Intermission.

3:20 876. *Ab initio* design of semiconductor nanowire synthesis. **M. Filler**

3:50 877. Interlayer interactions in 2D materials: From bulk to 2D and back. **S.C. Warren**

4:20 878. Formation and fluorescence of Wurtzite-CuInS₂. **J. Macdonald**

Synthesis & Application of Biofunctional Nanomaterials

Columbia Metropolitan Convention Center
Richland B

Cosponsored by COLL
Q. Wang, *Organizer, Presiding*

1:00 879. Core-shell nanoparticles as optically controlled synthetic muscle. **K. Salaita**, Y. Liu, Z. Liu

1:30 880. Photothermal stable dual responsive gold/mesoporous silica hybrid nanoparticle as a theranostic platform for cancer therapy. **P. Xu**

2:00 881. A plasmonic probe of distances for Biophysics: A biofunctionalized nanogold surface energy transfer molecular ruler. **G.F. Strouse**

2:30 882. Design and synthesis of J-aggregate nanotubes for biosensor applications. **J. Fang**

Molecules to Functional Supramolecular Materials

Hilton Columbia Center
Banquet 1

Cosponsored by ORGN
K. Shimizu, *Organizer*
L. S. Shimizu, *Organizer, Presiding*

2:00 883. Correlated structure and photophysics in donor-acceptor supramolecular polymer films. **A.B. Braunschweig**

2:30 884. Molecular balances for the study of non-covalent aromatic interactions. **K.D. Shimizu**

3:00 Intermission.

3:20 885. From host-guest chemistry to the nucleosome: Molecular recognition of methylated lysine and arginine. **M. Waters**

3:50 886. Self-assembling [2.2]paracyclophanes. D.E. Fagnani, M.J. Meese, Jr., K.A. Abboud, **R.K. Castellano**

4:20 887. Anion separation by selective crystallization of anion-water clusters with self-assembled guanidinium receptors. **R. Custelcean**, C. Seipp, N.J. Williams, A. Ivanov, V. Bryantsev

4:50 888. Supramolecular mechanochemistry. **S. Craig**

Colloid Chemistry Posters

Columbia Metropolitan Convention Center
Exhibit Hall

H. Zur Loye, *Organizer*

3:00 - 4:30

889. Effect of molecular weight on emulsification properties of water-soluble yellow mustard mucilage. A. Gao, **Y. Wu**

890. Tuning rod length during re-seeding through varying silver additions. **S.A. Canonico-May**, J.W. Stone

891. Preferential solvation model of Reichardt's dye in binary mixtures of organic solvents. **J. McFaddin**, L. Freeman, D.S. Boucher

892. Investigating the stability of P3HT solutions using light scattering and zeta-potential measurements. **M. Roesing**, I. Gould, J. Cobb, D.S. Boucher

Organic Chemistry Posters

Columbia Metropolitan Convention Center
Exhibit Hall

H. Zur Loye, *Organizer*

3:00 - 4:30

893. The synthesis and x-ray crystal structures of 1,1-dihalo-2,2,3,3-tetramethylcyclopropanes. E. Reinheimer, **C. Thurman**, M. Veers, L. Clark, W.C. Brown, J.R. Boone, **C. Clinger**

894. Stabilizing effects of electron withdrawing groups on the halogen bonding driven assemblies of semiconducting building blocks. **S. Nguyen**, K. Allen, N. Hammer, G.S. Tschumper, D. Watkins

895. Regioselective substitution reactions of indoles, controlled by "solvent polarity": A greener alternative. **S. Sutton**, A. Sood, S.M. Landge, A. Brown, J. Alonzo, B. Torok

896. New approach for the synthesis of vinyl phosphonates. **R. Mensah**, C.W. Alexander

897. Total synthesis of the *Morganella morganii* Zwitterionic polysaccharide repeating unit. **D.J. Keith**, S. Townsend

898. The influence of sterically demanding bis-(o-biphenyl)-phosphine ligands on gold(I) catalyzed reactivity and stability. **C. Griebel**, F. Liu, D. Hodges, A.C. Jones

899. Synthesis of phidianidine analogs containing 1,2,3-triazoles. B. Wakefield, **D. Laws**, D. King

- 900.** Development of novel ceramide analogs to target human acid ceramidase. J. Calkins, I. Lovett, A. Plotkin, S. Bataille, R. Land, T. Albers, **I. Lebedyeva**
- 901.** Enantioselective synthesis of spirocyclic and bicyclic lactones through desymmetrization. **K. Stingley**
- 902.** Synthesis of industrially useful dye intermediates. **P.D. Miller**, T. Neal
- 903.** Synthesis and derivatization of a human milk tetraose. **K.M. Craft**, S. Townsend
- 904.** Synthetic strategy toward β -Keto alkynes. B.D. Feske, S. Zingales, **M. Underwood**
- 906.** Novel resveratrol analog synthesis and using stilbenes to treat osteoporosis. **E. Barth**, D. Paull
- 907.** Studies toward the synthesis of dimeric derivatives of tadehaginoside. **C.M. Braun**, S. Townsend
- 908.** Bathochromic shifts in Schiff-base analogues of the highly emissive bipyrrrole moiety. **A. Finkelstein**, R. Kawano, T. Okawara
- 909.** One-pot synthesis of allylic esters and subsequent condition screening for ring-closure and dehydration to afford tetrahydroisobenzofurans. **B. Bashrum**, P. Wiget
- 910.** Oxidation of tricyclic ketones en route to marine-derive natural products. **E. Berry**, P. Wiget
- 911.** Asymmetric synthesis of enantioenriched cyclic compounds. **E. Minerali**, K.S. Petersen, J. Wilent
- 912.** Intermolecular Pauson-Khand reactions of *N*-substituted maleimides. **C.L. Brantley**, T.C. Coombs
- 913.** Development of a robust synthetic scheme to produce C9 analogs of the antibiotic pestalone. **M. Snyder**, A.L. Wolfe
- 914.** Organocatalyzed domino carbonyl-ene/Diels-Alder reactions. **A. McKinney**, H.A. Dahlmann, L. Davis
- 915.** Suzuki-Miyaura coupling for formation of asymmetric rhodamine derivatives with chiral sensing potential. **N.Y. Aleman**, D.C. Rich, N. Kamm, L.V. Odom, H. Nguyen, Q. Dang, C. Stephenson
- 916.** Synthesis of 2,3-butadiene ligands, metal organic frameworks, and investigation of their crystalline properties. **A.J. Stutesman**, B. Dinkelmeyer, C. Jones

