SERMACS PROGRAM

C. D. Sherrill, Program Chair

WEDNESDAY MORNING

Electronic Structure in Complex Environments

Large Systems and Molecular Properties

Loews Atlanta Hotel
Salon G

T. Crawford, Organizer
L. Slipchenko, Organizer, Presiding

8:00 Introductory Remarks.

8:05 1. Strategies for accurate calculations on large systems. M. Gordon

8:45 2. Beyond 'biologically relevant': Applying computationally tractable standards for noncovalent interactions to develop next-generation chemical databases. L. A. Burns, J. C. Faver, M. S. Marshall, Z. Zheng, C. D. Sherrill, K. M. Merz

9:05 Intermission.


10:05 4. Magnetic resonance parameter calculations: Gas phase vs solution vs solid state. J. Autschbach

Inorganic Chemistry General Session

Loews Atlanta Hotel
Pittman

J. Shaw, Organizer, Presiding

8:00 5. Acid-Base and aggregation behavior of water soluble N-confused porphyrin. J. L. Shaw, J. L. McMurry, E. H. Bennett, P. Salehi, A. Stovall


8:30 7. Photoacoustic calorimetry studies of the photoaquation of Ru(II)bis(2,2' bipyridine)(acetonitrile)_{2} and Ru(II)bis(2,2' bipyridine)(6,6' dimethyl 2,2' bipyridine)complexes. R. W. Larsen, A. Karolak, T. Word, M. T. Kemp, C. L. Whittington, A. van der Vaart

8:45 8. Building blocks for organosilver catalysis: Applications in renewable energy. B. K. Tate, C. M. Wyss, J. Bacsa, K. Kluge, L. Gelbaum, J. P. Sadighi

9:00 9. Long-lived excited state lifetime of a titanium(IV) oxo chromophore and the extension of its lifetime by use of new heterobimetallic charge transfer mechanisms. E. M. Goggins, T. T. Lekich, W. W. Weare

9:30 11. Synthesis and characterization of heterobimetallic systems containing d^0 titanium and d^1 vanadium acceptors for applications in solar energy conversion. X. Wu, T. Huang, T. Lekich, W. W. Weare


10:00 13. Bis(mercaptoimidazolyl)alkane complexes of zinc, cadmium and mercury. S. S. Zwayyer, D. Rabinovich


Medicinal Chemistry General Session

Loews Atlanta Hotel
Centennial

J. Arceneaux, Organizer, Presiding

8:00 15. Parthenolide promotes histone deacetylase I depletion and HDM2 hyperubiquitination independent of glutathione depletion and reactive oxygen species enrichment. E. Chanchorn, T. Lee, M. Clarke, M. W. Van Dyke


9:00 18. Triggered liposomal release via a synthetic phosphatidylcholine analog bearing a photocleavable moiety embedded within the sn-2 acyl chain. A. M. Bayer, S. Alam, S. Matthern-Schain, M. D. Best


Novel Bonding Types in Inorganic Chemistry

Main-Group Chemistry

Loews Atlanta Hotel
Chastain

J. Thrasher, Organizer
A. Arduengo, Presiding
8:00 Introductory Remarks.

8:05 23. One Electron Oxidations. **K. Seppelt**


9:25 Break.

9:40 25. Synthesis and applications of pentafluorosulfanyl difluoroacetic acid. A. V. Matsnev, M. A. Stanton, S. Qing, X. Wang, G. Haufe, **J. S. Thrasher**


**Physical Chemistry General Session**

Loews Atlanta Hotel
Inman

R. Fortenberry, A. Schrand, **Organizers, Presiding**

8:00 27. Integrating Concepts from Bio-Nano-Energetic Materials Research. **A. M. Schrand**


8:40 29. Stochastic potentials for coarse-grained solvents with varying softness. **G. T. Craven**, A. V. Popov, R. Hernandez

9:00 30. Thermal decomposition of metal oxalates. **T. C. DeVore**, N. Cooper

9:20 Break.


10:00 32. Dynamics of an ultrafast folding beta-hairpin in the context of WW-domain formation. **C. Davis**, B. Dyer

10:20 33. Zinc(II) 1,3,5-tris(4-carboxyphenyl)benzene metal organic frameworks templated by Ruthenium(II)tris(2,2'-bipyridine): Photophysical properties. **C. L. Whittington**, L. Wojtas, R. W. Larsen

**Recent Advances in Ion Mobility Mass Spectrometry**

Loews Atlanta Hotel
Salon I

J. McLean, F. Fernandez, **Organizers, Presiding**


9:00 36. Advances in comprehensive metabolomic strategies using structural mass spectrometry. **J. G. Forsythe**, C. R.
Goodwin, J. C. May, K. M. Hines, N. M. Lareau, J. A. McLean

9:30 37. Coupling Ambient MS Ion Sources with IMS. J. D. Keelor, P. Dwivedi, F. M. Fernandez

10:00 38. Structural mass spectrometry of protein modification by lipid electrophiles. L. Xu, J. G. Forsythe, N. A. Porter, J. A. McLean

Supramolecular Chemistry: From Little Things, Big Things Grow

Loews Atlanta Hotel
Dunwoody

K. Shimizu, Organizer
J. Lavigne, Organizer, Presiding

8:00 Introductory Remarks.


8:30 40. Fabrication of Superamphiphiles: From Micro-Sheets into Nano-Fibers by Charge Transfer Interaction. P. Wang, J. Hu, Q. Wang

8:45 41. Polymeric semiconductors: the impact of molecular ordering. E. Reichmanis, B. Fu, N. Kleinhenz, K. Nayani, J. Park, M. Srinivasarao

9:10 Intermission.

9:25 42. Multilayer thin films from renewable and/or environmentally-benign polyelectrolytes for flame retardant protection of polymeric substrates. J. C. Grunlan

10:05 43. Functional supramolecular materials and interactions: Sensors, solar cells, and stimuli-responsive vesicles. S. Saha

The Chemistry of Star and Planet Formation

Loews Atlanta Hotel
Ravinia

S. Widicus Weaver, Organizer, Presiding

8:00 44. Spectroscopy and astrochemistry with Herschel. D. C. Lis

8:30 45. Chemistry at the dawn of star formation. P. Caselli

9:00 Intermission.


10:00 47. Origins of chemical complexity in the early stages of star formation. K. Oberg

The RNA World
Loews Atlanta Hotel
Piedmont

L. Williams, Organizer

8:00 Introductory Remarks.

8:05 48. RNA World yes. RNA first maybe. S. A. Benner, H. Kim

8:30 49. RNA and protein - a match made in the Hadean. L. D. Williams

8:55 50. Evolutionary Landscapes of RNA. I. A. Chen

9:20 Break.

9:30 51. Embracing the mess: Consequences of product mixtures in model prebiotic reactions. A. Engelhart, M. W. Powner, J. W. Szostak


10:05 53. Ribozyme ligation of RNA in Ice. L. Lie, R. M. Wartell

10:15 Panel Discussion.

10:35 Concluding Remarks.

Posters: Biological Chemistry

Loews Atlanta Hotel
Over Look/Exhibit Hall

D. Sherrill, Organizer

9:00 - 11:00


60. Examination of the thermodynamic mechanism for E. coli ClpAP. **E. C. Duran**, A. L. Lucius

61. Kinetic mechanism of *Escherichia coli* ClpA catalyzed ATP hydrolysis and thermodynamic linkage to macromolecular assembly. **C. L. Weaver**, A. L. Lucius

62. Crystal structure of choline oxidase from *Arthrobacter globiformis* in complex with glycine betaine suggests the importance of the dimer interface for substrate access to the active site. **F. Salvi**, Y. Wang, I. Weber, G. Gadda

63. JNK binds to and regulates the activity of endothelial nitric oxide synthase. **K. E. Rhoades**, C. A. Chrestensen, J. C. Salerno, J. L. McMurry

64. Impact of single rNMP damage on DNA structure. **M. Evich**, A. M. Spring, K. D. Koh, F. Storici, M. W. Germann

65. Chemical modification and site-directed mutagensis of His48 in D-Arginine Dehydrogenase. **J. Ball**, D. Su, G. Gadda


69. Evidence for hydride tunneling in the human glycolate oxidase reaction: A stopped-flow study at various temperatures. **E. Romero**, G. Gadda

70. Targeting the Core of a Holliday Junction. **C. J. Hamilton**, M. W. Germann

71. Denaturation studies of heme-binding proteins using guanidine agents. **K. Bartlett**, D. Dixon


73. Multiple TIAR Proteins Bind to the 3′ Terminal Stem- loop of the West Nile Virus Minus-strand RNA. **J. Zhang**, **H. Liu**, M. A. Brinton, M. W. Germann

74. A novel assay to identify antibacterial compounds targeting bacterial topoisomerase I. **T. Annamalai**, C. Parra, Y. Tse-Dinh

75. Mapkap kinase 2 regulation by oxidation. **A. D. Duc**, E. Rye, C. A. Chrestensen

76. Design, Syntheses and GC Base-pair Binding Evaluation of Heterocyclic Benzamidazole Diamidines containing variable linkers. **A. S. Chaudhary**


78. Dynamic interactions in regulation of flagellar biogenesis in *H. pylori*. **L. M. Beasley**, J. L. McMurry


82. Circular dichroism studies of Mg(II) and Fe(II) binding to folded and unfolded RNA. **C. D. Okafor**, N. V. Hud, L. D. Williams


84. Diatoms and their silicon transporters. **D. Paudel**, P. Curnow, T. A. Nile

85. Post-Translational modifications: Regulating the regulator. **J. E. Morgan**, S. F. Greer


91. Synthetic receptors for post-translational modifications of proteins discovered using iterative redesign in dynamic combinatorial chemistry. **J. E. Beaver**, L. I. James, M. L. Waters

92. Biosynthetic studies of F430, the key coenzyme of methanogenesis. **B. R. Mueller**, X. Yang, S. O. Mansoorabadi

93. Isolation and characterization of Syndecan-1 mutants involved in cell wound migration. **L. V. Greene**, L. Chase, J. Koblinski


95. Optimization of the Extraction Procedures of Indigo from Selected Plants. **L. Misigaro**, B. Ooi


97. Selenium-derivatized nucleic acids (SeNA) for structure and function studies. **S. Jiang**, H. Sun, J. Sheng, J. Gan, Z. Huang

98. The influence of solution conditions on *E. coli* Hfq binding to RNA. **S. Y. Goo**, R. M. Wartell

99. Understanding Binding-Induced Conformational Change in Pin1. **H. G Yamfi**, N. C. Fitzkee, A. Bax, A. Grishaev

100. Hydrophobic drug binding by calmodulin is eliminated by methionine oxidation. **H. T. Niedermaier**, R. J. Bieber Urbauer, J. L. Urbauer


102. Investigations into the mutagenic potential of 8-oxo-2'-deoxyguanosine using Klenow Fragment and Human DNA
Polymerase β. **E. J. McFadden**


105. Role of C-terminus tail in the ligand binding and release mechanisms of *Antheraea polyphemus* pheromone binding protein1 (ApolPBP1). **S. Mazumder**, U. V. Katre, S. Mohanty


107. Single-molecule studies on loop-loop kissing interactions in guanine-sensing riboswitch. **V. Chandra**, H. Xu, M. Mandal


109. Synthesis and incorporation of S-(3-(acetylthio)propyl)-5-(mercaptomethyl)-2′-deoxyuridine triphosphate into DNA by DNA polymerase. **R. Esmaeili**, M. Kaur, Z. Huang


112. Discovery and identification of Hfq-binding nanoRNAs in *Escherichia coli*. **J. Patterson**, S. Cao, J. Clardy, C. Mura


115. Cationic porphyrin-ruthenium(II) conjugates as potential selective stabilizers of G-quadruplex. **C. Musettia**, T. Gianferrara, **C. Sissia**


**Plenary Session**

Loews Atlanta Hotel
Salon D/E/F

**11:00** **117.** DRIVE: An innovative, non-profit drug discovery company. **D. Liotta**

**WEDNESDAY AFTERNOON**

**Analytical Chemistry General Session**
Loews Atlanta Hotel
Ardmore

R. Wu, Organizer, Presiding

1:00 118. Electrochemical Analysis of Parathion-ethyl Pesticide by Zirconium Oxide-Laponite Composite Modified Glassy Carbon Electrode. M. N. Bui, S. S. Seo


2:00 121. Surface Enhanced Photoelectrochemical Performance Using Surface Plasmon Towards Solar Water Splitting. Z. Shan, S. Pan, D. Clayton, P. S. Archana, A. Gupta


2:40 123. Single-molecule spectroelectrochemistry (SMS-EC) of (4, 4'-difluoro-4-bora-3a, 4a-diaza-s-indacene) BODIPY dyes. J. Liu, S. Pan

3:00 124. High-resolution scanning electrochemical microscopy pH imaging using carbon-fiber ultramicroelectrodes modified by iridium-oxide-nanoparticles. H. Khani, D. O. Wipf

3:20 Intermission.


