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**


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


**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**


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.


1:40 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
toxicants. **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. Fabbrizzi, 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 liability 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


1:30 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.


3:30 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

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

Intermission.

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

Alpha substitution of nitriles mediated by trimethylsilyl trifluoromethanesulfonate. C.W. Downey

Calcium catalyzed Friedel-Craft and Mukaiyama-Mannich reactions. K.A. Nolin


Polymer Chemistry - Synthesis

Columbia Metropolitan Convention Center
Richland B

H. Zur Loye, Organizer
L. Yuan, Presiding

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

Polymer-grafted silica nanoparticles towards hybrid assemblies in one step. Y. Zheng


Linear poly(ethyleneimine) synthesized by living anionic polymerization. L. Reisman, C.P. Mbarushimana, S.J. Cassidy, E. Rowe, P. Rupar

Synthesis, characterization, and comparison of polyborafluorene and polyborafluorene copolymers. I.A. Adams, P. Rupar

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

Columbia Metropolitan Convention Center
Congaree A/B
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


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

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


68. Developing a fluorescence anisotropy immunoassay for real-time profiling of islet of Langerhans secretions. **J. Adablah**


70. Qualitative analysis of silicone contamination in market pulp using multi-temperature pyrolysis GC-MS. **T. Cotter**


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


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


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
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

Talk to an NSF Program Officer! T.B. Higgins

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

Scholarship program in science and mathematics at Kennesaw State University: Supporting the academic achievements of disadvantaged students. D. Tapu, A. Croicu

Chemisthenics: A literal VSEPR exercise. C. Rezsnyak

Evaluation of the procedure used for production of Canine Accelerant Detection training materials. D.W. Carpenetti, S. Giammona

Conceptual and calculation based experiments used to improve student understanding of equilibrium. A. Cook

Determining the antioxidant potential of Hedera helix extracts: Chemistry education through the Scots Science Scholars program. E. Burnham, A.D. Gibson, M. Siopsis

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

Meso-tetrakis(2-chloro-3-quinolyl)porphyrin and its water-soluble derivative, meso-tetrakis(2-chloro-4-sulfonato-3-quinolyl)porphyrin. A. Adeyemo

The synthesis and characterization of a new photosensitizer and its metal derivatives: Potential anticancer drugs. A. Adeyemo

The development of teaching and learning materials for cognition accelerating science classes for lower elementary students (I). K. Young Tae


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 (v2RDM)-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


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


114. Linear absorption spectra from explicitly time-dependent equation-of-motion coupled-cluster theory. D.R. Nascimento, A.E. DePrince


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 AnFₓ 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


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


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*

9:45 130. 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


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


### Asymmetric Chemistry throughout the Southeast

Columbia Metropolitan Convention Center
Congaree A

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


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


**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**


**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. Interfacial electron transfer in [Fe(CNC)_2]^2+-TiO_2 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-TiO_2 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**


**Materials Chemistry**

Columbia Metropolitan Convention Center
Hall of Fame

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


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


**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


9:45 171. Polydiacetylene-containing sensing systems. **T.W. Hanks**
10:15 172. Dual-functional antifogging/antimicrobial polymer coating. J. Zhao, W. Ming


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


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


**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


**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


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.


4:20 206. Organo-soluble Au$_{102}$(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**


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**


**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 [Fe(bpy)$_3$]$_{2+}$ and other tris-chelate polypyridyl complexes. **D.C. Ashley**, E. Jakubikova

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.


3:50 231. 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.


**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


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


3:00 Intermission.


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*


1:30 259. 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.


**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


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.


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


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


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


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


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


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**

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


295. Sequence, structure and function of small opioid peptides. **A.C. Schwartz**, M.W. Giuliano


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 is 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


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


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. Gilllan

315. Dehydrogenative coupling of a polysiloxane and dodecanethiol by way of the Piers-Rubinsztajn reaction. A. Abdul-Haqq, G. Mbah, T.W. Hanks


317. DMSO mediated cellular uptake of phenol red. H.I. Udo, K.K. Griffin, J.M. Meyers


322. Aldo-keto reductase YDL124w: Preliminary crystallization experiments. A. Neely, L. Lovelace, M. Weiland


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 Noxo1. **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**


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


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


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


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


350. Celebrating 30 years of our ACS student chapter at Francis Marion University. M. McCrimmon, C. Witt, J.G. Kelley


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**


3:00 Intermission.