- 917.** Selective mono-reduction of conjugated ester functional groups using lithium borohydride. **W. Rice**
- 918.** Synthesis of 1-aryl-1-alkenyl phosphonates. **S. Mize**, R. Mensah, **T. Gerschick**, J. Law, Z. Whitfield, C. Baum, C.W. Alexander
- 919.** Development, control, and application of the *o*-hydroxychalcone/flavanone molecular switch scaffold. **B. Muller**, M.J. Adler
- 920.** Synthesis of new cinnamaldehyde derivatives as potential anti-diabetic agents. **K. Blue**
- 921.** Production of chiral amines using enamine resistant substrates. **A. Vargas**, **S. Johnston**, B.D. Feske
- 922.** Improving heterogeneous catalysis of organic reactions: Unique properties of long-tethers to solid support. **S. George**
- 923.** Water-soluble 2-/3-formyl-BODIPY fluorophores to probe sulfites. **M. Isik**
- 924.** Withdrawn
- 925.** Investigation of the shape of atropisomers using dipolar couplings. **E.E. Schiller**, W. Carroll
- 926.** Taming silylium ions for synthesis: Applications in *N*-heterocycle synthesis *via* stereospecific C-C bond formation. **B.S. Moyer**, M.R. Gagne
- 927.** Reductive rail yard: Versatility of 1-hydrosilatane. **V. Skrypai**, S.E. Varjosaari, P. Suating, T.R. Gilbert, M.J. Adler
- 928.** Concise synthesis of difluorinated [6]-gingerol using selective C-C bond cleavage. **E. Kim**, E. Nazdrajic, C. West
- 929.** Synthesis and alkaline stability study of cationic perfluoroalkyl sulfonamide model compounds. **Y. Chen**
- 930.** Halogen bonded co-crystals of a pyridyl *bis*-urea macrocycle and diiodotetrafluorobenzenes. **B. Som**, S. Salpage, J. Son, B. Gu, M.D. Smith, L.S. Shimizu
- 931.** Progress toward phidianidine analogs containing oxazoles and isoxazoles. B. Wakefield, **A. Batten**
- 932.** Phidianidine analogues containing an isoxazole ring. B. Wakefield, **N. Stafford**
- 933.** Synthesis of phidianidine analogs containing 2,5-disubstituted oxazoles. B. Wakefield, **D. King**, A. Batten

- 934.** Application of C-H activation to the synthesis of disubstituted triazoles. **Y. Cao**, A. Neuman
- 935.** Purification and evaluation of immunomodulatory activity of polysaccharides isolated from *frankincense*. **N. Hosain**, R. Ghosh, P.C. Kline
- 936.** Three new aryl dihydronaphthalene type lignans isolated from *Bursera fagaroides* var. *fagaroides* and activity in zebrafish. **A.M. Rojas Sepulveda**
- 937.** Studies toward the synthesis of a novel rigid-core dendrimer nanostructure. **W.L. Robinson**
- 938.** Hydrocarboxylation of styrene's with CO₂ using chiral zinc and palladium complexes. **B.R. Hill**
- 939.** Preparation of 3-dimethylamino-1,2-diaryl-propenones and their application to the synthesis of highly functionalized pyrroles and pyrazoles. **J.T. Gupton**, A. Shimosono, J. Ortolani, S. Yeudall, E. Crawford, C. Heese
- 940.** Selected synthetic transformations of bismethoxy isoindenone and isoindene dimers. **J. Franklin**, A.D. Mills, M. Etzkorn
- 943.** Synthesis of natural product-inspired cyclopentanone-containing tricycles by heteroaromatic photo-Nazarov cyclization. **W. Ashley**, E. Timpy, T.C. Coombs
- 944.** Synthesis of functionalized alpha-sulfonamido aldehydes through organocatalysis. **R.J. McGorry**, M.D. Pitzen, **S.K. Allen**, T.C. Coombs
- 945.** Kinetic resolution of 2-arylcyclohexanols and understanding internal chirality transmission via Circular Dichroism. **L. Wang**, R. Akhiani, T. Zhang, B.K. Redden, C.I. Sheppard, R. Clark, M. Smith, S.L. Wiskur
- 946.** Selective mono-substitution of symmetric diols. **L. Daley**, D. Paull
- 947.** Resolution and crystal structure analysis of asymmetrical rhodamine derivatives with potential as chiral sensors. **D.C. Rich**, N.Y. Aleman, N. Kamm, H. Nguyen, Q. Dang, J.T. Mague, C.J. Stephenson
- 948.** Investigation of benzophenone *bis*-urea macrocycle via dynamic nuclear polarization surface enhanced NMR spectroscopy. **B.A. DeHaven**, J.T. Tokarski, C.R. Bowers, L.S. Shimizu
- 949.** Catalytic enantioselective (3+2)-cycloadditions α -keto ester enolates and nitrile oxides. **S.L. Bartlett**
- 950.** Towards the synthesis of hydroxytyrosol polyphenol. **E. Onobun**, I. Kady

951. Progress in the identification of the compounds in the kudzu bug, *Megacopta cribraria*.
H.V. Clontz, N. Rodgers, E. Niland

952. Preparation of 3-dimethylamino-2-aryl-acrylonitriles and their application to the synthesis of highly functionalized pyrroles and pyrazoles. **J.T. Gupton**, J. Wen, V. Moore-Stoll, E. Crawford, S. Yeudall, A. Lane

953. Preparation of 3-dimethylamino-2-arylacrylic acid esters and their application to the synthesis of highly functionalized pyrroles. **J.T. Gupton**, W. Curry, S. Yeudall, E. Crawford, E. Huff, V. Moore-Stoll

954. Structure-enantioselectivity correlation in NHC-Au(I) catalysis for 1,6-enynecyclizations.
R. Ma, B.W. Gung

955. Synthesis of novel thiazole-containing amino acids. **A.S. Bunev**

Polymer Chemistry Posters

Columbia Metropolitan Convention Center
Exhibit Hall

H. Zur Loye, *Organizer*

3:00 - 4:30

956. Brushing up on polymers: Controlling molecular weight distribution to manipulate polymer structure. **H. Davis**, D. Gentekos, B. Fors

957. Synthesis of β -cyclodextrin polymers crosslinked with organic chelating agents for the adsorption of organic and heavy metal pollutants from water. **E. Carter**

958. Synthesis and characterization of a silica nanoplate/polyethylene nanocomposite. **Y. Huang**, Y. Zheng, M.M. Khani, B.C. Benicewicz

959. Perfluorocyclobutyl (PFCB) aryl ether copolymers in proton exchange membrane fuel cells (PEMFCs). **K.D. Beard**

960. Anionic polymerization of Aziridines. **P. Mbarushimana**, P. Rugar

961. Waterborne non-leaching antimicrobial polymer coating. **L. Luo**, J. Zhao, W. Ming

962. A spectroscopic study of doping an electron-transport polymer. **T. Sutch**, G. Szulczewski, P. Rugar, M. Bowman, H. Chen, M. Lockart