3:55 126. Using temperature programmed analytical techniques to understand and optimize Fischer-Tropsch catalyst thermal treatments. K. Cook, W. Hecker, K. Keyvanloo

4:15 127. Highly ordered pillar arrays as platforms for planar chromatography. T. B. Kirchner, N. A. Hatab, N. A. Crane, D. R. Lincoln, N. V. Lavrik, M. J. Sepaniak

4:35 128. Electron transfer dissociation mass spectrometry of neutral peptides with alkyl side chains. C. Feng, C. J. Cassady

4:55 129. A novel, direct coupling of Simultaneous DSC/DTA-TGA (STA) and FTIR called Perseus™. T. Doll, R. Fidler


Biological Chemistry General Session

Enzymology, Protein Engineering, and Metabolism

Loews Atlanta Hotel
Inman

A. Reddi, Organizer, Presiding
1:00 131. Peroxygenase activity of dehaloperoxidase from *Amphitrite ornata*. **N. Lucas**


1:45 134. Solving the puzzle of a green flavin isolated from D-arginine dehydrogenase. **S. Gannavaram**, A. M. Spring, M. W. Germann, G. Gadda

2:00 135. Mechanistic study of D-arginine dehydrogenase I335H with pH profiles and rapid kinetics. **D. Ouedraogo**, G. Gadda

2:15 136. Thermodynamic analysis of the bacterial loop of E. coli β-glucuronidase. **S. E. Hickling**, S. Hengeli, K. Lane

2:30 137. Characterization of bacterial propionate 3-nitronate monooxygenase from Pseudomonas sp. Strain JS189. **D. Su**, K. Francis, G. Gadda


3:00 139. Transforming *in vitro* enzymatic reactions from flask into microbial cell: Production of polyhydroxylated molecules via engineered *E. coli*. **M. Wei**, Z. Li, L. Cai, B. Wu, P. Wang

3:15 140. Rescuing activity of an glycosyltransferase by glycosylation. **G. Zhao**, L. Li, T. Li, P. G. Wang

3:30 141. Bioorthogonal profiling of lysine acetylation with an engineered enzyme and derivatives of coenzyme A. **J. Mi**

3:45 142. A new role for an old copper enzyme in glucose and oxygen sensing. **A. Reddi**

4:00 143. Analysis of BCL-2 proteins during heart development. **T. A. Davis**, V. Del Gaizo Moore

4:15 144. Identification of powdery mildew resistance related metabolites in rootstocks of watermelon using NMR. **I. Mahmud**, R. Hassell, C. Kousik, K. Chowdhury, A. Boroujerdi

4:30 145. NMR-based metabolomics differences between nutrient uptake of embryogenic and non-embryogenic sugarcane calli from growth medium. I. Mahmud, **M. Thapaliya**, A. Boroujerdi, K. Chowdhury

4:45 146. Sugarcane (*Saccharum officinarum* L.) tissues have distinct NMR-based metabolomics profiles. **I. Mahmud**, **J. Pleasant**, A. Boroujerdi, K. Chowdhury

Frontiers in Nucleic Acid Chemistry

**Nucleic Acids 1**

Loews Atlanta Hotel
Piedmont

M. Germann, *Organizer*

1:30 148. Thermodynamic Signature to DNA Damage. B. Gold, M. Ganguly, M. W. Szulik, M. P. Stone


2:30 150. Structural Studies of the 2-Amino-3-methylimidazo[4,5-f]quinolone N²-dG DNA Adduct. M. P. Stone

3:00 Intermission.

3:15 151. Unfolding and Targeting Thermodynamics of DNA Stem-Loop Motifs. L. A. Marky, I. Khutsishvilli, I. Prislan

3:45 152. Monomeric HIV-1 Rev is an intrinsically disordered protein and folds upon self-association and RNA binding. M. Hennig, F. Casu, M. Marenchino, S. P. Edgcomb, B. M. Duggan

4:15 153. Structure and function of RNA processing and silencing enzymes in the CRISPR immunity. H. Li

4:45 154. Information Content in RNAs from the "Prebiotic Ribosome" to Modern Viruses. S. C. Harvey

Inorganic Chemistry General Session

Loews Atlanta Hotel
Pittman

J. Shaw, Organizer
C. Scarborough, Presiding

1:00 155. Carbene-stabilized unusual main group molecules: Synthesis, structure, and reactivity. R. J. Gilliard, Y. Wang, G. H. Robinson

1:15 156. Emerging chemistry of N-heterocyclic dicarbenes. Y. Wang, D. R. Sexton, G. H. Robinson


2:00 159. Synthesis and characterization of transition-metal-substituted polyoxometalates as water oxidation catalysts. G. Zhu, C. L. Hill

2:15 160. Phosphate ester hydrolysis of phosphatidylcholine in aqueous solutions of cerium(IV) and bis-tris propane. D. E. Williams, K. B. Grant

2:30 161. Bandgap engineering of germanium nanoparticles through tin alloying and quantum confinement effects. R. J. Esteves, I. Arachchige

2:45 162. Sol-Gel assembly of silver nanoshells into aerogel frameworks. X. Gao, I. U. Arachchige

3:00 163. Quinoxolinol salen ligands for spectrophotometric molecular recognition. M. DeVore II, A. Gorden, S. Kerns

3:15 164. Quinoxalinol salens: Ligands for actinide sensors and sensing polymers. A. E. Gorden

3:30 165. Structural and functional models of quercetin 2,3-dioxygenase using trisimidazolylphosphine complexes. W.
E. Lynch, D. Nivens, N. Peek, J. Stone

3:45 166. Development of new mixed-donor ligands for the preparation of synthetic analogues of methanobactin. D. Rabinovich

4:00 167. Sterically-demanding N-heterocyclic thiones (NHTs): Synthesis and reactivity. M. S. Styron, D. Rabinovich

4:15 168. Synthesis and coordination chemistry of new bis(pyridyl)-and bis(picolyl)thione ligands. N. K. Spencer, D. Rabinovich

Mass Spectrometry Applications in Clinical Chemistry and Environmental Health

Loews Atlanta Hotel
Salon I

V. De Jesus, Organizer, Presiding

1:00 169. Screening dried blood spots from newborns for inherited metabolic diseases using tandem mass spectrometry. D. H. Chace


2:00 171. LC-MS determination of molecular markers of water pollution from animal production. J. J. Harwood, S. L. Narayanan


3:00 173. Mass spectrometric identification of microRNA biomarkers with ultra-high accuracy. N. H. Chiu


4:00 175. Semi-automated solid phase extraction method for the mass spectrometric quantification of 12 specific metabolites of organophosphorus pesticides, synthetic pyrethroids, and select herbicides in human urine. M. D. Davis, L. Valentin-Blasini, E. Wade, W. Roman-Esteva, A. Calafat

Organic Chemistry General Session

Loews Atlanta Hotel
Candler

B. Feske, Organizer
L. Davis, Presiding

1:00 176. Phosphoric acid mediated tautomerism of imines: Addition of imines to aldehydes. L. O. Davis, M. Putri


2:00 179. Long-Range intramolecular S to N acyl migration: a study of the formation of native peptide. K. Ha, A. Katritzky

2:40 181. Ion-exchange chromatography to measure relative anion-pi binding of substituted benzenes. M. Lewis, C. Bagwill, S. Wirduaah

3:00 182. Synthesis of novel 2-[2-acylamidoethyl]-6(phenyl)pyridine analogues. J. G. Draper, T. Wenzler, R. Brun, D. W. Boykin


3:40 184. The glyoxoin reaction: A catalytic route to an abiotic citric acid cycle. C. J. Butch, E. D. Cope, P. Pollet, L. Gelbaum, R. Krishnamurthy, C. Liotta

4:00 185. Correlating N-alkyl group electronegativity with DFT-computed Parr global electrophilicity values of imidate ester analogs. J. M. Carr, A. P. Lathem, G. S. Tschumper

4:20 186. Revisit of a popular fluorophore: skeletal characterization and structural modification. H. Li, Q. Wang

4:40 187. Synthesis of symmetrical and unsymmetrical Bis-2,5-Diketopiperazines utilizing benzotriazole-mediated lactamization reactions. K. Martin

5:00 188. Addition of enol silanes, silyl ketene acetals, and zinc acetylides to nitrones under silylative conditions. C. Downey


Posters: Agricultural Chemistry

Loews Atlanta Hotel
Over Look/Exhibit Hall

D. Sherrill, Organizer

1:00 - 3:00

190. Reducing the allergenicity of wheat flour by proteases. Y. Li, J. Yu

191. In vitro Digestibility of macronutrients in the presence of grape pomace polyphenols. J. Yu, S. Ji, Y. Mi


Posters: Environmental Chemistry

Loews Atlanta Hotel
Over Look/Exhibit Hall

D. Sherrill, Organizer

1:00 - 3:00

193. Development of a protein-based system for the detection of organophosphates using the pH dependence of
enhanced green fluorescent protein. A. Henson, J. Harris, L. G. Puckett

194. Urinary diamines as biomarkers of exposure to diisocyanates. Y. Qiu, R. Newton, A. Udeni, B. Blount


196. Biosorption of Hexavalent Chromium from Aqueous Solutions Utilizing Agricultural Waste Products. A. M. Rizzuti, K. A. Wilson, L. W. Cosme

197. Investigation eutrophication of Lake Sinclair. J. Olmstead

198. Aqueous Cu(II) adsorption by modified and unmodified peanut hulls. K. O. Davis, C. L. Huffman


203. Ingested plastics as a transport medium for marine toxicants to the gastrointestinal tract of loggerhead sea turtles, Careta caretta. M. D. Wilbanks, P. J. Seaton

Posters: Medicinal Chemistry

Loews Atlanta Hotel
Over Look/Exhibit Hall

D. Sherrill, Organizer

1:00 - 3:00

204. Synthesis and thermal stability evaluation of six-membered cyclic triphosphates containing three nucleotides. Y. A. Beni, K. Parang

205. Design and synthesis of potential CXCR4 antagonists. T. Gaines, S. Mooring


209. Applying desorption electrospray ionization to streamline the discovery of bioactive compounds from fungi. V. Sica, N. Oberlies, B. Ehrmann, H. Raja, T. El-Elimat

210. Polyamine-anthracene conjugates: the effects of high ionic strength on DNA interactions and photocleavage. K. Nguyen, J. J. Archer, O. Phanstiel IV, K. B. Grant


217. SAR Studies of pyrimidine SecA inhibitors as potential antimicrobial agents. **A. S. Chaudhary**


226. Potent chiral Inhibitor of histone deacetylase. **J. hou**


229. Glucosamine conjugates of a minor-groove methylating agent: DNA-reactivity and cell toxicity. T. Goodwin, M.


232. Polyethylene Glycol containing ROMP Polymers for the modification of neuro-protective Hemoglobin. A. L. McCollum, H. J. Schanz


234. Microgel encapsulated methylene blue for the treatment of breast cancer cell by photodynamic therapy. A. Khanal, S. S. Seo

Supramolecular Chemistry: From Little Things, Big Things Grow

Loews Atlanta Hotel
Dunwoody

J. Lavigne, K. Shimizu, Organizers

1:00 235. Polydiacetylenes for sensor applications. W. T. Pennington, S. C. Hill, P. L. Dawson, T. W. Hanks

1:25 236. FRET-based indicators for zinc ions. L. Zhu

1:50 237. Iterative redesign in DCC: Identification of a new synthetic receptor that recognizes trimethyllysine with nanomolar affinity. N. K. Pinkin, M. L. Waters

2:05 238. Sensing anions with fluorescent ureas. W. E. Allen

2:30 239. Molecular probes for Zinc(II) and Iron(III) ions. K. J. Wallace, E. Manandhar

2:55 Intermission.

3:10 240. Supramolecular approaches to developing sensors for modified amino acids in proteins. M. L. Waters

3:50 241. Molecular probes based on the supramolecular interactions of rhodamine B derivatives with organic analytes. C. Stephenson


4:30 243. Experimental studies of the effect of polarizability on the $\pi$-$\pi$ interaction. J. Hwang, B. Dial, M. Kozik, K. D. Shimizu

4:45 244. From “little” boronate ester sensors grow “big” supramolecular boronate sensors (with tiny pores). J. J. Lavigne

5:10 Concluding Remarks.

The Chemistry of Star and Planet Formation

Loews Atlanta Hotel
Ravinia

S. Widicus Weaver, Organizer, Presiding

1:00 245. The formation of complex interstellar molecules. E. Herbst

1:30 246. Excitation of carbon monoxide: Full-dimensional structure and dynamics for inelastic scattering. P. Stancil

2:00 247. Ab initio ro-vibrational IR spectra of H$_5^+$ D$_5^+$ and HOCO. J. Bowman, S. Carter, Y. Wang

2:30 248. Computational prediction of l-C$_3$H$^+$ in the Horsehead Nebula PDR. R. C. Fortenberry, X. Huang, D. Crawford, T. J. Lee

3:00 Intermission.

3:30 249. Vacuum Ultraviolet photon-stimulated formation of CO$_2$ at buried ice: graphite grain interfaces. T. M. Orlando, J. Shi, G. Grieves

4:00 250. Phosphorus in planet formation. M. A. Pasek

4:30 251. Chirped-pulse spectroscopy from 110 - 170 GHz with real-time digitizers. L. Bernier, S. Shipman

Novel Bonding Types in Inorganic Chemistry

New Materials and Catalysts for Energy Conversion and Storage

Loews Atlanta Hotel
Chastain

J. Thrasher, Organizer
T. Gunnoe, Presiding

1:10 252. Mechanism-based design of precursors for the deposition of inorganic films and nanoparticles. L. McElwee-White


2:30 254. Synthesis of mono-oxo bridged first row transition metal heterobimetallic molecules as long-lived, redox-tunable chromophores. W. W. Weare

3:10 Break.

3:30 255. Ionic and metallic carbides grown in metal fluxes. S. Latturner

4:10 256. Oxyfunctionalization with Cp*Ir complexes. E. A. Ison

4:50 257. Harnessing redox-active ligands for low-barrier radical coupling reactions at oxidizing oxo complexes. J. D. Soper

Chemical Patent and Trademark Law
Loews Atlanta Hotel  
Salon H  

M. Katz, Organizer, Presiding  

1:20 Introductory Remarks.  