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


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 SiO$_2$ nanoparticles as an antibiotic delivery vehicle. **R.B. Fletcher**, J.G. Pribyl, B.C. Benicewicz


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**

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


375. White light from hybrid water soluble Au (I) phosphor systems for OLED applications. C. Williams, S.B. Marpu, M.A. Omary


378. Employing a flexible tritopic linker to construct metal-organic frameworks. C.R. Martin, G.J. McManus


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.


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


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


395. Copper-catalyzed radical cascade trifluoromethylation reaction. J.L. Biaco, T.J. Barker


397. Synthesis of substituted urazole radicals. K.S. Aktepe


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


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


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


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


419. Halogen-directed Co-catalyzed hydroacylation. P. Chavis, D. Wilger


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


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**


440. Fuel cell catalyst formation by simultaneous reduction of platinum and graphene oxide. **T. Kusumadjaja, W. Zhou**


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. Gorensek, 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**

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

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


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

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

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**


3:50 453. 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
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**

Redox dopamine sensing with chitosan-catechol modified electrodes. **B. McDowell, H. Ben-Yoav, N. Peixoto, A. Silue**

Using cotton plant waste to remove cadmium from aqueous solutions. **A. Rizzuti, K. Mouzone**

Photoacoustic microscopy with carbon black: Sound generation by pure elemental carbon. **A. Korshun, H. Park**

UPLC-MS characterization of membrane phospholipids from *Vibrio* species following exposure to exogenous fatty acids. **D. Anderson, Z.J. Avello, S. Symes, D. Giles**

HPLC method development for separation of methanol extracts from yellowstriped oakworm. **J. Howell, M. Melnychuk, J. Ellenburg, P.B. Nolibos, A. Thomas**

Atomic absorption analysis of electrolyte content in sports drinks and food products utilized by athletes for muscle cramp relief. **K. Dowlatshahi, S.E. Hooper**

Elemental analysis of cigarette butt leachates in seawater. **M. DeMailly, G.E. Potts**

Development of an inexpensive atomic emission spectrometer for the detection of easily ionizable elements. **D.A. Free, J.P. Troutman, C.E. Dahm**

GC-MS analysis of commercially available food products containing mint flavoring. **V.R. Griffin, C.E. Dahm**

A first-generation amperometric galactose biosensor. **C. Steele, T. Munoz, S. Borum, W. Case, M.C. Leopold**

Carboxylic acid multi-walled carbon nanotubes modified with β-cyclodextrin for the detection of uric acid on an electrochemical sensor. **M.A. Schwarzmann, S.D. Gillespie, M.B. Wayu, M.C. Leopold**


Fluorescence studies of aromatic and polycyclic aromatic compounds. **N. Dos Santos, H.V. Clontz**

469. Effects of solvent on electrochemistry of biogenic amines in non-mammalian systems. **S.M. Wright**, N.J. Kuklinski


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


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**


487. Identifying conjugated molecules from mixtures by mass spectrometry with selective excitation. **R. Ford**, R.B. Grubbs


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


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. Rupar, 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**


**507.** Effect of golf course on water quality. A. Walton, **S.A. Myers**


**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 pentamethycyclopentadienyl. **P.A. Dean, J.P. Lee**

517. Designing alkynyl bridged FeII-TiIV complexes that are inert to oxidative decomposition. **D. Agakidou, J. Pienkos, 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**


522. New transition-metal complexes of polycyclic thioureas. **R. Hooper, O. Kuykendall, 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**


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**


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**

43
532. Withdrawn


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


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


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


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


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. Samaranayake, 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


9:45 561. 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


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


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*


9:45 573. 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**

**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. McMahen, 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

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


**Materials Chemistry - Nanoparticles**

Columbia Metropolitan Convention Center
Carolina B

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


9:45 588. Withdrawn


**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**


11:45 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


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


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 Aβ 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