963. Synthesis of bifuran-based derivatives. **H. Cao**, P. Rugar

- 964.** Functionalization of polyacrylates with TEMPO and PEG moieties for the modification of hemoglobin-based oxygen carriers. **O. Al Omainy**, H.J. Schanz
- 965.** Using multi-step synthesis for the production of hydrogels with adhesive properties. **M. Alcantar**, **J. Deardorff**, **J. Mathis**, C.H. Lisse
- 966.** Synthesis and characterization of bio-based polyurethane foams. **E. Day**, N. Tonks, B. Stephens, B. Snyder, P. Cotterillo
- 967.** Novel terpene-based stickers as adjuvants for agricultural applications. **T. Clark**
- 968.** Polychloroprene grafted silica nanoparticles for polymer nanocomposites. **Z.M. Abbas**, Y. Zheng, B.C. Benicewicz
- 969.** Thiol-ene click chemistry toward sustainable polyamides from plant oils. **A. Eta**, Z. Wang, L. Yuan, C. Tang
- 970.** Antimicrobial cobaltocenium metallopolymers materials against multidrug-resistant bacteria. **P. Yang**, Y. Chen, P. Pageni, M. Bam, M. Nagarkatti, A.W. Decho, C. Tang
- 971.** Antimicrobial applications of itaconic acid and its derivatives. **L. Mercado**, M.S. Ganewatta, P. Mehrpouya-Bahrami, Y.P. Chen, M. Nagarkatti, A.W. Decho, C. Tang
- 972.** Investigation of new heteroleptic lanthanide catalysts for ring-opening homopolymerization of α -methylene- γ -butyrolactone to obtain biodegradable cross-linkable polyesters. **D. Guthrie**
- 973.** Polymerization of MBL via aluminum catalyst-(Al(CH₃)₃). **T.N. Campbell**, P. Binda
- 974.** Polymerization of alpha-methylene-gamma-butyrolactone using Ca[N(SiMe₃)₂]₂. **K. Parrish**, P. Binda
- 975.** Synthesis of precision sulfone containing polyethylene via ADMET polymerization. **H. Hester**, M.H. Bell, T.W. Gaines, K.B. Wagener
- 976.** Silica grafted cobaltocenium-containing nanoparticles for antimicrobials. **P. Pageni**, P. Yang, Y. Chen, J. Wang, M. Kabir, A.W. Decho, C. Tang
- 977.** Rational design and preparation of thiophene polymers for dielectric energy storage. **T. Zhu**
- 978.** Hydrogen-bonding bio-based soy polymers. **M. Lamm**, N. Trenor, L. Yuan, C. Tang
- 979.** Renewable rosin containing tri- and pentablock copolymers for tough thermoplastics. **M. Rahman**, M.S. Ganewatta, L. Yuan, C. Tang

Cutting Edge of Biological Inorganic Chemistry

Columbia Metropolitan Convention Center
Richland A

J. H. Dawson, *Organizer*
A. Rogers, *Organizer, Presiding*

3:20 980. Metal properties control sulfur and selenium antioxidant activity. M. Kimani, M.T. Zimmerman, B. Stadelman, A.M. Owen, C.A. Bayse, **J.L. Brumaghim**

3:50 981. Identification of key residues within the cytochrome P450 BM-3 reductase domain that facilitate “transferable” improvements in catalysis. **R.L. Osborne**, E. Milczek

4:20 982. Nickel-binding mediates structural changes and decreases the inhibitor role of metalloregulatory protein YqjI in *E. coli*. **M. Blahut**, S. Wang, S. Dzul, A. Kandegedara, T. Stemmler, F.W. Outten

4:50 983. Fe-S clusters as signaling molecules: Mechanistic insights into regulation of iron metabolism in yeast. **A.N. Albetel**, H. Li, C.E. Outten

Synthesis & Application of Biofunctional Nanomaterials

Columbia Metropolitan Convention Center
Richland B

Cosponsored by COLL
Q. Wang, *Organizer*
K. Metavarayuth, Q. Wang, *Presiding*

3:20 984. Silicon nanowired human cardiac spheroids for heart repair. **Y. Mei**, D. Richards

3:35 985. Microwave heating of antibody-functionalized carbon nanotubes as a feasible cancer treatment. A. Cowan, B. Beckler, N. Farrar, A. Murawski, A. Robinson, A. Diamanduros, K. Scarpinato, V. Sittaramane, **R.L. Quirino**

3:50 986. Microwave-assisted synthesis and characterization of nanomaterials. **P.N. Njoki**, P. Nwokogu, T. Williams, R. Yehdego

4:05 987. Development of core–shell nanostructures by in situ assembly of pyridine-grafted diblock copolymer and transferrin for drug delivery applications. **L. Lu**, L. Yuan, J. Yan, C. Tang, Q. Wang

4:20 988. Enhanced carrier for hydrophobic molecules in aqueous systems: Synthesis and characterization. **O. Klep**, S.H. Foulger

4:35 989. Nano-biosensors: Probing intracellular response to nanoparticle therapy via live cell fluorescence microscopy. **K. Carnevale**, G.F. Strouse

WEDNESDAY MORNING

Plenary Session

Columbia Metropolitan Convention Center
Ballroom A/B

L. Shimizu, *Organizer*
L. M. Campos, *Presiding*

8:00 990. Amphidynamic materials and molecular machines: Supramolecular architectures. S. Perez Estrada, X. Jiang, **M.A. Garcia-Garibay**

Biological Chemistry - Drug/Assay Development

Columbia Metropolitan Convention Center
Ballroom B

H. Zur Loye, *Organizer*
M. Rahman, *Presiding*

9:15 991. Antibody drug conjugates: Guided missiles deployed to fight cancer. **S. Silverman**

9:45 992. Targeted intrinsic protein fluorescence, an approach towards high-throughput drug screening and mechanistic evaluation of Tuberculosis sikimate kinase. **R. Fuanta**, J. Simithy, G. Gill, T. Childers, A. Calderon, D.C. Goodwin

10:15 993. Design and synthesis of peptide conjugates and cyclic peptides as potential pharmacophores. **S. Panda**

10:45 994. Protein-coated DNA nanostructures: Applications in drug delivery. **D. Li**

11:15 995. New fast and efficient biotinylation platform: Both water-soluble and traceable. **A. Fessler**, C. Garmon, A. Fowler, C. Ogle

Catalysis & Biocatalysis

Columbia Metropolitan Convention Center
Richland A

T. M. Makris, *Organizer*
A. K. Vannucci, *Presiding*

9:15 996. Structural biology of redox partner binding: Simple and complicated. **T.L. Poulos**

9:45 997. What makes cytochrome P450 move. **D. Goodin**

10:15 998. Surprising influence of proximal heme pocket on distal-side chemoselectivity of heme thiolate enzymes P450cam and CPO: QM and QM/MM studies of epoxidation vs hydroxylation. **D.C. Chatfield**

10:45 999. Catalytic activity of non-heme diiron monooxygenases. **R.N. Austin**, A. Su, J. Austin

11:15 1000. Engineered biomolecular catalysts for small molecule activation. **K. Bren**, B. Kandemir, Y. Guo, S. Chakraborty, C. Dickerson

Cope Symposium: Molecules to Functional Supramolecular Materials

Hilton Columbia Center
Banquet 1

Cosponsored by ORGN
K. Shimizu, *Organizer*
L. S. Shimizu, *Organizer, Presiding*

9:15 1001. In silico design: Tailoring functional materials. **C.M. Colina**

10:05 Discussion.