1:30 258. Chemical inventorship. D. B. Shortell  


2:30 260. Patents: Obviousness in chemical inventions. K. W. Hathcock  

3:00 Intermission.  


3:50 262. All you need to know about trademarks. W. H. Needle  

Electronic Structure in Complex Environments  

Biological Environments and Energy Conversion  

Loews Atlanta Hotel  
Salon G  

L. Slipchenko, T. Crawford, Organizers  
L. Burns, Presiding  

1:20 263. A flickering resonance mechanism for biological charge transfer. D. N. Beratan  

2:00 264. Using quantum mechanics in biological structure refinement. K. M. Merz  

2:40 265. Electron transport and transfer through molecular-resolved interfaces: Insight by ab-initio modeling. B. D. Dunietz  

3:20 Intermission.  


4:20 267. The on-the-path random walk sampling to enable multi-step-multi-coordinate enzymatic reaction simulations. L. Cao, W. Yang  

5:00 268. How does catalase release nitric oxide? Elucidating the reaction mechanism with QM/MM. F. L. Kearns, S. Vankayala, H. Woodcock  

Neuropeptergic Targets for CNS Disorders  

Loews Atlanta Hotel  
Centennial  

F. Carroll, Organizer, Presiding
1:30 Introductory Remarks.

1:35 269. Neoclerodane diterpenes as novel treatments for drug abuse. T. E. Prisinzano


2:35 271. Evaluation of ligand bias at the kappa opioid receptor: Spanning compound development to effects in neurons. L. M. Bohn


3:35 Concluding Remarks.

Posters: Organic Chemistry

Loews Atlanta Hotel
Over Look/Exhibit Hall

D. Sherrill, Organizer

4:00 - 6:00


276. Total synthesis of (±)-2-methoxy-6-octadecenoic acid, identified in the Caribbean sponge Spheciospongia cuspidifera, as possible therapeutic agent against neuroblastoma cells. N. Montano, W. O. Marrero, N. M. Carballeira


278. Synthesis of cyclic peptides by intra-molecular lactamization and cyclo-oligomerization of dipeptidyl benzotriazolides. S. Hamedzadeh, K. Ha

279. Pyrimidine based potential liquid crystals. T. A. Bradshaw, Z. A. Ratka, B. S. Clark, S. Q. Smith

280. Total synthesis of Hibiscone C. A. G. Boyd

281. Efficient benzotriazole–mediated route to C₂ symmetric cyclo-tetrapeptides containing β-amino acids. R. E. Quinones, K. Ha

282. Hypervalent-iodine mediated substitution of aromatic compounds with sodium periodate. P. A. Shelton, H. Kim, K. Kim, W. Crosby

283. Solvent-free synthesis of oxindole derivatives through C-H activation in air. S. Son, J. Lee, W. Lee

284. Withdrawn.

286. Synthesis of cysteine ester macrocyclic peptoids by benzotriazole methodology. **L. Nhon**

287. Gold(I) Catalyzed Racemization of 1,3 disubstituted Allenes. **R. J. Harris**, R. A. Widenhoefer


289. Simple One Step Oxidation of Steroidal Olefins. **W. Grainger**, E. Parish

290. Progress toward the Synthesis of Callophycolide A, an Antimalarial Benzene Diterpenoid. **R. E. Key**, S. France


294. Lewis acid-catalyzed interrupted formal homo-Nazarov cyclization. **R. Shenje**


297. Lewis acid-catalyzed ring opening annihilations of polarized strained rings in the presence of amines. **M. C. Martin**


299. Chemoenzymatic synthesis of homogenous activity-reversible biotinylated ultralow molecular weight (ULMW) heparin. **B. Wu**, V. Thon, T. Li, P. G. Wang

300. Oxidation of Hibiscone C towards synthesis of recently discovered Natural Products. **J. H. Tryon**

301. Oxa-dibenzocyclooctyne (ODIBO): The most reactive cyclooctyne for uncatalyzed alkyne azide reactions. **C. D. McNitt**, V. V. Popik


303. Further Insight into the Generation of Cyanocarbenes. **M. A. Maxwell**, M. Croatt, I. F. Hyatt

304. Chemo-enzymatic Synthesis of Polysaccharides. **T. Li**


306. Towards the synthesis of a tripyrromethane derivative mimicking the active site of coenzyme F430. **C. Crooks**, A. Gorden


309. Synthesis of (+)-Bakuchiol using the desymmetrization of a prochiral hydroxy diester with a bulky Brønsted acid. A. T. Stacy, K. S. Petersen

310. Probing the Binding Properties of Dendrimers as Supramolecular Hosts. A. Jolly

311. Intramolecular Photochemical Cyclizations of Dihydropyridones. S. Kiren, D. Butler

312. Atom-modified fluorescent labels for nucleic acid based detection. M. Kaur, J. Caton-Williams, Z. Huang

313. Synthesis, characterization, and biological applications of Nile red derivatives. V. Martinez, E. Alsolmy, M. Henary


**THURSDAY MORNING**

**Plenary Session**

Loews Atlanta Hotel
Salon D/E/F

8:00 315. Academia-Industry-Government Relations in Practice. D. P. Duncan

**Organic Chemistry General Session**

Loews Atlanta Hotel
Candler

B. Feske, *Organizer, Presiding*

9:00 316. Synthesis of complex alkaloids as a driving force for discovery. J. G. Pierce


9:40 318. Calcium catalyzed addition reactions. K. Nolin

10:00 319. Total Synthesis and Biological Activity of Hibiscone C. B. C. Goess

10:20 320. Facile synthesis of enantioenriched hydroxy esters through Brønsted acid catalyzed kinetic resolution. A. Benavides, G. Qabaja, K. Petersen

10:40 321. Highly selective Lactonization of racemic Diesters to yield enantioenriched \(\gamma\)-Lactones. J. E. Wilent, K. Petersen

11:00 322. Lewis Acid/Brønsted Acid-Catalyzed \(Csp^3\)-H Bond Functionalization of 2-Methyl Azaarenes. A. Shaikh


11:40 324. Silver-promoted [2,3]-rearrangement reactions of O-allylhydroxylamines. J. B. Vu

**Synthesis, Structure, and Properties of f-element materials**

f-element intermetallics
Loews Atlanta Hotel
Inman

T. Albrecht-Schmitt, Organizer
S. Lattuner, Organizer, Presiding

9:15 Introductory Remarks.


10:00 326. Nd₂Co₂SiC and other intermetallics grown from rare earth / transition metal melts. S. Zhou, T. Mishra, S. E. Lattuner

10:25 Intermission.

10:35 327. Magnetism in giant unit cells: does cobalt participate in magnetic ordering in $R_{117}Co_{52+\delta}Sn_{112+\gamma}$ structures? M. Shatruk, P. Chai, K. Kovnir

11:15 328. Synthesis of rare-earth cobalt arsenides from Bi flux. X. Tan, C. M. Thompson, K. Kovnir, M. Shatruk

11:40 329. Magnetic properties of $R_{21}Fe_8M_7C_{12}$ (R = La, Ce; M = Si, Ge, Sn) intermetallic phases. S. E. Lattuner, T. Mishra

Approaches to Organic Synthesis Across Disciplines

Loews Atlanta Hotel
Salon H

D. Whitehead, S. Wiskur, Organizers

9:20 Introductory Remarks.

9:25 330. Towards the synthesis of the malagashanine alkaloids – Molecules with a stereochemically unique framework that have the potential to impact malaria chemotherapy. S. B. Blakey

10:10 331. Taking advantage of the chemistry of heterocycles in advanced catalyst ligand supports. A. E. Gorden

10:30 Intermission.

10:45 332. Chelation-assisted, copper(II) acetate-catalyzed azide-alkyne cycloaddition and amine dehydrogenation. L. Zhu

11:05 333. Gold(I)-catalyzed functionalization of C=C bonds. R. A. Widenhoefer

Biological Chemistry General Session

Chemical Biology, Metabolism, and Nucleic Acids

Loews Atlanta Hotel
Ravinia

A. Reddi, Organizer, Presiding

9:35 335. NMR-based metabolomics approach for the biochemical characterization of embryogenic and non-embryogenic calli of *Saccharum officinarum* L. I. Mahmud, **B. Shrestha**, A. Boroujerdi, K. Chowdhury


10:35 339. Designing a novel class of protein-based MRI contrast agents (ProCAs) for metastatic tumors in liver and molecular imaging of disease biomarkers. J. Qiao, S. Xue, F. Pu, **J. Yang**


11:05 341. *In vitro* study of assembly events during bovine leukemia virus replication. **D. F. Qualley**


**Electronic Structure in Complex Environments**

**Potential Surfaces and Excited States**

Loews Atlanta Hotel
Salon G

L. Slipchenko, T. Crawford, *Organizers*
G. Tschumper, *Presiding*


10:00 345. Spatial partitioning of symmetry adapted perturbation theory: the A-SAPT heuristic. **R. M. Parrish**, C. D. Sherrill

10:20 Intermission.


**Frontiers in Nucleic Acid Chemistry**

**Nucleic Acids 2**
Loews Atlanta Hotel
Piedmont

M. Germann, Organizer


10:20 Intermission.


NanoElectrochemistry in Biomedical Research and Energy Technology

General Topics

Loews Atlanta Hotel
Centennial

L. Bottomley, J. Stickney, G. Wang, Organizers, Presiding

9:20 Introductory Remarks.

9:25 352. Mechanistic Electrochemistry with Cyclic Square Wave Voltammetry. L. A. Bottomley, M. A. Mann


10:45 355. Electrodeposition of non-dendritic lithium by addition of alkaline earth metals. J. K. Stark, P. A. Kohl


11:25 357. Imaging and measuring single molecular specific interactions by single molecule recognition and force spectroscopy. B. Xu, B. Wang, C. Guo

New Opportunities for Chemical Businesses

Loews Atlanta Hotel
Pittman

M. Beug-Deeb, Organizer, Presiding

9:20 Introductory Remarks.
9:30 358. An Overview of 3D Printing and an Introduction to Some Emerging Additive Manufacturing Technologies with Disruptive Potential. **S. Das**

10:10 359. International Trade Services and Chemical Exports from Georgia; and The Benefits of Georgia. **T. Ponce**, **W. R. Harrison**

10:50 360. Accelerating Medical Device Commercialization in the Southeast. **T. W. Karp**

11:30 361. Local Content --- Opportunities for Business Expansion – A New Way to Market. **P. Dismer**, **M. Beug-Deeb**

**Novel Bonding Types in Inorganic Chemistry**

**NHC Chemistry**

Loews Atlanta Hotel
Chastain

J. Thrasher, *Organizer*
K. Seppelt, *Presiding*


10:40 Break.

11:00 364. Evolving Main Group Chemistry of N-Heterocyclic Carbenes. **G. H. Robinson**


**Physical Chemistry General Session**

Loews Atlanta Hotel
Ardmore

A. Schrand, R. Fortenberry, *Organizers*


10:00 368. Photoreactivity and singlet oxygen generation of select mononitrofluoranthenes. **S. Gavalda**, R. Arce


10:40 Break.


11:40 372. Widely accessible fast mixer to study biophysical reactions. M. J. Reddish, B. Dyer

Supramolecular Chemistry: From Little Things, Big Things Grow

Loews Atlanta Hotel
Dunwoody

J. Lavigne, K. Shimizu, Organizers

9:20 Introductory Remarks.

9:25 373. Biomolecular synthesis of the conducting polymer PEDOT:PSS. C. Payne

9:50 374. Noncovalent polymerization in water by monomers that were inspired by the nucleobases. B. J. Cafferty, M. C. Chen, I. Gállego, N. V. Hud

10:05 375. Controlling the structure and dynamics of supramolecular G-quadruplexes from the nano- to the micro-scale. J. M. Rivera

10:30 Intermission.