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


618. Ionic interactions that stabilize and denature protein and peptide structures. A. Lorts, A.L. Stewart


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


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


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**


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. Bouthilette**, A.L. Wolfe


642. Eukaryotic heme a synthase: Importance of oligomerization. **N.J. Harris**, N.G. Taylor, O. Khalimonchuk, J.L. Fox


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 17α-ethinylestradiol using *Lentinula edodes* and *Phanerochaete chrysosporium*. **A. Milliken**, C.M. Johnson


655. Investigating mutagenic forms of cytochrome P450 BSβ for biofuel application. **C. Rutland**, J.A. Amaya, T.M. Makris


658. Molecular mechanism for polypeptide translocation catalyzed by domain I & II of ClpA. **N. Scull**, A.L. Lucius


660. Role of ferritins in iron donation to Suf Fe-S cluster assembly in *Escherichia coli*. **N. Bolaji**, P.A. Lindahl, F. Outten

Cellular uptake of polyphenols in a bacterial protein expression system. **B. Griffin**


Eukaryotic heme $\alpha$ synthase: Roles of conserved amino acid residues. **N.G. Taylor**, N.J. Harris, O. Khalimonchuk, J.L. Fox

Effect of mitochondrial reactive oxygen species on pre-adipocyte differentiation. **C.M. Matzie**


Synthesis and characterization of meso-tetrakis(2-fluoro-4-methoxyphenyl)porphyrin. **A. Adeyemo**

Fluorescence and UV-VIS studies of quinone-induced protein modifications. **C. Thomas**, M. Booker, T.V. Albu, J. Kim

Characterization of the DNA binding activity of bacterial response regulator BfmR from *Acinetobacter baumannii*. **M. Milton**, G. Draughn, R. Thompson, J. Cavanagh


Comparison of structure and function of 2-methylcitrate synthase (mcsA) from *Aspergillus fumigatus* and citrate synthase (HCS) from *Homo sapiens*. **C. Schlachter**, M. Chruszcz

Lipophilic optimization of peptoid library design. **J. Turkett**, K. Fisher, K. Bicker

Biomolecular interaction determination and quantification by microscale thermophoresis. **E. Lee**, A. Lazic, S. Duhr, D. Breirsprecher

Characterization of the monooxygenase subunit of dimethylsulfide monooxygenase from *Hyphomicrobium 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. Gorensek, 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


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


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-Fe₂₋ₓMnₓO₃ 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


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


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-nilutamide 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


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


**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**


1:45 715. 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 [Ca $^{2+}$] 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.


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


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.


3:50 734. Withdrawn


**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


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.


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


2:30 747. 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


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

3:00 Intermission.

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


**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 M₂AX₄ (M=Li,Na; A=Be,Mg,B⁺,Al⁺; X=H,F) and carbon and silicon hydrides YₘHₙ (Y=C,Si; m,n=2,3,4,6). D.A. Clabo

3:00 Intermission.


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

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

Nanohybrids for the determination of fundamental aspects of nanoparticle effects on the environment. **J. Lead**

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

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


Intermission.

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


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

Environmental Chemistry Posters

H. Columbia Metropolitan Convention Center
Exhibit Hall

Zur Loye, Organizer

1:00 - 2:30


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 NOx 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


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

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.


3:50 792. 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 Bi_{13-x}Sb_xS_{18}I_2 and Bi_{1-x}Sb_xS_I. R.A. Groom, A. Jacobs, M. Cepada, R. Drummey, S.E. Lattturner

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

3:00 Intermission.

3:20 797. Cage opening of the closo-carborane ligands: The reaction of closo-o-C_2B_{10}H_{10} with triosmium carbonyl cluster complexes. J. Kiprotich, R.D. Adams


Materials Chemistry Posters

Columbia Metropolitan Convention Center
Exhibit Hall

H. Zur Loye, Organizer

1:00 - 2:30


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**


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


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


815. Artificial peptides for improved synthesis and performance of lithium ion battery electrodes. **A. Winton**, M.A. Allen


820. Graphene oxide modified macroporous TiO$_2$-CeO$_2$ 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**


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


**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


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

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


851. Analysis of the decomposition of a nerve agent simulant, dimethyl methylphosphonate (DMMP), by the Lindqvist polyoxometalate: Cs₁₈[Nb₆O₁₉]. C. Gottschau, M.B. Mitchell

852. The rovibronic spectrum of c-C₃H₅. 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 pKa of the nitroxide pH EPR probe 2,2,3,4,5,5-hexamethyldiazolidin-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
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 TiO$_2$/Au(111) inverse model catalysts. D.T. Boyle, J.A. Wilke, V.H. Lam, A. Baber


3:00 Intermission.