Electrocatalysis

Hilton Columbia Center
Breakout 1/2

A. K. Vannucci, *Organizer, Presiding*

9:15 1002. Probing the rates of consecutive ET events and counter cation effects in polyoxometalate-catalyzed water oxidation. **C.L. Hill**, Y.V. Geletii, M. Wieliczko, Z. Xu, S. Lauinger, E.N. Glass, H. Lv, J. Bacsá, D.G. Musaev, T. Lian

9:45 1003. Electrochemically-promoted catalytic asymmetric hydrogenation using chiral rhodium complexes. **B.T. Donovan-Merkert**

10:15 1004. Electrocatalytic hydrogen production with [2Fe2S] clusters yielding high turnover frequencies and numbers. **D.L. Lichtenberger**, K.E. Clary, J.M. Marx, D.H. Evans, R.S. Glass

10:45 1005. Mechanistic studies of molecular photoelectrocatalysts for hydrogen evolution. **A.J. Miller**, M. Chambers, C. Pitman

11:15 1006. Linear free energy relationships in the elementary reactions steps of the hydrogen evolution reaction. **J.L. Dempsey**, N. Elgrishi, W.C. Howland, K. Lee, B. McCarthy, E.S. Rountree

Electronic Structure: Concepts & Applications

Columbia Metropolitan Convention Center
Richland C

Cosponsored by COMP and PHYS
S. Garashchuk, *Organizer*
V. Rassolov, *Organizer, Presiding*

9:15 1007. Development of multicomponent coupled-cluster theory for treating electron-hole correlation in multiexcitonic systems. B.H. Ellis, **A. Chakraborty**

9:45 1008. New developments in symmetry-adapted perturbation theory. **K. Patkowski**

10:15 1009. Reactions of CO₂ and H₂O mediated by metal dications for the geological sequestration of CO₂. **K. Thanthiriwatte**, V.E. Jackson, M. Chen, D.A. Dixon

10:45 1010. Differential hydration in the DNA minor groove and at the protein-DNA interface drive PU.1 and Ets-1 sequence recognition. **B. Kossmann**, E.K. Carter, K. Huang, G.M. Poon, I.N. Ivanov

11:00 1011. Integrative modeling of pre-initiation complex (PIC) assembles at the core promoter. **C. Yan**, Y. He, I.N. Ivanov, E. Nogales

11:15 1012. Impact of differential sequence length separation on PU.1 binding and transcription. **K. Huang**, G.M. Poon

Environmental Chemistry

Columbia Metropolitan Convention Center
Carolina B

H. Zur Loye, *Organizer*
S. Kimura-Hara, *Presiding*

9:15 1013. Is there a disinfection by-product problem in Flint? **J. Allen**, A. Cuthbertson, S. Kimura-Hara, M. Franco, S. Richardson

9:45 1014. Impacts of hydraulic fracturing on drinking water: New disinfection by-products. **H.K. Liberatore**, S.D. Richardson, J.M. Vanbriesen, M.J. Plewa, D.B. Burnett, L.H. Cizmas

10:15 1015. Possible demethylation of methamphetamine by ultraviolet treatment at a wastewater treatment plant. **L.M. Newberry**, T.H. Boles

10:45 1016. Removal and transformation of persistent priority emerging contaminants via advanced oxidation techniques and transformation product identification using mass spectrometry. **K. Cochran**, J. Casado, D. Russo, D. Spasiano, M. Vaccaro, R. Andreozzi, R. Marotta, N.M. Reis, G. Li Puma, D. Schlenk, D.D. Dionysiou, S. Richardson

11:15 1017. Adaptation of a mass balance box model to estimate the rate constants of mercury (Hg(II)) photoreduction in a lake. **L. Kocher**, H. Zhang

Frontiers in Nucleic Acid Chemistry

Columbia Metropolitan Convention Center
Lexington A

W. Wilson, *Organizer*

M. W. Germann, *Organizer, Presiding*

9:15 1018. Nucleic acid NMR made simple(r). **M.W. Germann**

9:45 1019. Current trends and applications in NMR for nucleic acids: Novel hardware, methods and software tools. **C. Anklin**

10:15 1020. Biacore 8K - the high-throughput, high-sensitivity solution for the study of molecular interactions involving nucleic acids. **E. Roush**

10:45 1021. Topological structure determination of RNAs using small angle X-ray scattering. **Y. Bhandari**, L. Fan, J. Stagno, E. Stahlberg, W. Jiang, C.D. Schwieters, Y. Wang

11:15 1022. Frozen in time: The intertwined histories of RNA and protein. **L.D. Williams**

Inorganic Chemistry Posters

Columbia Metropolitan Convention Center
Exhibit Hall

H. Zur Loye, *Organizer*

9:15 - 10:45

1023. Copper 5, 10, 15, 10-tetrakis-(3,4-bis-benzyloxyphenyl) porphyrin. **L.D. Mathews**, W.G. Stephens, C.P. Tidwell, P. Bharara

1024. Metal catalyzed reactions of hydrocarbons with carbon dioxide: An approach to study the mitigation of greenhouse gases. **A. Rahman**, K.M. Nicholas

- 1025.** Inhibition of cancer cell growth by ruthenium complexes. **E.T. Bell-Loncella**, J. Iida, M. Purazo, C.D. Shriver
- 1026.** Mercury(II) complexes of a new bulky N-heterocyclic thione (NHT). **B.C. Park**, J.J. Flanagan, D. Rabinovich
- 1027.** Stability of cyclopentapnictide adducts. **J.W. Hall**, M.T. Griffin, J.R. Wasson
- 1028.** Precise control of polyhydroxamate ligand topology for selective actinide coordination. **K. Sockwell**, M. Wetzler
- 1029.** Cation and anion binding in host selenaza macrocycles. **U. Patel**
- 1030.** Unusual coordination of heptadentate tripodal Schiff-base lanthanide complexes. **K. Seidler**
- 1031.** Synthesis of multi-metallic clusters of lithium, iron, and zinc supported by 2,6-bis(trimethylsilylamino)pyridine. **G.W. Durrell**, J.A. Rave, G. Guillet
- 1032.** The first corannulene-based metal-organic framework. **W.B. Fellows**, A. Rice, N.B. Shustova
- 1033.** Bimetallic MOFs: Control of material electronic properties. **E.A. Dolgoplova**, O. Egebabwo, A. Brandt, T.D. Maddumapatabandi, D.A. Chen, N.B. Shustova
- 1034.** Synthesis of precursor molecules for novel heterocyclic based materials. M.P. Washington, **T. Jones**, A. Barr-Cook
- 1035.** Synthesis, characterization, and *in vivo* cellular imaging of Eu(III)-doped zinc oxide nanoparticles. **J. Lee**, N.A. Dragan, G. Martin, R. Youker, C.R. De Silva
- 1036.** Photoluminescent studies of europium thenoyltrifluoroacetone complexes using dipyrrophenazine type ligand derivatives. **R. Downing**, A. Lillie, C. Jensen, J. Lee, B. Dinkelmeyer, C.R. De Silva
- 1037.** Synthesis, characterization, and cytotoxicity studies of europium metal-doped zinc oxide nanoparticles for potential clinical applications. **J. Spell**, N.A. Dragan, H. Coan, C.R. De Silva
- 1038.** Comparison of eight different iron-gall ink mixtures with respect to value of the inks as determined using a Munsell scale and the resulting effects of different environmental conditions on the dried ink samples. **M.S. Morton**, D. Noortajalli
- 1039.** Synthesis of NCN-Pincer ligands via the Staudinger reaction designed to support low-coordinate nickel complexes. **O.N. Nelson**, A.L. Rogers, J.A. Yates, **G. Guillet**