10:45 376. Post-synthesis DNA modifications with the boronic acid moiety for sensing applications. B. Wang

11:25 377. Water-Soluble Polyelectrolytes as Supramolecular Hosts. M. Bonizzoni

Posters: Nanochemistry and Spectroscopy: Symposium Honoring Mostafa El-Sayed

Loews Atlanta Hotel
Over Look/Exhibit Hall

P. Wine, Z. Zhang, Organizers

10:00 - 12:00


379. Proton coupled electron transfer in biomimetic beta hairpin peptides. C. V. Pagba, J. Yohannan, T. McCaslin, M. McDaniels, B. A. Barry

380. The role of surface diffusion in determining the shape of noble-metal nanocrystals. X. Xia, S. Xie, M. Liu, Y. Xia

381. Synthesis of Cationic Polyamine and Polyguanidine Type Polymer-Capped Gold Nanoparticles: Heterogeneous Catalysis. C. Padgett, N. A. Green, G. J. Gabriel, B. Baruah*

382. Quantitative analysis of the coverage density of Br⁻ ions on Pd{100} facets and its role in controlling the shape of Pd nanocrystals. H. Peng, Y. Xia

383. Kinetically controlled synthesis of palladium icosahedra and their catalytic properties. T. Lv, Y. Wang, S. Choi, Y. Xia

384. Surfactant-Coated Nanoparticles as Substrates for Surface Enhanced Raman Spectroscopy. B. S. Thompson, K.
Wulkowicz, B. Baruah

385. Development of highly luminescent europium-based silica nanomaterials for biomedical applications. A. N. Darsanasiri, I. Bose, C. R. De Silva

386. Complete water splitting with hybrid nanoparticles and hole-extracting ligands. A. D. La Croix, J. Macdonald

387. Progress towards synthesis of Au@SiO$_2$---Cu$_{2-x}$Se hybrid nanoparticles for surface plasmon interaction studies. S. L. Arrowood, J. Macdonald

388. Size- and shape-controlled synthesis of wurtzite CuInS$_2$ nanoparticles for photocatalytic reduction of water. B. C. Howard, E. Hernández-Pagan, J. Macdonald


390. Electrochemical formation of tungsten nanosharp tips. M. Nave, B. Rubin, V. Maximov, S. Creager, K. Kornev

391. Determination of the maximum dopant threshold of cobalt ferrite spinels with gadolinium as the dopant. P. A. Edmonds, Z. J. Zhang

392. Change of magnetic properties in nanoparticles for surface detection. J. Robbins, Z. J. Zhang

393. Using self-assembled DNA nanostructures to stimulate cell surface receptors. R. Pedersen, T. H. Labea, E. G. Loba

394. Hollow gold nanorectangles: The roles of polarization, substrate and orientation. R. Near, M. El-Sayed


396. Plasmonic Coupling Of Three Pairs Of Sharp Corners Of Solid Cubes, Two Pairs Are Homogeneous (Au or Ag) And The Third Pair Is Of Silver And Gold. N. Hooshmand, D. O'Neil, M. El-Sayed


399. Determining the mechanism of solution metallic nanocatalysis with solid and hollow nanoparticles: homogeneous or heterogeneous. B. Garlyyev, M. Mahmoud, M. El-Sayed


402. Study on Faraday Rotation Spectra for Cobalt Ferrite Thin Films. H. i. Doo, Z. J. Zhang

403. Platinum-silver alloy nanocage catalysts exhibit low activation energies with minimal platinum content. J. A. Bordley, M. A. El-Sayed

404. Synthesis of Lipid-Capped Nanoparticles as SERS Substrates. J. A. Law, C. Megedyuk, B. Baruah


407. Capture and detection of cancer cells in whole blood with magnetic–optical nanoovals. **S. Bhana**, E. Chaffin, Y. Wang, X. Huang

408. Kinetic control: a versatile and powerful route to controlling the shape of metal nanocrystals. **X. Xia**, Y. Xia

409. Particle size effect on the photocatalytic activity of BiNbO₄. **S. P. Adhikari**, K. Senevirathne, A. Lachgar

410. Probing of local photoelectrochemical events on single crystal TiO₂ with nanometer scale resolution. **D. A. Clayton**, G. J. Szulczewski, S. Pan

**Posters: Computational Chemistry**

Loews Atlanta Hotel
Over Look/Exhibit Hall

D. Sherrill, *Organizer*

**10:00 - 12:00**


413. Discovery of potent inhibitors targeting protein arginine methyltransferases using in silico virtual screening. **C. Yan**, L. Yan, Y. G. Zheng, I. Ivanov


416. Using Adaptive Steered Molecular Dynamics (ASMD) to determine the energetics of secondary structures in peptides. **H. Bureau**, E. Hershokvitz, R. Hernandez, D. Merz, S. Quirk


419. Docking studies of Modafinil to neurological receptors. **K. Huang**, P. G. Wang, N. W. Allen


423. DFT of RDX fragmentation pathways: Computational evidence for the lack of molecular ion peak in RDX mass spectrum. K. A. Duncan, Y. A. Jeilani

424. PRMT1: Exploring the mechanism and product specificity from molecular dynamics simulations. S. Gathiaka, J. Hevel, O. Acevedo

425. Highly accurate potential energy surface for the He-H₂ dimer. B. W. Bakr, D. G. Smith, K. Patkowski

426. Vesicle phase transition dynamics in a coarse-grained simulation. L. A. Patel, J. T. Kindt

427. Molecular mechanism of dynamic recognition of octamer-binding transcription factor (OCT4) to its target DNA. L. Li, L. Luo, C. Luo, K. K. Li

428. Structurally distinct complexes of ubiquitin and SUMO-modified PCNA lead to distinct functional outcomes. C. Yan, X. Xu, I. Ivanov

Posters: Physical Chemistry

Loews Atlanta Hotel
Over Look/Exhibit Hall

D. Sherrill, Organizer

10:00 - 12:00

429. Temperature dependence of the thermodynamics for binding histone H1₀, its carboxyl domain (H₁₀-C), or its globular domain (H₁₀-G) to calf-thymus DNA. V. Machha

430. Electron spin resonance investigation of matrix isolated C₂H₆⁺. C. Burton, J. J. Banisaukas, III, L. B. Knight, Jr

431. Synthesis of Silver Cyanide by Pulsed Laser Ablation in N,N-dimethylformamide. S. Lee, M. Y. Choi

432. Enhanced dechlorination of m-dichlorobenzene using Fe/Pd/C nanoparticles Produced by Pulsed Laser Ablation in Liquid(PLAL). Y. Yu, M. Y. Choi


434. Photochemical reduction of CO₂ on sphalerite (ZnS) mineral surfaces. R. Zhou, M. I. Guzman

435. Tuning bipolaron populations in PEDOT:PSS via biological catalysts. J. Morris, C. Payne


437. Spectral characterization of intermediate species in the catalytic degradation of hydroxyurea by horse heart myoglobin. P. Huhta, R. Larsen


439. Photo-initiating the enzymatic reaction of mushroom Tyrosinase utilizing the Ru(II)bis(2'2-Bipyridine)(Tyramine)₂ complex as a substrate photo-releasing agent. V. Fuillerat, T. Word, P. Huhta, R. W. Larsen

441. Effect of shape and symmetry of gold and silver nanoparticles on their mechanical properties. D. O'Neil, M. Mahmoud, M. El-Sayed

442. Time resolved fluorescence measurements to study electron transfer in DMPD-Pro-Coumarin and two coumarin control compounds. M. Fekhry, R. Abdel Malak Rached, E. Castner, J. Wishart

THURSDAY AFTERNOON

Minority Affairs Committee Luncheon

(Ticketed event)

Loews Atlanta Hotel
Salon A

J. Green, K. Jackson, Organizers

12:00 443. Considering the chemistry of a crisis. K. Bobb

Frontiers in Nucleic Acid Chemistry

Nucleic Acids 3

Loews Atlanta Hotel
Piedmont

M. Germann, Organizer

1:00 444. DNA-Encapsulated Silver Clusters. J. Petty, D. Nicholson, O. Sergev


2:00 446. Development of Benzimidazoles alkynes in Nucleic Acid Recognition. D. P. Arya, N. Ranjan

2:30 447. Nucleic Acid NMR, new Tools and Methods. C. Anklin

3:00 Intermission.

3:15 448. Identification of new, biologically relevant, G-quadruplexes formed within the critical promoter of kRAS as promising molecular targets. C. A. Hockings, T. A. Brooks

3:35 449. Integrative modeling of complex nucleic acids assemblies. C. Yan, X. Xu, I. Ivanov

3:55 450. DNA origami: Constructing nanomaterials and nanorobotics from DNA. R. M. Wadkins, J. Waller

4:15 451. Supercooled aqueous NMR. A. M. Spring

Minority Serving Institutions and their Role in the STEM Pipeline

Loews Atlanta Hotel
Candler

K. Jackson, Organizer

1:00 Introductory Remarks.

1:10 453. The contributions of HBCUs to the STEM pipeline: Challenges and opportunities. W. Pearson

1:40 454. Role of HBCU's in the education and employment of African American women chemists. J. E. Brown

2:10 455. Sustaining the Legacy: The Role of Spelman College in Diversifying the STEM Pipeline. L. Winfield

2:40 456. Can a Solid Undergraduate Research Program in STEM Help a Hispanic Serving Institution Become Tier One? L. E. Echegoyen

3:10 Intermission.


3:55 458. Diversifying the STEM Enterprise. D. Barnes

4:25 459. STEM education praxis: Role performance of MSIs in K12 education. A. T. Tucker Blackmon

4:55 Panel Discussion.

Nanochemistry and Spectroscopy: Symposium Honoring Mostafa El-Sayed

Loews Atlanta Hotel
Salon I

P. Wine, Organizer
Z. Zhang, Organizer, Presiding
G. Schatz, Presiding

1:00 460. Reflections on Mostafa's Contributions to Physical and Materials Chemistry. J. D. Simon

1:20 461. For Mostafa – with energy and charge. M. Ratner

2:00 462. The structure and dynamics of patterned nanospheres. R. Hernandez

2:20 463. Tuning the optical properties of iron oxide-gold core-shell nanoparticles for cancer detection and treatment. E. Chaffin, S. Bhana, X. Huang, Y. Wang

2:40 464. Energy transfer in collisions of highly excited allyl radical in Argon. R. Conte, P. L. Houston, J. M. Bowman

3:00 Intermission.


3:40 466. Solar energy conversion using artificial atoms, molecules and solids. T. Lian
4:00 467. Reformulation of disulfiram with Au nanoparticles for targeted drug delivery in cancer therapy. J. Mi, J. Song, X. Peng, S. Nie, D. M. Shin


4:40 469. A Chemist's Approach to Nanofabrication: Towards a “Desktop Fab”. C. A. Mirkin

New Opportunities for Chemical Businesses

Loews Atlanta Hotel
Pittman

M. Beug-Deeb, Organizer, Presiding

1:00 470. Current Trends in Shale Oil and Gas Exploration Including Hydraulic Fracturing Operations. C. L. Alfaro

1:40 471. US Shale Gas – Implications for the Global Chemical Industry. H. Disteldorf

2:20 472. New Chemical Business Opportunities in Saudi Arabia and Gulf States. T. M. Deeb

3:00 Intermission.

3:10 473. The Business Case for Sustainability. F. M. Clark

3:50 474. Crowdfunding Your Way to Success. A. Cape

Supramolecular Chemistry: From Little Things, Big Things Grow

Loews Atlanta Hotel
Dunwoody

J. Lavigne, K. Shimizu, Organizers

1:00 475. Creating Complex Interfaces Using Orthogonal Click Reactions. J. Locklin


2:05 478. Self-assembled bis-urea macrocycle hosts as functional molecular containers. L. S. Shimizu


2:55 Intermission.

3:10 480. How breaking bonds can keep materials whole. S. L. Craig

4:05 482. Preparation, structures and host-guest chemistry of selected fluorinated frameworks. **M. Etzkorn**, J. C. Timmerman, M. D. Brooker, D. T. Nguyen, C. M. Kane, D. S. Jones, M. Gerken


4:45 484. Versatile model system for studying non-covalent interactions of aromatic surfaces. **K. D. Shimizu**

5:10 Concluding Remarks.

**Novel Bonding Types in Inorganic Chemistry**

**Halogen Bonding**

Loews Atlanta Hotel
Chastain

J. Thrasher, *Organizer, Presiding*

1:10 485. From crystal engineering to function engineering with halogen bonding. **P. Metrangolo**, G. Cavallo, G. Resnati, G. Terraneo

1:50 486. Halogen bonding of bromosubstituted electrophiles with halides, pseudohalides and halometallates: from charge-transfer complexes to electron-transfer reactions. **S. Rosokha**


3:10 Break.


**Southern Chemistry History Lessons for 21st Century America**

Loews Atlanta Hotel
Ardmore

D. Hicks, *Organizer, Presiding*

1:10 Introductory Remarks.

1:15 491. Accidental crusader for the world's largest(USA) chemistry based industry. **D. G. Hicks**

1:50 492. National Historic Chemical Landmarks in the South. **W. R. Oliver**


3:00 Intermission.
3:20 494. Chemistry-related industries of the southern USA: Then and Now. M. P. Walls

3:55 495. Georgia Research Alliance: An economic development model for the South and nation. C. L. Liotta

4:30 496. Captain Charlie's keys to 21st Century STEM career success. E. Reichmanis

5:05 Concluding Remarks.

Electronic Structure in Complex Environments

Condensed-Phase Environments

Loews Atlanta Hotel
Salon G

L. Slipchenko, Organizer
T. Crawford, Organizer, Presiding


2:00 498. Electronic optical activity: Intrinsic behavior and environmental perturbations. P. Lahiri, K. B. Wiberg, P. H. Vaccaro


3:00 500. Harmonic vibrational frequencies for hydrogen bonded clusters: Towards the CCSD(T) complete basis set limit for explicit solvation. G. S. Tschumper

3:20 Intermission.

3:40 501. Towards the Accurate Simulation of UV/Vis Spectra in Solution. M. Caricato

4:20 502. Chemical reactions at aqueous surfaces and in ionic liquids from QM/MM simulations. O. Acevedo

5:00 503. Evaluation of implicit solvation models for the prediction of solution-phase intramolecular CH/π interactions. T. M. Parker, N. Pokhrel, S. Janardan, A. E. DePrince, C. D. Sherrill

Synthesis, Structure, and Properties of f-element materials

f-element oxides, arsenides, etc

Loews Atlanta Hotel
Inman

S. Latturner, Organizer
T. Albrecht-Schmitt, Organizer, Presiding
A. Sefat, Presiding


2:25 506. Crystal growth, structure determination and physical properties of new uranium containing complex oxides and oxy-chlorides. **H. zur Loye**

3:05 Intermission.


4:50 510. Evidence of filamentary superconductivity in praseodymium-doped CaFe$_2$As$_2$ crystals. **A. Sefat**

**Approaches to Organic Synthesis Across Disciplines**

Loews Atlanta Hotel
Salon H

D. Whitehead, S. Wiskur, *Organizers*


3:00 Intermission.