3:20 864. Radical chain reduction of CCl$_4$ initiated by illumination of SPEEK solutions. M. Islam


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**


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**


2:45 875. 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
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


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 weigh 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


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


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) catalyst 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

901. Enantioselective synthesis of spirocyclic and bicyclic lactones through desymmetrization. K. Stingley

902. Synthesis of industrially useful dye intermediates. P.D. Miller, T. Neal


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


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


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


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


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**


940. Selected synthetic transformations of bismethoxy isoindenone and isoindene dimers. **J. Franklin**, A.D. Mills, M. Etzkorn


944. Selective mono-substitution of symmetric diols. **L. Daley**, D. Paull


947. Catalytic enantioselective (3+2)-cycloadditions α-keto ester enolates and nitrile oxides. **S.L. Bartlett**

948. Towards the synthesis of hydroxytyrosol polyphenol. **E. Onobun**, I. Kady


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


**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


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


964. Functionalization of polyacrylates with TEMPO and PEG moieties for the modification of hemoglobin-based oxygen carriers. **O. Al Omainy, H.J. Schanz**


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**


972. Investigation of new heteroleptic lanthanide catalysts for ring-opening homopolymerization of $\alpha$-methylene-$\gamma$-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(SiMe $\text{3}$) 2] 2. **K. Parrish, P. Binda**


977. Rational design and preparation of thiophene polymers for dielectric energy storage. **T. Zhu**


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


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


4:50 983. 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


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


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


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


Catalysis & Biocatalysis

Columbia Metropolitan Convention Center
Richland A

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

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*


10:05 Discussion.

**Electrocatalysis**

Hilton Columbia Center
Breakout 1/2

A. K. Vannucci, *Organizer, Presiding*


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


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


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


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


**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 fur 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**


**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-benzyloxypyphenyl) 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


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


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


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 $^{15}$N ESEEM experiments in actinide and lanthanide complexes. **D. Dan**, T.E. Albrecht-Schmitt


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 organoiiodine hybrid salts. K. Khadijatul, A. Miller, A.M. Siegfried, T.W. Hanks, **W.T. Pennington**


1051. Reactivity of ($\eta^6$-para-cymene)Ru(Ph)(I)(P(OCH$_2$)$_3$CEt) 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


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. Dolgopolova, 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


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 selone ligands. A.M. Allen, M. Kocherga, D. Rabinovich


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*


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**


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 K₂M(SO₄)₂·6H₂O (M = Mg, Co, Zn, Ni, Cu). **T.C. Devore**, A. Morales, B.A. Reisner


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


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


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


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

New recipes for biocatalysis: Expanding the cytochrome P450 chemical landscape. E.M. Brustad

Oxygen-dependent activation of diguanylate cyclase-containing globin coupled sensors. E.E. Weinert

Structural studies of cellulolytic redox enzymes using neutron scattering and diffraction. F. Meilleur, A. Bodenheimer, W. ODell

Intermission.

Theoretical investigation of the aziridination mechanism of tetracarbene iron catalysts. J.L. Kern, S. Roy


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

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

Iron complexes for hydrogen generation in aqueous solutions. W. McNamara

Efficient electrocatalytic hydrogen evolution enabled by multiple non-innocent ligands. J.D. Blakemore

Electrocatalytic conversion of CO₂ using Mn(I)-NHC compounds. J. Agarwal

Intermission.

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. NOₓ 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.


**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


3:00 Intermission.


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-tBu)18 nanomolecules and their relation to Au30S(S-tBu)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. Guiton
Towards the utilization of hole trapping ligands on nanorods for oxidative reactions.


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


3:00 Intermission.


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


Organic Chemistry

Columbia Metropolitan Convention Center
Carolina A
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 $^4$He. 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


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

3:00 Intermission.


3:50 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


3:00 Intermission.


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


4:50 1189. Withdrawn