- 1040.** Electrochemical characterization of hexakis(urea)chromium(III) chloride and *cis*-dichlorobis(ethylenediamine)chromium(III) chloride. **K. Wells**, M.L. Pajski, J.J. Pajski
- 1041.** Synthesis of cationic vinyl imido complexes of Ta(V) upon deprotonation of nitriles. **M.M. Rahman**, D.V. Peryshkov
- 1042.** Synthesis of bis-triazinyl pyridine (BTPs) ligands for ¹⁵N ESEEM experiments in actinide and lanthanide complexes. **D. Dan**, T.E. Albrecht-Schmitt
- 1043.** Synthesis and optical properties of phosphonate-substituted rotationally locked bithiophenes. **D.N. French**, G.M. Gray
- 1044.** Probing the electrochemical behavior of rare-earth and actinide dipicolinic acid complexes. **M.L. Marsh**, D.E. Hobart, T.E. Albrecht-Schmitt
- 1045.** Noninnocent reactivity and interconversion of boron coordinated carborane, carboranyl, and carboryne complexes. **B.J. Eleazer**, D.V. Peryshkov
- 1046.** Metal-free B–H and O–H bond activation driven by cage rearrangements in icosahedral boron clusters. **Y. Wong**
- 1047.** X-panded polyiodides and triiodide × asymmetry in organoiodine hybrid salts. K. Khadijatul, A. Miller, A.M. Siegfried, T.W. Hanks, **W.T. Pennington**
- 1049.** Photophysics of fulleretic metal-organic frameworks. **D.E. Williams**, C. Risner, D. Godfrey, N.B. Shustova
- 1050.** Synthesis and spectroscopic investigations of the zinc and manganese complexes of 5,10,15,20-tetra[3,4-dibenzyloxy]porphyrin. C.P. Tidwell, **P. Bharara**, H. Palacio, A. Ezell, T. Tidwell
- 1051.** Reactivity of (η^6 -*para*-cymene)Ru(Ph)(I)(P(OCH₂)₃CEt) and its derivatives. B.P. Quillian, **A.E. Fields**, D. Zurwell
- 1052.** Synthesis, characterization, and structures of ruthenium(II) and ruthenium(IV) complexes with multiple solvato ligands. **M.A. Abbas**, J.L. Brumaghim
- 1053.** Toward the synthesis of a novel class of trisNHCs. **R. Justice**, **A. Berry**, O. Kuykendall, R. Hooper, D. Tapu
- 1054.** Synthesis of mercury(II) complexes of new bulky N-heterocyclic chalcogenone ligands. **A.J. Peterson**, J. Patterson, D. Rabinovich
- 1055.** Photophysics of corannulene-based metal-organic frameworks. **A. Rice**, W. Fellows, B.J. Yarbrough, N.B. Shustova

- 1056.** Crystallographic and luminescence property investigation of new non-centrosymmetric lanthanide silicates. **L.D. Sanjeewa**, K. Fulle, C. McMillen, J.W. Kolis
- 1057.** Synthesis and thermal analysis of modular polyphosphonates with potential in nonlinear optical hydroformylation catalysis and ionic conduction studies. **T.R. Totsch**
- 1058.** Identification of reaction intermediates in the mechanism of a classic ligand substitution reaction on Vaska's complex. **C. Durango Garcia**
- 1059.** Rigid mimics of GFP-based systems for efficient energy transfer. **E.A. Dolgoplova**, O. Ejegbavwo, N.B. Shustova
- 1060.** New multifunctional bis(amidine) ligands for highly luminescent coinage metal assemblies. **O. Ugarte Trejo**, **A. Calderón Díaz**, N. Bhuvanesh, **M. Stollenz**
- 1061.** Deoxygenation of phenolic compounds through the use of nickel-based homogeneous catalysts. **N.A. DeLucia**, E. Moon, A.K. Vannucci
- 1062.** Synthesis of a novel ditopic nonchelating N-heterocyclic carbene. **A. Carter**, M. Baker, A. Mason, D. Bettler, A. Changas, D. Tapu
- 1063.** Electrochemical synthesis of N-substituted indazoles. **M.M. Dissanayake**
- 1064.** Recent developments in the coordination chemistry of caffeine chalcogenones. **E.M. Grimm**, M. Styron, D. Rabinovich
- 1065.** Coordination chemistry of dialkylbenzimidazole chalcogenones. **K.K. Lugli**, L. Hernandez, D. Rabinovich
- 1066.** Copper(I) complexes with bulky thione and selenone ligands. **A.M. Allen**, M. Kocherga, D. Rabinovich
- 1067.** Rational design of novel Mn(I)-NHC molecular catalysts for CO₂ reduction. **C.J. Stanton**, G. Majetich, H.F. Schaefer, J. Agarwal
- 1068.** Charged and confused: *meso*-Tetrakis(*p*-methoxycarbonylphenyl)N-confused porphyrin as a precursor to water soluble variants. **J. Shaw**, V. Nemykin, S. Doble, N. Akbar

Interdisciplinary Chemistry Posters

Columbia Metropolitan Convention Center
Exhibit Hall

H. Zur Loye, *Organizer*

9:15 - 10:45

- 1069.** Grape pomace content and oxidative stability of extruded food products. **J. Yu**, I. Smith, G. Chen
- 1070.** Influence of grape pomace in the diet on nutrient absorption in rats fed high cholesterol diet. I. Smith, **J. Yu**, S. Hurley
- 1071.** Plastics to oil: NMR and GC/MS characterization of oils produced from a variety of plastics under a variety of reactor conditions. **P.J. Seaton**, M. Anttila, B. Monteleone, J. Bledsoe, R.N. Mead
- 1072.** Rheology and botanical origin of Ethiopian monofloral honey. A. Belay, G.D. Haki, M. Birringer, H. Borck, A. Addi, K. Baye, **S.M. Abegaz**
- 1073.** Evolution of functionality of the polycomb repressive complex (PRC2). **Z. Barnes**
- 1074.** Effects of particle size of grape seed flour on the polyphenols composition and sensory properties of cookies. **J. Yu**, R. Maman
- 1075.** Synthesis of cationic photosensitizers for the photodynamic inactivation of *Escherichia Coli*. **A. Hurst**, J.L. Vivero
- 1076.** Calibrating alcohol breath testers using commercially available liquors as reference solutions. S. Kim, **J. Lee**