3:15 513. Lewis acid-catalyzed ring-opening annulation approaches to fused benzene rings. **S. France**

4:00 514. Chemo-, regio-, and stereoselective reactions of Grignard and organozincate reagents for generating small molecular synthons. **R. Dieter**

4:45 515. Vanadium oxide catalysis for organic synthesis. **D. C. Whitehead**

**NanoElectrochemistry in Biomedical Research and Energy Technology**

**Biomedical/Bioanalytical**

Loews Atlanta Hotel
Centennial

J. Stickney, *Organizer*
L. Bottomley, G. Wang, *Organizers, Presiding*


2:00 517. Visualizing hydrogen oxidation reaction activity of polycrystalline platinum by scanning electrochemical
microscopy (SECM). **Y. Wang, D. O. Wipf**

2:20 **518.** Carbon nanotube yarn microelectrodes for enhanced detection of neurotransmitter dynamics in live brain tissue. A. C. Schmidt, X. Wang, Y. Zhu, **L. A. Sombers**

2:50 **519.** Silver nanoparticles-enhanced light absorption and photoelectrochemical performance of hematite (α-Fe₂O₃) thin-film electrodes for water splitting. **J. Wang, S. Pan**


3:30 Intermission.


4:15 **522.** Enhanced neurotransmitter detection with nanostructured-carbon microelectrodes. **C. B. Jacobs, A. Zestos, B. Venton**

4:45 **523.** Biomimetic nanomaterials for energy technologies. **M. R. Knecht**

5:15 **524.** Redox and optical activities in the dithiolate and monothiolate stabilized gold complexes and nanoclusters. **J. Jiang, C. V. Conroy, T. Ahuja, J. W. Padelford, T. Wang, G. Wang**

**Posters: Analytical Chemistry**

Loews Atlanta Hotel
Over Look/Exhibit Hall

D. Sherrill, *Organizer*

1:30 - 3:30

525. Withdrawn.

526. An automated dual stage solid phase extraction procedure for 15 F2t-isoprostane (8-iso Prostaglandin2a) from BSA and human serum as lipid markers of oxidative stress. J. Bosken, F. Kero, V. Vandell, T. Enzweiler, **M. Cherrier**

527. Sol-gel Thin Film of Zirconium Oxide for Detection of Organophosphate Compounds and Pesticides. **M. N. Bui, S. S. Seo**


530. Determination of arsenic, cadmium and chromium in commercial wine samples. K. Smith, **S. Melaku Abegaz**


532. Determination of the Conformation of Specific Residues in a Model Peptide by C₁₃ Isotope Edited ATR-FTIR in Regular Water. **S. Potana, C. Wang**

534. Development of a Raman spectroscopic database of artists' pigments. C. E. Phipps, S. W. Huffman


536. Creating an ongoing learning environment through experimentation and root cause investigation to understand sources of variation in measurements of Opiate analyte concentrations obtained via LCMS/MS analysis. J. Supica, J. Hull

537. Optimizing return on investment for LCMSMS consumable components in a high throughput toxicology laboratory using Six Sigma methodologies. J. Hull, J. Supica

538. Higher Order Derivative Voltammetry For Irreversible Processes at Spherical Electrode. T. Hong, I. Rusodimos, M. Kim


541. Determination of trace and heavy metals in some herbal teas and spices. J. Mierzwa


543. GC-MS method for the accurate quantitation of trans-fatty acids. N. Wei, H. C. Kuiper, H. W. Vesper


548. Identification of Flavonoid Content in Poplar and Sourwood Honey. M. Martin, S. Mastromarino, E. Grimley

549. Analysis of Kentucky bluegrass and rye grass pollen glycans using Mass Spectrometry. K. Stumpo

550. Development and implementation of dynamic IEF. R. Montgomery

551. Gold coated TiO₂ nanotubes as a visible light surface enhanced photocatalyst for water splitting applications. A. S. Panikar, Z. Shan, S. Pan, A. Gupta

552. Separation and characterization of high mannose glycan isomers from bovine Ribonuclease B. J. Qu, B. Dun, P. G. Wang

553. Effects of lanthanide metal cationization on electron transfer dissociation mass spectrometry of the acidic peptide Fibrinopeptide B. J. J. Commodore, C. J. Cassady

554. Towards pattern-based recognition with self-assembled receptors. A. Mallet, M. Bonizzoni
555. In-vitro calibration of microiontophoresis pipets. P. A. Flowers

556. Properties of the SPI/HPMC blending films. M. Chen, Q. Huang, J. Ye, J. Xiong


558. Removal of molecular adsorbates on silver nanoparticles using sodium borohydride in water. H. S. Perera

559. Adsorption, desorption, exchange, and reaction of adenine and 2-mercaptobenzimidazole (MBI) on aggregated gold nanoparticles (AuNPs). M. Gadogbe, W. E. Collier, D. Zhang

Posters: Polymer Chemistry

Loews Atlanta Hotel
Over Look/Exhibit Hall

D. Sherrill, Organizer

1:30 - 3:30

560. Modulating the temperature responsivity of thermoresponsive microgel thin films. K. C. Clarke, L. A. Lyon

561. π-Stacked models for conjugated polymers. E. M. Henry, D. M. Collard

562. Fluorescent liposome-based multiplexing biosensor system. M. Evans, C. Hansen, D. Ebzery, T. Hanks, C. Wright


565. Functional poly(lactic acid)s: Synthesis and potential applications for bone tissue engineering. P. P. Kalelkar, G. R. Alas, D. M. Collard

566. Patterned Surface Modification of Conducting Polymer Films. B. Toney, P. Molino, T. Hanks

567. Exploring the liquid crystallinity of poly(3-alkylthiophene)s. B. E. Cox, D. M. Collard

568. Molecular weight effects on PBT-6 charge carrier mobility. A. Ravi Sankar, E. Reichmanis, B. Fu

569. Polystyrene Coated Silver Nanoparticles with Applications in Optical Data Storage. L. Zhu, G. Zhang, E. Zlibut

570. Adsorption of heavy metals by modified agricultural waste materials. Z. M. Akhtar, I. N. Urhoghide

571. Binding of As, Ni, and Mn metal ions by grafted carboxyl methyl- containing cellulosic materials. G. Pacareu, I. N. Urhoghide

572. Separation of heavy metal ions from solution using modified cellulosic materials. I. N. Urhoghide, G. Pacareu, J. Vettaparambil

573. Protein and cell resistant brush polymer on medical grade stainless steel. G. R. Alas, D. M. Collard, A. J. Garcia

574. Interfacial Polymerization Synthesis of Polyamide-Polyetheramide (PAPEA) Thin-Film Composite Reverse Osmosis Membranes. A. F. Olatokunbo


577. Ternary nanocomposites based on poly(n-butyl methacrylate), cellulose acetate butyrate and an Algerian bentonite. S. Djadoun, K. Ouaad, N. Ziani, Y. Ouchelli

Small Business Innovation Research Seminar

Loews Atlanta Hotel
Ravinia

3:30 578. Understanding how to tap into federal funds through the small business innovation research (SBIR) and small business technology transfer (STTR) programs. C. G. Casteel

Posters: Inorganic Chemistry

Loews Atlanta Hotel
Over Look/Exhibit Hall

D. Sherrill, Organizer

4:30 - 6:30


583. Structural diversity in the reactions of mixed-donor ligands with bromine and iodine. J. Velasco, D. Rabinovich

584. The synthesis and reactivity of a hydride-bridged dicopper cation supported by an N-heterocyclic carbene ligand. C. M. Wyss, B. K. Tate, J. Bacsza, T. G. Gray, J. P. Sadighi


586. Synthesis and characterization of model square planar platinum group metal complexes with asymmetric α,ω-bis(phosphite)-polyether ligands for use in the Rh catalyzed hydroformylation of styrene. E. C. Cagle, G. M. Gray

587. Metal-oxo complexes with redox-active ligands: Toward oxyl reactivity. A. M. McDaniel, J. D. Soper

588. Redox-active N-heterocyclic carbene nickel complexes as cross-coupling catalysts. C. F. Harris, J. D. Soper

589. Bis(pyridyl)selone complexes of tin(IV) and lead(II). A. Fowler, D. Rabinovich

591. Use of Ligand Functionalized Resins for Metal Extractions. C. D. Tutson, A. E. Gorden

592. Unconventional high temperature synthesis of two water-soluble Keggin-based salt inclusion solids (SISs): Cs₂Cl₂Na(PMoVI₁₀MoV₂O₄₀) (1) and Cs₆IClNa(PMoVI₁₀MoV₂O₄₀) (2). D. Sulejmanovic, S. Hwu

593. Metallathiacrown ethers: Transition metal complexes of α,ω-bis(phosphite)-polythiaether ligands as sensors for environmental pollutants. J. R. Martin, G. M. Gray


595. Synthesis and x-ray structure determination of transition metal complexes using tris-1-ethyl-4-methylimidazolylphosphine. N. Peek, W. Lynch

596. Synthetic approaches to new emissive transition metal alkynyl complexes. D. Crapps, P. S. Wagenknecht


599. Mechanochemical synthesis of halogen-bonded cocrystals involving bis(diphenylphosphino)alkane disulfides/selenides and tetraiodoethylene. A. M. Siegfried, H. D. Arman, W. T. Pennington


601. Synthesis and characterization of of a two-dimensional antiferromagnetic oxyphosphate: Sr₁.₂₅Na₁.₅Fe₂O₂(PO₄)₅. L. D. Sanjeewa, C. M. Brown, J. He, D. Hitchcock, S. Hwu, A. Pfirman


603. POM-based catalytic gelating nanoarray for the decontamination of mustard agent analogs. K. Sullivan, D. Hillesheim, W. Neiwert, H. Zeng, C. L. Hill

604. Withdrawn.

605. Synthesis and characterization of two dirhenium compounds that contain bis(diphenylphosphino)acetonitrile. D. R. Derringer, C. M. Ammermann


Posters: Materials Chemistry

Loews Atlanta Hotel
Over Look/Exhibit Hall
D. Sherrill, Organizer

4:30 - 6:30

607. Porphyrin-Based Polysilsesquioxane Nanoparticles to Improve Photodynamic Therapy for Cancer Treatment. L. K. Fritts, D. Vega, J. Vivero-Escoto

608. MCM-NaTaO$_3$ composite catalysts for photocatalytic organic molecule conversion. K. Senevirathne, L. Zhang, R. T. Williams, A. Lachgar

609. Electrospun Si/TiO$_2$ composite nanofibers for advanced lithium ion batteries. K. R. McCormac, T. Tran, J. Wu

610. SYNTHESIS OF PbS/TiO$_2$ NANOCOMPOSITES USING THE SOL-GEL PROCESS FROM COVALENTLY INCORPORATED LEAD THIOLATES. K. Patel, J. T. Moore

611. Development of redox-responsive silica-based nanoparticles for photodynamic therapy applications. D. L. Vega, J. L. Vivero-Escoto

612. Development of sustainable nanotechnology for environmental remediation. S. I. Kuriyavar, T. Joell, A. Apblett

613. Processing and Applications of Sol-Gel Materials. K. Ehret

614. Peptide seeding reshapes the energy landscape of self assembly. C. Liang, N. Li, S. Johnson, A. Metha, D. G. Lynn

615. Assessing the ability of dye conjugated gold nanorods to recognize and bind to cell surface receptors. K. Mills, J. Wilson, M. Turnage, K. Walker, J. W. Stone


617. Rescinnamine as a promising drug therapeutic against advanced, chemotherapy-resistant prostate cancer. B. Crowe, A. Diamanduros, J. W. Stone, K. Scarpinato

618. Mesogenic flavones. A. J. Jordan, D. J. Timmons


FRIDAY MORNING

Biological Simulations using Molecular Dynamics, Monte Carlo, and Multiscale Approaches

Loews Atlanta Hotel
Salon G
O. Acevedo, Organizer, Presiding

8:00 623. Probing the Intricate Coupling between Enzyme dynamics and Catalysis. D. Hamelberg

8:30 624. Development of HIV inhibitors targeting cyclophilin A guided by free energy perturbation calculations. O. Acevedo

9:00 625. "Bicelle" lipid mixtures: Atomistic, coarse-grained, and thermodynamic modeling. J. T. Kindt

9:30 626. Molecular dynamics of biomolecules in the times of GPUs and Replica exchange: What dreams are made of... A. E. Roitberg

10:00 Intermission.

10:20 627. Determining free energy curves of proteins through adaptive steered molecular dynamics (ASMD). R. Hernandez

10:50 628. The orthogonal space sampling scheme to enable quantitative free energy simulations. L. Zheng, W. Yang


Chemistry Education General Session

Loews Atlanta Hotel
Ardmore

M. Koether, Organizer, Presiding

8:00 630. Implementation of a project-based guided inquiry approach to general chemistry labs. L. B. Wheeler, B. Barnhill, C. Lariviere, C. Grisham

8:15 631. Authentic Chemistry Experiments(ACE) in the general chemistry lab curriculum: Design, implementation and the role of teaching assistants in the freshman laboratory. V. Lykourinou, A. Villalta-Cerdas, T. Gatlin


8:45 633. Coupling DFT calculations with experimental measurements in the physical chemistry lab. T. C. DeVore, A. C. Bagley

9:00 634. Comparison of student performance on various laboratory assessments following the creation of a self-created technique video. M. A. Erdmann, J. L. March

9:15 635. Development and assessment of a hybrid introductory chemistry laboratory course. J. L. Poteat

9:30 636. Using electronic laboratory notebooks to improve student learning outcomes. M. C. Koether

9:45 637. Contextualizing chemistry with art. A. Gaquere-Parker

10:00 638. Using Marzano's taxonomy to assess and improve learning outcomes. T. D. Shepherd

10:15 639. Organic chemistry students' knowledge structures of fundamental general chemistry concepts: Lewis structures and bonding. S. R. Mooring, N. L. Burrows
10:30 Intermission.