Materials Chemistry - Solid State

Columbia Metropolitan Convention Center
Carolina A

H. Zur Loye, *Organizer*
T. Ragsdale, *Presiding*

- 9:15 1077.** Materials discovery by crystal growth: New transition metal and uranium containing fluoride crystals from mild synthetic techniques. **J.B. Felder**, J. Yeon, M.D. Smith, H. Zur Loye
- 9:45 1078.** Enhanced flux technique for the synthesis of salt-inclusion uranyl silicates. **G. Morrison**, M. Smith, H. Zur Loye
- 10:15 1079.** *In situ* reduction of early transition metal oxides via hydrothermal and molten flux methods: Crystal growth, structural characterization, and neutron studies. **D. Abeyasinghe**, M. Smith, H. Zur Loye
- 10:45 1080.** Crystal chemistry and magnetic properties of complex transition metal oxides. **T. Ferreira**, S. Calder, G. Morrison, J. Yeon, H. Zur Loye

11:15 1081. Specific effects in microwave chemistry explored through reactor vessel design, theory, and spectroscopy. **B. Ashley**, L. Derek, Y. Chiu, H. Gao, J. Owens, G.F. Strouse

Nuclear Power & Safety

Columbia Metropolitan Convention Center
Hall of Fame

D. Cain, *Organizer, Presiding*

9:15 1082. Power plant chemistry. **D. Cain**

9:45 1083. Chemistry and materials science of nuclear fuel. **T. Bessmann**

10:15 1084. Chemical aspects of the MOX fuel fabrication facility. **P. Henry**, B. Karmioli

10:45 1085. Complexation of holmium with tributyl phosphate in bis(trifluoromethylsulfonyl)imide ionic liquid solutions. **D.S. Meeker**, C.L. Klug

11:00 1086. A natural history of the Chernobyl ecosystem. **R. Mancke**

Physical Chemistry - Theory/Computation

Columbia Metropolitan Convention Center
Ballroom A

H. Zur Loye, *Organizer*
D. A. Clabo, *Presiding*

9:15 1087. Dehydration pathways for the Tutton salts $K_2M(SO_4)_2 \cdot 6 H_2O$ (M = Mg, Co, Zn, Ni, Cu). **T.C. Devore**, A. Morales, B.A. Reisner

9:45 1088. Equation of state for solids. **E.E. Gordon**, J. Köhler, M. Whangbo

10:15 1089. Utilization of molecular dynamics to examine the physical properties of different hydrocarbons for alternative fuels. **J. Winkler**, T. Knippenberg

10:30 1090. Investigation of the crystal structure of the 3,4-dichlorophenol and imidazole co-crystal. **C.J. Wright**, K. Martin

10:45 1091. Withdrawn

Polymer Chemistry - Materials

Columbia Metropolitan Convention Center
Ballroom C

H. Zur Loye, *Organizer*
M. S. Ganewatta, *Presiding*

9:15 1092. Polyoxometalate-based tunable gelating networks for entrapment, detection, and decontamination. **K. Sullivan**, A.K. Mehta, Q. Yin, S. Vivek, P. Yin, E.R. Weeks, T. Liu, C.L. Hill

9:45 1093. Comparison between two post-modification approaches for polybenzimidazoles with improved gas permeability. **R.M. Joseph**, A. Fraser, R. Liu, S. Roy Choudhury, J.S. Riffle, J.D. Moon, B.D. Freeman

10:15 1094. Novel sulfonyl-containing monomer based polybenzimidazoles and post-modification for high temperature gas separation membranes. **R. Liu**, R.M. Joseph, J.D. Moon, S. Roy Choudhury, H. Borjigin, K.A. Stevens, B.D. Freeman, J.S. Riffle

10:45 1095. Diversifying the chitin economy: Different sources of biomass for chitin extraction and biomaterial formation. **E.C. Achinivu**, J.L. Shamshina, R.D. Rogers

11:15 1096. Boronic acid-modified poly(amidoamine) dendrimers as sugar sensors. **X. Liang**, M. Bonizzoni

Small-Molecule Inorganic Chemistry in the Southeast: Honoring Jerome Odom

Hilton Columbia Center
Banquet 2

J. O. Boles, J. M. Iriarte-Gross, *Organizers, Presiding*

9:15 Introductory Remarks.

9:25 1097. Adventures with Jerry Odom in small molecule chemistry and NMR spectroscopy. **P.D. Ellis**

9:50 1098. Small molecule inorganic chemistry has taken me on a wild ride from germanium to grits. **J.M. Iriarte-Gross**

10:15 1099. Small-molecule main group chemistry, Jerry Odom, and a career in comprehensive universities. **T. Moore**

10:40 1100. From small molecule chemistry to microscale chemistry to President at a small college. **Z. Szafran**

11:05 1101. Synthesis and incorporation of selenium and tellurium-containing amino acids into proteins. **J.O. Boles**

11:30 1102. How industry university engagement can catalyze small chemistry research and commercialization. **A.M. Boccanfuso**

11:55 Concluding Remarks.

Structural & Functional Characterization of Proteins

Columbia Metropolitan Convention Center
Richland B

M. Chruszcz, *Organizer, Presiding*

9:15 1103. Reproducibility in biomedical sciences. **W. Minor**

9:45 1104. Structural maturation of HIV-1 reverse transcriptase. **R. London**, X. Zheng, G. Mueller, E.F. Derose, L. Pedersen

10:15 1105. Species-dependent ISG15 variation impacts viral protease function. **S.D. Pegan**

10:45 1106. MauG catalysis: A tale of ferryl iron, radicals and long distance hopping. **C.M. Wilmot**, E. Yukl, V.L. Davidson

11:15 1107. Structure determination of a protein-protein complex based on joint NMR and X-ray data. **T. Cierpicki**

Molecules to Functional Supramolecular Materials

Hilton Columbia Center
Banquet 1

Cosponsored by ORGN
K. Shimizu, L. S. Shimizu, *Organizers*
D. Watkins, *Presiding*

10:15 1109. Theoretical insight into non-covalent interactions using functional-group partitioning of energy component analysis. **C.D. Sherrill**

10:45 1108. Photochemistry in confined spaces: Medium is the message. **V. Ramamurthy**

11:15 1110. Modifying dendritic polymers for supramolecular analytical applications. **M. Bonizzoni**

WEDNESDAY AFTERNOON

Biological Chemistry - Drug Development & Redox Biology

Columbia Metropolitan Convention Center
Ballroom B

H. Zur Loye, *Organizer*
S. M. Strickland, *Presiding*

1:00 1111. Development and analysis of a novel targeting strategy for bacterial sugars. **K.M. Erickson**, J.M. Troutman

1:30 1112. Thermodynamic profiling of the inhibition of HMGA binding to AT rich DNA by netropsin. **R. White**, C. Quandt, J. Schoen, A.H. Gorensek, K.L. Buchmueller

1:45 1113. Towards further understanding of kinase activity during oxidative stress: Synthesis of the highly active ERK2 substrates Sub-D and Sub-F. **O. Tornow**, A.J. Wommack

2:00 1114. Quantifiable DNA damage prevention by hydrophobic compounds under biologically relevant conditions: Evaluation of selenium glutathione peroxidase mimics. **A.A. Gaertner**, H.M. Gordhan, D.C. Whitehead, J.L. Brumaghim

2:30 1115. Understanding antioxidant prevention of iron-mediated cell death in *E. coli*: The role of NADH. **S. Goodman**, J.L. Brumaghim

3:00 Intermission.

3:20 1116. Selones as novel, multifunctional antioxidants. **U. Patel**

3:50 1117. Metabolic analysis of watermelon varieties and germplasm lines using NMR spectroscopy. **S. Shrestha**, A. Battiste, M.K. Mandal, C. Kousik, A. Boroujerdi

4:05 1118. Exploring the metabolome of a yeast model for Parkinson's disease. **K. Goldston**, R. Chosed, D. Boroujerdi

4:20 1119. Exploring the role of Tat-SF1 as an HIV-1 host factor. **M. Warrick**, H.B. Miller

Catalysis & Biocatalysis

Columbia Metropolitan Convention Center
Richland A

T. M. Makris, *Organizer*
A. K. Vannucci, *Presiding*

1:00 1120. Multiple enzymatic activities of the dehaloperoxidase hemoglobin from *Amphitrite ornata*. **R.A. Ghiladi**, N.L. McCombs, L.M. Carey

1:30 1121. New recipes for biocatalysis: Expanding the cytochrome P450 chemical landscape. **E.M. Brustad**

2:00 1122. Oxygen-dependent activation of diguanylate cyclase-containing globin coupled sensors. **E.E. Weinert**

2:30 1123. Structural studies of cellulolytic redox enzymes using neutron scattering and diffraction. **F. Meilleur**, A. Bodenheimer, W. ODell

3:00 Intermission.

3:20 1124. Theoretical investigation of the aziridination mechanism of tetracarbene iron catalysts. **J.L. Kern**, S. Roy

3:50 1125. Mechanistic study of the effect of aryl halide and aryl amine steric properties on Pd(PNP₃)₂ catalyzed Buchwald-Hartwig amination. **H.U. Hu**, K.H. Shaughnessy

4:20 1126. Cu-Catalyzed Nitrene Transfer Reactions of Olefins using PhINTs in the Presence of an Ionic Liquid. **H.U. Valle**, K.M. Riley, J.P. Emerson

4:50 1127. Quantitative study of catalytic activity of colloidal gold nanoparticles and supported gold nanoparticles. **S. Chakraborty**, S.M. Ansar

Electrocatalysis

Hilton Columbia Center
Breakout 1/2

A. K. Vannucci, *Organizer, Presiding*

1:00 1128. Hydrogen production catalyzed by molecular Co complexes with pentadentate ligands in aqueous solution. **X. Zhao**, P. Wang, Y. Sun, L. Duan, M. Long, D. Reese, A. Bah, C. James

1:30 1129. Iron complexes for hydrogen generation in aqueous solutions. **W. McNamara**

2:00 1130. Efficient electrocatalytic hydrogen evolution enabled by multiple non-innocent ligands. **J.D. Blakemore**

2:30 1131. Electrocatalytic conversion of CO₂ using Mn(I)-NHC compounds. **J. Agarwal**

3:00 Intermission.

3:20 1132. Robust molecular electrocatalysts for carbon dioxide reduction featuring rigid dinucleating ligand scaffolds. **J.W. Jurss**, W. Yang, S. Sinha Roy

3:50 1133. Electrochemical generation of hexavalent americium, and progress towards its selective separation: Applications to nuclear fuel cycle technology. **C. Dares**, B.J. Mincher

4:20 1134. Earth-abundant iron diboride (FeB₂) nanoparticles as a highly active bifunctional electrocatalyst for overall water splitting. **H. Li**

Environmental Chemistry

Columbia Metropolitan Convention Center
Carolina B

H. Zur Loye, *Organizer*
S. Kimura-Hara, *Presiding*

1:00 1135. Identification and measurement of some opioids in wastewater by SPE and LC-MS/MS and determination of their structure in solution by NMR and RDC. **F. Mahmoudi**

1:30 1136. NO_x formation in post-flame gases during syngas/air combustion at atmospheric pressure. **N. Asgari**, S. Ahmed, T. Farouk, B. Padak

2:00 1137. Investigation of sulfur trioxide formation in oxy-combustion of coal. **N.N. Choudhury**, B. Padak

2:30 1138. Analysis of phytoplankton community structure in ocean samples using a fluorescence imaging photometer. **S.T. Faulkner**, C. Rekully, S. Tazik, E. Lachenmyer, T.J. Shaw, T. Richardson, M. Myrick

3:00 Intermission.

3:20 1139. Theoretical investigation of sulfur adsorption on calcium oxide. **B. Galloway**, A. Maymi, A. Bland, B. Padak

Frontiers in Nucleic Acid Chemistry

Columbia Metropolitan Convention Center
Lexington A

M. W. Germann, *Organizer*
W. Wilson, *Organizer, Presiding*

1:00 1140. Orphan transcription factor discovery by the combinatorial approach REPSA. **M. Van Dyke**, E. Clay, K. Hiam, M. Lee

1:30 1141. DNA-encapsulated silver clusters. **J.T. Petty**, M. Ganguly, I. Rankine, M. Gilllan, Y. Wang, E. Baucum, M. Fuenmayor Llanos

2:00 1142. Probing nucleic acid grooves with fluorescent aminosugars. **D.P. Arya**

2:30 1143. Negatively cooperative self-titration: A novel mechanism of transcription factor regulation. S. Esaki, M. Evich, S. Xhani, N. Erlitzki, M.W. Germann, **G.M. Poon**

3:00 Intermission.

3:20 1144. History of the ribosome and the origin of translation. **K.A. Lanier**, L.D. Williams

3:50 1145. Design and investigation of a DNA alkylating molecule capable of producing DNA double strand breaks. **S. Varadarajan**, N. East, I. Campos, A. Frampton

Materials Chemistry - General

Columbia Metropolitan Convention Center
Ballroom A

H. Zur Loye, *Organizer*
M. M. Khani, *Presiding*

1:00 1146. Enhanced visible light photocatalytic water reduction of a g-C₃N₄/SrTa₂O₆ heterojunction. **S.P. Adhikari**, A. Lachgar

1:30 1147. Nanoporous asymmetric membranes for stabilizing high capacity lithium ion battery anodes. **J. Wu**

2:00 1148. Novel electrode architecture for high energy density lithium ion batteries. **L. Ventrapragada**, R.C. Biswal, M.A. Ghadkolai, R. Podila, A.M. Rao, R.K. Bordia, S.E. Creager

2:30 1149. Electrochemical characterization of novel complexes for supercapacitor applications. **C. McNeill**

2:45 1150. Aqueous synthesis and characterization of novel nanostructures for water purification. **T. Eldred**, J.C. Poler

3:00 Intermission.