11:00 640. Nomenclature – The “mail man” analogy: Organic chemistry. **S. Landge**

11:15 641. Role of iPads in chemistry curriculum at Anderson University. **D. A. Abramovitch**

11:30 642. Forensic science track at Georgia Regents University. **S. Myers**

11:45 643. Pedagogical view of metrology in analytical forensic science. **J. Messman**

**New Pedagogy and Approaches to Improve Student Learning Outcomes in Undergraduate Chemistry Education**

Loews Atlanta Hotel
Dunwoody

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

8:00 644. Computer animations in chemistry: How chemical education research can help chemistry instructors. **M. J. Sanger**

8:30 645. Engaging students in the inorganic chemistry classroom with well-defined learning objectives: Interactive learning through group activities, literature discussions, and even field trips. **J. P. Lee**

9:00 646. New computational physical chemistry experiments: Using POGIL techniques with ab initio and molecular dynamics calculations. **M. S. Reeves, R. M. Whitnell**

9:20 647. Integrated approach for development of scientific writing skills in undergraduate organic lab. **E. C. Duran, C. L. Weaver, J. A. Nikles**

9:40 648. Use of the enzyme-substrate interactions concept inventory to measure biochemistry students' misconceptions. **K. Linenberger, S. Lowery Bretz**

10:10 Intermission.

10:30 649. Can a PLTL teaching reform targeting General Chemistry improve student progression throughout a Chemistry curriculum? **S. E. Lewis**

11:00 650. Let's give them something to talk about: participation strategies that improve student engagement and learning. **K. D. Kloepper**


**Polymer Chemistry General Session**

Loews Atlanta Hotel
Ravinia

X. Zhang, *Organizer, Presiding*

8:00 652. Direct Visualization of Polyelectrolyte Mobility in Microgel Thin Films. **E. S. Herman, L. A. Lyon**

8:40 654. Synthesis and characterization of Phosphonated-bisphenolA dopants for solid state proton conduction in polyfunctional acid membranes. K. Reid

9:00 655. One-step synthesis and characterization of Poly(o-toluidine) nanofiber/metal nanoparticle composite networks as non-enzymatic biosensors. S. Poyraz, Y. Liu, N. Lu, Z. Liu, M. Kim, X. Zhang


10:00 658. Improved methodology for observing the molecular weight distributions of wood components in original and processed wood. T. Leskinen, S. Kelley, D. S. Argyropoulos


10:40 660. Synthesis and characterization of bisphenol A tetrachlorocyclotriphosphazene poly(arylene ether sulfone) hybrid copolymers for proton exchange membrane fuel cells. T. N. Thompson, N. Arnett

11:00 661. Poly(n-alkyl methacrylates)/Algerian bentonite nanocomposites prepared via in situ polymerization, initiated by a novel complex. S. Djadoun, K. Ouaad

11:20 662. Nanostructure, ion transport, and mechanical properties of LiTFSI and PVDF based solid polymer electrolyte. J. Chen

11:40 663. Optimizing of UV coatings and their curing behavior by means of Thermal Analysis. T. Doll

Nanochemistry and Spectroscopy: Symposium Honoring Mostafa El-Sayed

Loews Atlanta Hotel
Salon I

P. Wine, Z. Zhang, Organizers
C. Landes, S. Link, Presiding

8:20 664. Nanoscale manipulation of light: New physical insights and technological opportunities. N. Halas

9:00 665. Elucidating chemical transformations one nanocrystal at a time. P. K. Jain

9:20 666. Role of Ligand Coordination Geometry in Controlling Binding of Thiolated Target Molecules to Quantum Dot Surfaces. C. D. Heyes

9:40 667. A monolayer graphene;Au surface enhance Raman spectroscopy platform for DNA damage studies. T. M. Orlando, A. Sidorov

10:00 Intermission.

10:20 668. Mostafa and the golden age. C. J. Murphy

11:00 669. Nanoparticle surface charge directs the cellular binding of nanoparticle-protein complexes. C. C. Fleischer, C. K. Payne

11:40 671. A Water-Soluble High-Contrast Cu(I)-Selective Fluorescent Probe with Parts-Per-Trillion Sensitivity. M. T. Morgan, A. M. McCallum, C. J. Fahrni

NanoElectrochemistry in Biomedical Research and Energy Technology

General Topics

Loews Atlanta Hotel
Centennial

L. Bottomley, J. Stickney, G. Wang, Organizers, Presiding


9:00 673. Enhanced charge storage capacity of conducting polymer electrodes by the entrapment of p-benzoquinone. M. R. Arcila-Velez, M. E. Roberts


9:50 675. Single molecule spectroelectrochemistry of MEH-PPV on nanostructured TiO₂ surfaces. C. M. Hill, S. Pan

10:10 Intermission.

10:25 676. The Use of Gold Nanoparticles in Dye-Sensitized Solar Cells and Biosensing. F. P. Zamborini, T. Luitel, S. Beeram, L. Bao, A. Fang


Posters: Undergraduate Research

Analytical/Inorganic/Environmental Chemistry

Loews Atlanta Hotel
Over Look/Exhibit Hall

V. Singh, Organizer

8:30 - 10:00

680. Modification of Polysaccharides with Attachment of Iron Chelating Ligands. A. Parker, C. J. Fowler


683. Enhancing biomolecular class separation in complex sample analysis using ion mobility-mass spectrometry (IM-MS). **R. M. Reyes**, N. M. Lareau, J. C. May, J. A. McLean


686. Isolation and derivatization of pentobarbital. **A. Farooq**, S. F. Hornbuckle

687. The Addition of Thiols to Electron-Deficient Cyclopropanes Catalyzed by a Ca (II) Complex. **C. Braun**, K. Nolin

688. Thiol Additions to Epoxides Catalyzed by a Rhenium(V)-Oxo Complex. **A. Badiceanu**, K. Nolin

689. Heteroleptic palladium(II) and platinum(II) complexes containing a crown thioether and monodentate phosphines. **T. P. Latendresse**, J. P. Lee, C. L. Keller, G. J. Grant


691. Hydrogen uptake on palladium catalysts. **C. E. Milliron**

692. Analysis of Cold and Flu Medications Found in DayQuil™ and NyQuil™ Using HPLC and Cyclic Voltammetry. **J. Stewart**, C. E. Dahm, K. R. Wilson

693. Copper and zinc acetylacetonate: How one electron changes everything. **A. Brown**, L. Pinelo, B. S. Ault

694. Detection of Naturally Produced Organohalogen Compounds in Marine Sponges from the Bahamas and Florida Coast. **S. D. Shaw**, N. Rosenfelder, J. R. Pawlik, J. Kucklick

695. Seeded Growth of Pd Nanocrystals: The Influence of Surface Capping Agent. **Z. Li**, H. Peng, Y. Xia

696. Studying imidazole coordination to Mn(III) porphyrins by UV-Vis absorption spectroscopy. **L. L. Cyr**, L. Arnold, G. B. Ray


698. Quantification of ethanol in rainwater using solid-phase microextraction (SPME). **C. Andreacchi**, K. M. Mullaugh


700. Studies of DNA binding interactions with \([\text{Rh}(9S3)\text{Cl}_3,] [\text{Rh}(9S2O)\text{Cl}_3]\), and \([\text{Ir}(9S3)\text{Cl}_3]\) using fluorescence spectroscopy. **H. J. Greve**, J. Kim

701. Study of the binding between \( \text{Fe}^{2+}/\text{Fe}^{3+} \) and the fluoroquinolones. **M. A. Addo**, U. Kalapathy, H. Fan-Hagenstein

702. Characterization of chemical and biological properties of extracts from American Pokeweed. **B. L. Parker, G. S. Barrett**, D. Ivankovic, D. A. Abramovitch

703. Optimization of glycan labeling for plant pollen protein analysis by UPLC. **P. Wesner**, K. Stumpo


706. Quantification of the uremic toxin p-cresol in serum of ESRD and normal patients. J. M. Murphy, M. F. Santiago, S. R. Whitson

707. Rhodium and iridium complexes of NHC as catalysts in hydrosylation reactions. Z. McCarty, D. Woodruff, D. Lee, D. Tapu


709. Analysis of Thiocyanates in Wasabia Japonica. C. R. Dockery, J. Lu, M. Giedd, B. Patterson

710. Automated spectrophotometric titrations and the determination of chemical equilibria. J. C. Hammond, J. A. Lynch


712. Mutational Analysis of Bovine Leukemia Virus Nucleocapsid Protein. V. Sokolove


715. Mosquito repellent to heavy metals: Chemical impacts on local neighborhoods. L. M. Bianco, M. B. Bowen, I. D. Patel, C. R. Wilson, J. L. Look

716. Application of coffee as an electron donor to reduce hexavalent chromium: column test. S. A. Fatima, C. Kim, S. Park


718. Photoactivated hydrazone metal chelation: The HAPI approach. R. McAtee

719. Spectroscopic analysis of metal desorption from industrial Georgia clay. C. L. Quattlebaum, E. L. Oliver, K. A. Knapper, B. Cicerchi, D. Ma, R. Carter, K. D. Kloepper


722. Method development for metabolomic analysis of Saccharomyces cerevisiae by LC-MS. S. M. Elcik, W. C. Cory, J. L. Fox

723. Determination of Enzyme Kinetics Using Electrophoretically Mediated Microanalysis. K. J. Woodard, L. G. Puckett

724. Investigation of casein kinase II via mass spectrometry. E. DeVlieger, J. Hunter, L. Bedard, A. Mosley

725. Solid phase extraction method for the simultaneous determination of an aminoglycoside and a glycopeptide from a
biodegradable medical implant. P. O'Brien, C. Quinn, S. Symes


728. Quantitative analysis of minerals in vitamins and fortified cereal centered on child nutrition from before birth to preteen years. T. Brown, B. Cook, R. Thompson, S. A. Wasileski


731. Development of an activity-based probe for cystathionine gamma lyase. S. Bowhay, C. M. Johnson

732. Analysis of intact proteins from gels using mass spectrometry. A. Balius, B. Rollins, R. Montgomery

733. Novel Biosensor for point-of-care medical diagnostics. A. Wilkes

734. Can variations in chromatographic peak asymmetry factors and peak retention times give insight into the dependence of DOM–surface interactions on DOM surface coverage in liquid chromatographic studies of DOM adsorption? S. Z. Sutton, G. Whitetree, Y. Wu, D. Kreller

735. Comparison of two analytical methods for the measurement of nitrate concentrations in standard solutions and environmental samples. G. Prusky, M. S. Morton, D. Carbonell

736. Synthesis and characterization of cis-disubstituted tetracarbonylmolybdenum(0) complexes with binaphthol-based chlorophosphite ligands. R. D. Davidson, S. D. Hastings, G. M. Gray

737. Cyclic voltammetry of carotenoids. W. M. Potter, A. Focsan

738. Synthesis of a Cationic Metal-Organic Solid Solutions Based on CO(II) and Zn(II) and their applications in Chromate trapping. G. Hernandez, H. =. Fei, S. Oliver

739. Neonicotinoids: Chemistry behind the controversy. W. F. Davis, J. M. Carr


742. Simultaneous detection of glucose and lactic acid in flowing environments. A. T. Harding, A. H. Suroviec

743. Fluorescence and electrophoresis studies on lysozyme modifications induced by pbenzoquinone. J. W. McDonald, H. Greeve, J. Kim, T. V. Albu

744. Quantitative analysis of pesticide tank rinses for residues. K. D. Swanson, P. P. Osborne, L. Xu, T. Walker


746. Broad survey reveals tolerance of Fe-S clusters to substitution in [NiFe] hydrogenase. B. R. Clarkson, I. T. Yonemoto, P. D. Weyman
747. Characterization of a customized thin layer flow cell interfaced to an ion trap mass spectrometer for electrospray ionization mass spectral studies of self-assembled monolayers. **S. K. Hartman, A. B. Murphy, B. W. Gregory**

748. One-pot enol silane formation-Mukaiyama aldol and Mukaiyama-Mannich reactions of ketones and thioesters. **C. M. Dombrowski, J. A. Ingersoll, C. Downey**

749. TMSOTf-accelerated opening of epoxides with halogens and α-hydroxylation of ketones. **A. T. Barnett, N. C. Yeutter, C. Downey**

**Advancing Graduate Education in the Chemical Sciences**

Loews Atlanta Hotel
Candler

P. Houston, *Organizer*

9:00 750. Advancing graduate education in the chemical sciences. **B. Z. Shakhashiri**

9:15 751. ACS Commission on Advancing Graduate Education in the Chemical Sciences: Overview and responses to big questions. **L. R. Faulkner**

9:40 752. Overview of the symposium and recommendations of the ACS Commission on Graduate Education. **P. L. Houston**

10:05 753. Reformation of Graduate Education in Chemistry: A 40 Years Journey The Best Predictor of Future Behavior is Past Behavior. **G. B. Schuster**

10:30 Intermission.

10:45 754. Comments on the Commission's Report from the Perspective of the National Science Foundation. **J. Ferrini-Mundy**

11:15 Panel Discussion.

**Approaches to Organic Synthesis Across Disciplines**

Loews Atlanta Hotel
Salon H

D. Whitehead, S. Wiskur, *Organizers*

9:00 755. Brønsted acid catalyzed enantioselective lactonization strategies. **K. S. Petersen**

9:45 756. From molasses to biogasoline: A synthetic approach. **S. Emelife, M. Raja, C. Gwengo, B. White, L. Ambrosia**

10:05 Intermission.