3:20 1151. Crystal structure and theoretical analysis of green gold Au₃₀(S- *t*Bu)₁₈ nanomolecules and their relation to Au₃₀S(S- *t*Bu)₁₈. **T.C. Jones**

3:50 1152. Direct observation of manganese-containing nanowire formation with spinel crystal structure in *in situ* TEM. **L. Yu**, Y. Zhang, D. Kim, B.S. Gupton

4:20 1153. Towards the utilization of hole trapping ligands on nanorods for oxidative reactions. **A.D. LaCroix**, A. O'Hara, K.R. Reid, N. Orfield, S. Pantelides, S.J. Rosenthal, J. Macdonald

Molecules to Functional Supramolecular Materials

Hilton Columbia Center
Banquet 1

Cosponsored by ORGN
L. S. Shimizu, *Organizer*
K. Shimizu, *Organizer, Presiding*

1:00 1154. Probing the energetics and spectroscopic signatures of non-covalent interactions in (supra)molecular assemblies. **G.S. Tschumper**

1:30 1155. Novel thin film morphologies of semi-crystalline polymer and polymer blends. **J. Albert**, G. Kelly

2:00 1156. Elucidating the synergic effects of sigma-hole interactions and pi-pi stacking within organic electronic materials for applications in OFETs and OPVs. **D.L. Watkins**, N. Hammer, G. Hill, G.S. Tschumper

2:30 1157. Polydiacetylenes: Sensor applications and reversible thermochromism. **W.T. Pennington**, K. Khadijatul, P. Dawson, T.W. Hanks, R. Jelinek, J. Northcutt

3:00 Intermission.

3:20 1158. Using the supramolecular interactions of rhodamine derivatives with amino alcohols to develop chiral sensors. D.C. Rich, N.Y. Aleman, J. Romaine, N. Kamm, **C. Stephenson**

3:50 1159. Functional materials from self-assembling *bis*-urea macrocycles. **L.S. Shimizu**

4:20 1160. Triazoles as controlled molecular switches with logic gate functions. **S.M. Landge**, A. Atkinson, J. Gibson, W. Ming, K.S. Aiken, D. Ghosh

4:50 1161. Dual sensibility of phenanthrene based 1,2,3-triazole chemosensor. **D. Ghosh**, D.Y. Lazare, D. Winder, S.M. Landge, K.S. Aiken

5:05 1162. The effect of molecular dipole moment on the electrical properties of molecular rectifiers. **A.D. Broadnax**, Z.A. Lamport, O. Jurchescu, M.E. Welker

Organic Chemistry

Columbia Metropolitan Convention Center
Carolina A

H. Zur Loye, *Organizer*
B. A. Van Horn, *Presiding*

1:00 1163. Conformationally restricted macrocyclic nucleosides for RNA-based therapeutic applications. **A.M. Dmytrejchuk**, B.L. Merner

1:30 1164. Highly efficient green color dual anchor & dual donor dyes for dye-sensitized solar cells. **A. Peddapuram**

2:00 1165. Small-molecule models of poly(amidoamine) dendrimers. **N. White**, M. Bonizzoni

2:30 1166. Conformational analysis of Thiosemicarbazone ligands and their metal complexes in solution using residual dipolar couplings (RDCs). **S. Gukathasan**, W. Carroll

3:00 Intermission.

3:20 1167. Synthesis of Dilantin. **V. Sublett**, D.J. Swartling

3:50 1168. Dynamic kinetic arylation of carbonyl derivatives. **S.L. Bartlett**

Physical Chemistry - Theory/Computation

Hilton Columbia Center
Banquet 2

H. Zur Loye, *Organizer*
D. A. Clabo, *Presiding*

1:00 1169. Enthalpy of formation of $K_2M(SO_4)_2 \cdot 6 H_2O$ (M = Mg, Co, Ni, Cu, Zn). **T.C. Devore**, A.C. Molales, N. Cooper, B.A. Reisner

1:00 1170. Influence of three-body interactions on the low-temperature equation of state and elastic constants of HCP solid 4He . **A.L. Barnes**, R.J. Hinde

1:00 1171. Structure and properties of gold doped silicon clusters. **J.T. Lyon**

Polymer Chemistry - Physical

Columbia Metropolitan Convention Center
Ballroom C

H. Zur Loye, *Organizer*
W. Zheng, *Presiding*

1:00 1172. Fluorinated ionomers and their membranes for fuel cell. **I. Sharif**, S.E. Creager, J.S. Thrasher, D.D. Des Marteau

1:30 1173. High molecular weight biobased plastics and elastomers from renewable resin acids. **M.S. Ganewatta**, W. Ding, M. Rahman, L. Yuan, Z. Wang, N. Hamidi, M.L. Robertson, C. Tang

2:00 1174. Poly(arylene ether sulfone) statistical copolymers: Alternative hydrocarbon-based proton exchange membranes for perfluorosulfonic acids in water electrolysis cells. **A. Daryaei**, J. Willey, S. Roy Choudhury, C. Mittelsteadt, J.S. Riffle

2:30 1175. Tailored block ionomer architectures via gel-state functionalization. **G. Fahs**

3:00 Intermission.

3:20 1176. Synthesis of poly(4-vinyl pyridine) grafted HIPE foams towards an improved ion-exchange material. **J.G. Pribyl**, R.B. Fletcher, W.P. Steckle, K.M. Taylor-Pashow, T.C. Shehee, B.C. Benicewicz

3:35 1177. Withdrawn

3:50 1178. Synthesis of multifunctional polyacrylates and binding to hemoglobin. **M.E. Michaud**, H.J. Schanz

4:05 1179. Thermal analysis of linear high molecular weight poly-DCPD (Dicyclopentadiene) and its brominated derivatives. **D. Barvaliya**, H.J. Schanz

4:20 1180. Analysis of the reaction between thiol macromolecules and polyaniline nanofibers. **B. DiTullio**, P. Molino, T.W. Hanks

4:50 1181. Silicone acrylate coatings as a model system for predictive surface free energy analyses. A. Alkazzaz, R. Brooks, E. Henry, W. Wei, **T.B. Cavitt**

Structural & Functional Characterization of Proteins

Columbia Metropolitan Convention Center
Richland B

M. Chruszcz, *Organizer, Presiding*

1:00 1182. Three-dimensional structure of asthma-associated allergens for diagnosis and immunotherapy. **A. Pomes**

1:30 1183. Structure and function of the peanut panallergen Ara h 8. **B.K. Hurlburt**

2:00 1184. Structural and functional characterization of indoor allergens from dust mites and cockroaches. **G. Mueller**, L. Pedersen, P. Thompson, T. Randall, R. London, A. Pomes

2:30 1185. Novel hybrid molecular docking approach for determining drug-protein complexes: The future of drug design and development. **L.A. Wilt**, A.G. Roberts

3:00 Intermission.

3:20 1186. Structure-based development of menin-MLL inhibitors for cancer therapies. **J. Grembecka**

3:50 1187. Targeting the phospholipid-sensing nuclear receptor LRH-1 with synthetic agonists. **E. Ortlund**

4:20 1188. Gaining antibiotic resistance without loss of essential function: The balancing act negotiated by *N. gonorrhoeae* penicillin-binding protein 2. A. Fedarovich, J. Tomberg, R.A. Nicholas, **C. Davies**

4:50 1189. Withdrawn