10:40 758. Silylation-based kinetic resolutions: Substrate scope and mechanistic investigations. **S. L. Wiskur**

**Synthesis, Structure, and Properties of f-element materials**
f-element coordination polymers

Loews Atlanta Hotel
Inman

S. Latturner, T. Albrecht-Schmitt, Organizers
C. Cahill, D. de Lill, Presiding

9:00 759. Supramolecular assembly of f-element hybrid materials. C. L. Cahill, R. G. Surbella

9:40 760. Observing the NC bridge of the actinide tetracyanometallate compounds. B. A. Maynard, R. E. Sykora, A. E. Gorden

10:05 Intermission.

10:15 761. Non-aqueous and high-temperature solvent synthesis and crystal growth of rare-earth metal organics and rare-earth double phosphates. L. A. Boatner


11:20 763. Examining the antenna effect within lanthanide coordination polymers. D. T. de Lill

Undergraduate Research Symposium

Undergraduate Keynote Speaker and Research Symposium 1

Loews Atlanta Hotel
Piedmont

N. Kirk, Organizer

9:00 764. Undergraduate Reseach Symposium Keynote Talk. Extracting Value From Patents: Lessons Learned From a Six Year Litigation. D. C. Liotta

9:45 Intermission.

10:00 765. Separation and detection of 19 neurochemically significant biogenic amines and acids in non-mammalian systems. E. C. Marder, S. Steagall, C. Dorismond, C. D. Hallman, N. J. Kuklinski


10:45 768. Utilization of metathesis to achieve water solubility of nanoparticles. L. G. Mast, J. E. Macdonald, M. J. Turo

11:00 769. Synthesis of Large Polyacenes. K. D. Gebhard, S. Miao

11:30 771. Pyrene-based organic semiconductors. J. Ji, S. Miao

11:45 772. Solution aggregation and polymorphism of platinum(II) bipyridine complexes. M. H. Hudson, R. E. Bachman*

Undergraduate Research Symposium

Undergraduate Research Symposium 2

Loews Atlanta Hotel
Chastain

N. Kirk, Organizer

10:00 773. Copper(I)-catalyzed azide-alkyne cycloadditions for functionation of enzyme packaged viral nanoparticles. R. Hincapie, C. McKay, M. Finn

10:15 774. Determining the mechanism of periodic precipitation (Liesegang) reactions. A. W. Bruch, A. Sowell, J. M. Karty

10:30 775. Synthesis of hydroxy substituted indole chalcones. C. M. Bridges, H. L. Holt, Jr.


11:00 777. Rational design of platinum complexes with enhanced nonlinear optical properties. D. C. Yost, K. Martin, S. Kilina, W. Sun

11:15 778. Estrogenic hormones: Their interactions with Lactoperoxidase and potential for DNA mutations. N. M. Clark, K. M. Matera

11:30 779. Polymer functionalization of single-wall carbon nanotubes for nano-resin water purification. W. M. Payne, J. E. Amburgey, J. C. Poler


Posters: Undergraduate Research

Organic/Medicinal Chemistry

Loews Atlanta Hotel
Over Look/Exhibit Hall

V. Singh, Organizer

10:30 - 12:00


783. Inhibition of Copper Thiostrepton's Oxidation of DTBC to DTBQ. S. Herrera, J. Moses, L. Li-June Ming

784. Synthesis of glycosaminoglycans and mimics to explore binding affinity to malarial proteins. C. J. White, B. G. Trogden, G. Geist, K. Ferrill, J. Hoggges

785. Analysis of secondary metabolites in *Carpinus caroliniana* and *Ostrya virginiana*. J. A. Boudell, S. F. Hornbuckle, J. M. Mikula

786. Catalytic homologous conjugate additions of heteroaromatic nucleophiles to electron-deficient cyclopropanes. C. Dulin, K. Murphy, K. Nolin

787. One-pot deoxygenation of crude Grignard adducts and similar compounds. A. P. Honeycutt, B. W. Love, J. M. Gibson, H. V. Clontz


790. Synthesis of 2-amino-7-benzyl-6-hydroxy-7H-purin-8(9H)-one derivatives as potential inhibitors of folate requiring enzymes. A. Jackson, E. Brazil, R. Vaden, P. S. Ray

791. Connecting halomethane analogues and Lewis bases: Sigma hole interaction trends. M. Tawfik, K. J. Donald


793. (BPA)RuBr(PPh₃)₂ as a multipurpose reagent: Alcohol dehydration/oxidation and alkene isomerization. M. Sharma, D. Chace, B. Quillian

794. New ruthenium(II) complexes supported by bis(pyrazolyl)acetate as intermediates to olefin hydroarylation catalysts: Synthesis, characterization and structure. M. Trivitayakhun, B. Quillian

795. Effect of Acetaminophen to Cyclodextrin Ratios in the Presence of Polymeric Excipients on Crystal Morphology. B. Collins, R. Wilcox


802. Polydiacetylene Liposomes Encapsulation of Trifluoroethanol and Fluoride Salts. I. Miller, J. Rapley, C. Wright, T. Hanks


806. Microwave Deprotection of Boc-Protected Amino Acids Under Mildly Acidic Conditions. **S. Sedberry**, M. I. Moore, K. R. Wilson

807. Structure activity relationship study of phenolic antioxidants. **S. Obeng**, A. Roberts, B. Scruggs, V. J. Geisler


809. Ring-closing metathesis reactions of novel dienes. **P. Carey**, K. Knight


812. Overexpression and characterization of manganese catalase from *L. plantarum*. **R. Murphy**, P. Riggs-Gelasco

813. Synthesis towards IL-supported hypervalent iodine compounds. **W. B. Unthank**, T. R. Hayden

814. Studies toward a convergent total synthesis of Motualevic Acids A-E. **F. A. Diaz**, **K. Black**


817. Catalyst development for a Sonogashira catalyst transfer polycondensation. **K. Singer**, P. Lundin

818. Benzotriazole-Mediated synthesis of symmetrical and unsymmetrical bis-2,5-diketopiperazines. **A. Nasajpour**


822. Cysteine modification via nucleophilic aromatic substitution. **J. Kapp**, M. Forconi


824. Role of conserved amino acid residues in heme *α* synthase. **F. D. Esquivel**, **L. R. Penland**, O. Khalimonchuk, J. L. Fox
825. Production of Biodiesel via Hydrocracking. M. Hilliard, K. Dickens, K. McGill

826. Microwave-assisted synthesis of 4 and 4'-substituted 3,5-diphenylisoxazoles. Y. Zhang, S. Son, N. L. Powell

827. The exploratory synthesis of glutamate lipid-derived naphthalene and perylene organogelators. R. R. Denham, R. E. Bachman

828. Mutagenic analysis of the oligomerization of E. coli β-glucuronidase. G. Burchett, K. T. Lane


831. Developing strategies for the preparation of rationally designed analogs of the furanosteroid family of natural products. D. Vogt, B. Goess


833. Synthesis of bromo-substituted dipyridosiloles. P. Hang, P. Wei, D. M. Peloquin, T. A. Schmedake


836. Investigation of Novel Amine Dehydrogenases for the Asymmetric Synthesis of Amines. J. Groover, B. Bomarius, A. Bommaris, B. D. Feske

837. The monofluorination of Diethyl Cyanomethylphosphonate. D. Singleton, T. Hizer, B. D. Feske

838. Synthesis of the pharmaceutical Bepreve using biocatalysis as the key asymmetric step. A. Casas, B. Weaver, J. Groover, B. D. Feske


842. Metalloradical catalyzed N=N bond formation with fluoroaryl azides: A new approach to the synthesis of fluoroazobenzene compounds. T. N. Arzua, L. Jin, P. Zhang


846. Exploring the Chlorination of Diethyl cyanophosphonate. A. Dykes, T. Hizer, B. D. Feske

847. Ditopic N-heterocyclic carbene ligands: 9,10-anthracene linked imidazolylidenes. A. A. Kellum, A. Mangalum, A. G. Tennyson

848. Trans-chelating N-heterocyclic carbene ligands: Dialkyl-amine linked benzimidazolylidenes. A. C. Rollings, A. Mangalum, Y. Htet, A. G. Tennyson

849. Development of Brønsted acid catalyzed intramolecular imino-ene reaction. M. Putri, L. Davis


851. Zinc acetylides in the presence of TMSOTf: Addition to nitrones and alkylation with methyl ethers. E. N. Maxwell, D. C. Obenschain, C. Downey

FRIDAY AFTERNOON

Approaches to Organic Synthesis Across Disciplines

Loews Atlanta Hotel
Salon H

D. Whitehead, S. Wiskur, Organizers

1:00 852. Recent progress in alkaloids synthesis. V. H. Rawal

1:45 853. New ligand space through novel hydrophosphinations. C. Busacca

2:30 Intermission.

2:45 854. New synthetic methods as an entrée to biological discovery. S. E. Schaus

3:30 855. Synthesis of chiral allylboron and enolborane reagents via allene and acrylamide hydroboration reactions, and applications to the synthesis of natural products. W. R. Roush

4:15 Concluding Remarks.

CHED Chemistry Education General Session

Loews Atlanta Hotel
Ardmore

M. Koether, Organizer, Presiding
M. Dean, Presiding

1:00 856. Impact of the Chemistry Scholars Program at UNC Asheville on recruitment and retention of majors and department culture. S. A. Wasileski, J. M. Schmeltzer, H. Holt


1:30 858. Alternative method to enhance student performance and retention in STEM majors at Georgia Perimeter College. J. Lee-Joyer, A. Steinau, I. Rickets
1:45 859. Use of problem solving to elicit self-explaining in General Chemistry. A. Villalta-Cerdas, S. Sandi-Urena

2:00 860. Online homework with targeted instructional feedback leads to improved student learning outcomes. J. E. Bara

2:15 861. In-class demonstrations by students enhance learning in general chemistry course. P. M. Todebush

2:30 862. Approach to flipping the classroom to enhance student participation in large chemistry courses. M. Lewis


3:00 Intermission.


3:45 865. Understanding the obstacles to incorporation of graphing and graphing-related mathematics into the general chemistry curriculum. D. W. Carpenetti II, A. Woolfer, Z. B. Snead, H. N. Tran, M. Weber

4:00 866. Engaging general chemistry students with POGIL and climate change. G. H. Webster, D. King, J. E. Lewis, K. Anderson, D. Latch, S. Sutheimer, C. Middlecamp, R. Moog

4:15 867. Tales from the other side of the podium: How to use a flipped classroom model to increase student learning and engagement in organic chemistry. K. Daus


4:45 869. Chemistry in Berlin, Germany - a study abroad program experience for majors. R. Fietkau

Computational Chemistry General Session

Loews Atlanta Hotel
Salon G

A. DePrince, Organizer, Presiding

1:00 870. Calculation of standard enthalpies of formation. 1 Hydrocarbons. R. Bacaloglu, L. Cotarca


1:40 872. New structural framework for integrating replication protein A into DNA processing machinery. C. Yan, C. A. Brosey, I. Ivanov, W. J. Chazin

2:00 873. Anisotropy in the Debye-Waller factor of hcp solid $^4$He. A. L. Barnes, R. Hinde

2:15 874. Computational insights for the AlkD base extrusion strategy. B. Kossmann, I. Ivanov

2:30 Intermission.

2:40 875. Spin-orbit transitions of halogen atom dopants in solid parahydrogen matrices. R. Hinde

3:00 876. Characterization of a stripe liquid crystal phase in simple binary water solutions. T. D. Shepherd, M. Parry, R. Okumu, V. Molinero
3:20 877. Roaming trajectories in a reduced-dimensional model of ketene. I. S. Ulusoy, J. F. Stanton, R. Hernandez

3:40 878. Opening pathways of the DNA clamps proliferating cell nuclear antigen and Rad9-Rad1-Hus1. X. Xu

3:55 879. Density functional calculations of an inhomogenous $^{4}$He system. M. Dutra, R. Hinde

4:10 Intermission.


5:10 883. Density-fitted singles and doubles coupled cluster theory on graphics processing units. E. DePrince, D. Sherrill

Environmental Chemistry General Session

Loews Atlanta Hotel
Candler

A. Suroviec, Organizer, Presiding

1:00 884. Neighborhood chemistry: Combining undergraduate research, analytical chemistry and service learning to understand local environmental issues. J. L. Look


1:30 886. Photochemical Degradation and Environmental Fate of Pharmaceutically Active Compounds in Simulated Natural Water Samples. W. Cory

1:45 887. Conversion of iodide to hypoiodous acid and molecular iodine at the air-water interface. M. I. Guzman, E. A. Pillar

2:00 888. Photolysis of 2-oxopropanoic acid: A study of intermediates and products. A. J. Eugene, S. Xia, M. I. Guzman


2:45 891. Soil Quality Analysis Using Qualitative and Quantitative Analytical Methods. S. C. Miller

3:00 Intermission.


3:30 893. Predicting organic carbon chromatograms and monitoring adsorptive fractionation using dual-wavelength UV

**3:45 894.** Does the method of predicting [DOC] from UV absorbance at two wavelengths work in liquid chromatography? **G. Whitetree**, S. Sutton, Y. Wu, D. Kreller

**4:00 895.** Measuring a UV-VIS absorption spectrum of aerosols and greenhouse gases using a photoacoustic spectrometer. **J. R. Wiegand**

**4:15 896.** Incoherent broadband cavity enhanced spectroscopy for measuring extinction coefficients of atmospheric species throughout the UV-visible spectrum. **D. A. Fischer**, G. D. Smith

**4:30 897.** Retrieval of Complex Refractive for an Absorbing Aerosol Binary Mixture Using Cavity Ringdown Spectroscopy at 355nm. **K. Schuldt**

**4:45 898.** Origin of optical absorptivity in brown carbon aerosols. **S. Phillips**

**Materials Chemistry General Session**

**Chemistry of Materials**

Loews Atlanta Hotel
Pittman

B. Baruah, *Organizer*
I. U. Arachchige, *Presiding*

**1:00 899.** Controlling the Interfacial Junction Properties of Hybrid Organic/Inorganic PEDOT:PSS / n-, p-, and n⁺-Si Devices for Solar Energy Conversion Applications. **M. G. Walter**

**1:15 900.** Photoinduced Inter-Cavity Electron Transfer between Ru(II)tris(2,2'-bipyridine) and Co(II)tris(2,2'-bipyridine) Co-Encapsulated within a Zn(II)-Trimesic Acid Metal Organic Framework. **R. W. Larsen**, L. Wojtas

**1:30 901.** Crystal-bound vs. surface-bound thiols on semiconductor nanoparticle surfaces: achieving water solubility and charge transfer properties. **M. J. Turo**, J. E. Macdonald

**1:45 902.** Small molecule organic dye synthesis and design based on ullazine for Dye Sensitized Solar Cells. **J. Delcamp**, A. Yella, M. Nazeeruddin, M. Grätzel

**2:00 903.** Introducing New Fully-Integrated TGA-GC-MS and TGA-FTIR Systems for Characterization of Materials Including Polymers, Biomass and More. **T. Doll**

**2:15 904.** Increased efficiency of gold conversion via a re-seeding approach. **J. W. Stone**, S. Canonico-May, K. Beavers, C. Duvall

**2:30 905.** Bio-based materials to synthesize a novel surfactant in the production of polyurethane foams. **B. S. Snyder**, N. Tonks

**2:45 Intermission.**

**2:55 906.** New Materials Based on Cellulose and Natural Biopolymers. **R. Kotek**, R. Boy


**3:25 908.** Self-healing microgel coatings. **M. W. Spears Jr.**, L. Lyon


4:40 913. Microwave approach to ultrafast synthesis of nanomaterials. X. Zhang


5:10 915. Anisotropic growth of metallic nanocrystals by high frequency mechanical stirring. M. Mahmoud, M. El-Sayed, U. Landman

Nanochemistry and Spectroscopy: Symposium Honoring Mostafa El-Sayed

Loews Atlanta Hotel
Salon I

Z. Zhang, Organizer
P. Wine, Organizer, Presiding
R. Dickson, Presiding

1:00 916. Multifunctional mesoporous inorganic nanoparticles controlled by nanomachines for in vitro and in vivo drug delivery. J. I. Zink


2:00 918. Hollow metallic nanoparticles in nanocatalysis: High catalytic efficiency and studying the mechanism of the solution catalysis. M. Mahmoud, M. El-Sayed


2:40 920. Ionic Rectifier Based on Carbon Nanotube Membranes. B. Patel, M. Patel, M. Bassett, S. Landge, J. Wu

3:00 Intermission.

3:20 921. New developments in the synthesis of colloidal noble-metal nanocrystals. Y. Xia

4:00 922. Silver Atom Doping to Ultra-Small and Plasmonic Gold Nanomolecules. C. Kumara, D. Cullen, A. Dass

4:20 923. Transformation of Ag nanocubes into Ag-Au hollow nanostructures with enriched Ag contents to improve SERS activity and chemical stability. D. Qin, Y. Yang

4:40 924. Nanoparticles Immobilized on Cellulose Fibers: SERS Substrate and Catalytic Reaction. B. Baruah

Perspectives in Undergraduate Forensic Chemistry Education
Loews Atlanta Hotel
Dunwoody

H. Msimanga, C. Dockery, Organizers, Presiding

1:00 925. Perspectives in Undergraduate Forensic Chemistry Education. Z. Oommen

1:30 926. Multivariate analysis techniques in teaching forensic analytical chemistry at the undergraduate level. H. Z. Msimanga, C. R. Dockery

2:00 927. Introductory and advanced forensic chemistry. W. E. Brewer

2:30 928. From classroom to laboratory: Creating an effective transition for scientists. D. Wallace-Duckworth

3:00 Intermission.

3:15 929. Forensic toxicology education. O. A. Vanderpuye

3:45 930. Development of specialty courses on forensic toxicology and forensic microscopy. L. G. Puckett

4:15 931. The CSI effect on college curricula: Educational considerations for scientists entering the field of forensics. R. J. Ollis

4:45 Panel Discussion.

NanoElectrochemistry in Biomedical Research and Energy Technology

Energy/Materials

Loews Atlanta Hotel
Centennial

L. Bottomley, Organizer
J. Stickney, G. Wang, Organizers, Presiding

1:30 932. Toward a new generation of solid oxide fuel cells: Recent progress, challenges, and perspectives. M. Liu

2:10 933. Polypyrrole/Poly(4-Styrenesulfonic Acid) Supercapitor Electrodes for Energy Storage Applications. K. P. Diaz-Orellana, M. E. Roberts

2:30 934. Transient Ion Transport Against Concentration Gradient through Conical Nanopipettes. G. Wang, Y. Li, D. Wang, M. Kvetny, W. Brown

3:00 Intermission.


3:45 936. Dimension dependent near-surface phase transitions in Pt and their effect in electrocatalytic properties. F. M. Alamgir, A. Vitale


Synthesis, Structure, and Properties of f-element materials
f-element materials: theory and applications

Loews Atlanta Hotel
Inman

S. Latturner, Organizer
T. Albrecht-Schmitt, Organizer, Presiding

1:30 938. New directions in the molecular chemistry of high valent uranium and cerium. E. J. Schelter

2:10 939. Synthesis and characterization of holmium and dysprosium containing garnet nanoparticles for radiotherapy. K. Balkus, I. Munaweera, A. DePasqua, Y. Shi

2:40 Intermission.

2:55 940. Probing actinide bonding using multiphoton excitation and photoelectron spectroscopy. M. C. Heaven

3:35 941. Lanthanide-based nanomaterials with improved luminescence properties for potential biomedical applications. C. R. De Silva, G. Attanayake, A. N. Darsanasiri, M. Clark

Undergraduate Research Symposium

Undergraduate Research Symposium 3

Loews Atlanta Hotel
Piedmont

N. Kirk, Organizer


2:15 945. Comparative Study of Gold Nanoparticle Structure Modifications Induced by Aggregation Reagents. E. Stafford, S. M. Ansar, D. Zhang

2:30 946. Modeling lactate dehydrogenase enzyme kinetics with temperature jump spectroscopy. K. Panwar

2:45 947. Effect of the hydrophobic environment on the retro-aldol reaction: Comparison to a computationally-designed enzyme. J. Schmidt, C. Ehasz, M. Epperson, M. Forconi

3:00 Intermission.

3:30 948. Aromatic organothiol interactions with silver nanoparticles in water. G. E. Salomon, S. Ansar, D. Zhang

3:45 949. Towards quantum information in a cryogenic ion trap. K. A. Burkhardt

4:00 950. Energetic contribution of poly(C) binding protein-2 (PCBP-2) in the formation of the i-Motif. C. R. Funk, Y. Bhavsar-Jog, R. M. Wadkins

4:15 951. Computational analysis of water...2-aminopyrimidine hydrogen bonding interactions with protein kinase
GSK-3β. L. E. Jobe, K. M. Elokely, R. J. Doerksen

4:30 952. Synthesis, purification and analysis of novel "zone 4" sphingosine kinase-1 inhibitors. L. Mount, T. Grattan

4:45 953. A menthol-derived synthon for preparing homoallylic alcohols bearing three contiguous elements of stereochemistry. N. A. Ochs, K. Carroll, F. E. McDonald

5:00 954. Synthesis and morphology of NiO and CoO nanoplate - carbon nanotube materials for energy storage. D. Brokaw, J. C. Poler

Undergraduate Research Symposium

Undergraduate Research Symposium 4

Loews Atlanta Hotel
Chastain

N. Kirk, Organizer


1:45 956. Characterization of copper (I) binding thermodynamics to small molecules. D. Johnson, N. Grossoehme

2:00 957. Effects of zinc and clioquinol on oligomerization of Alzheimer's amyloid-β peptide. K. McLaurin, E. Amenson, A. Bradner, M. Humphrey, R. K. Lammi

2:15 958. Molecular Docking Studies of Novel Flavonoid Derivatives as Acetylcholinesterase Inhibitors. O. M. Newman

2:30 959. Effects of aflatoxin B1 on Jurkat T-cell function. L. E. Sutherland, T. Laakko Train

2:45 960. Utilizing heat capacity to understand the competition between netropsin and A/T hook for DNA. C. Quandt, A. Gorensek, K. L. Buchmueller

3:00 Intermission.


3:45 962. Insight Into the Hydrophobic Effect by 1H NMR Analysis of the Hofmeister Series. R. S. Carnegie, C. L. Gibb, B. C. Gibb

4:00 963. Synthesis and biological activity of hibiscone C. D. P. Rhinehart, B. C. Goess, J. S. Rawlings

4:15 964. Spin crossover in Fe(II) complexes with dicyanometalate bridging ligands. A. Arroyave, O. Hietsoi, H. Stout, C. Achim, M. Shatruk

4:30 965. Progress towards “brilliant” materials: Iron core, gold shell nanoparticles with engineered optical, magnetic, and biological functionality. B. Rittgers, T. Jewett, D. A. Stuart

4:45 966. ROMP Monomers and Polymers Containing a Primary Amino Functionality. M. E. Mullens, H. J. Schanz

5:00 967. ROMP Polymers Containing Organic Radicals for Treatment of Traumatic Brain Injuries. C. H. Feriante, H. J. Schanz
Posters: Undergraduate Research

Material/Polymer/Biochemistry

Loews Atlanta Hotel
Over Look/Exhibit Hall

V. Singh, Organizer

2:00 - 3:30

968. Synthesis of Alginate/Conducting Polymer Composites for Fabrication of Tissue Scaffolds. T. Pannell, C. Yore, C. Wright, B. Zhang, T. Hanks

969. Polymer Impregnation of Graphite Rods for Reducing Interfacial Capacitance. A. B. Reed, S. E. Creager

970. Toward new inorganic/organic conjugate dyes for solar harvesting. S. A. Parks, R. E. Bachman*


975. Studies on Polymer Coated Magnetite for Drug Targeting. B. N. Louthen, R. D. Wilcox


977. Phosphonated cationic polymers with flame-resistant properties. K. B. Nottke, G. J. Gabriel


979. Progress towards the synthesis of an enhanced donor-acceptor nanotubular assembly. A. Seal, A. H. Coffman

980. Synthesis and Characterization of Phosphonated Bisphenol A as a Precursor for Proton Exchange Membranes in Fuel Cells. M. C. Boyer, K. Reid, N. Arnett

981. Synthesis of Bisphenol-A Tetrachlorocyclotriphosphazene (BATCCP) from Bisphenol-A and Hexachlorocyclotriphosphazene: The Effect of Reaction Solvent. S. E. Davies

982. Cellular binding of anionic gold nanoparticles as a function of surface modification. C. Thompson, C. Fleischer, C. Payne

983. Study of the effects of chemical etchants on the quality of silver nanowires grown on periodically poled lithium niobate. J. C. Snow, J. M. Schmeltzer, J. R. Perkins


986. Interfacial polymerization of bisphenol A tetrachlorocyclotriphosphazene monomers to synthesize poly (arylene ether sulfone) hybrid copolymers. J. Robertson, T. Thompson, N. Y. Arnett


988. Tuning Iodine Content in Poly(epsilon-caprolactone): Synthetic Hydroxylamines for Grafting. L. L. Davis, S. E. Nicolau, C. C. Duncan, B. A. Van Horn


993. Investigating cellular death mechanisms in response to targeted gold and silver nanospheres. L. A. Austin, S. Ahmad, M. Mahmoud, M. A. El-Sayed


999. Controlled Zwitterionic Polymer Growth on Conducting Polymer Films. L. Pendleton, T. Hanks

1000. Molecular engineering of aquaporin to improve stability. T. A. Combs, C. Ye, Y. Wei

1001. Determination of the photoproducts of amphiphilic cyanine dyes in monomeric and aggregated forms. R. Kozlowski, J. Womick


1003. Preliminary results for the crystallization of the yeast aldo-keto reductase family member YDL-124w. W. Mojadedi, Y. Nguyen, M. H. Weiland

1004. Characterization and Determination of Inhibitor Interaction with Streptomyces griseus Aminopeptidase. L. Vang, J. Moses, L. Ming

1005. Antimicrobial secondary metabolites from endophytic fungal isolates of Goldenseal (Hydrastis canadensis). J. M.

1006. Progress towards the synthesis of a pyrimidodiazepine-based folate as a potential inhibitor of glycinamid ribonucleotide formyltransferase. A. Gann, L. Gonzalez, P. S. Ray

1007. Investigations into the incorporation of 5'-triphosphate-8-oxo-2'-deoxyguanosine (OdGTP) and related analogues with polymerase RB69. A. M. Weaver, M. Hamm

1008. Investigation of the incorporation efficiency of OdGTP and its analogues opposite dC and dA with polymerase BF. K. Alexander, M. Hamm


1011. Examinations of the Incorporation of 8-Oxo-2'-deoxyguanosine with the A-family Polymerase Klenow Fragment. J. Capalbo, M. Hamm


1014. Interactions between creatinine and serum albumin: a study of free and bound nitrogenous uremic toxins. S. A. Harris, S. R. Whitson, M. F. Santiago

1015. Purple Urine Bag Syndrome: Regulation of Pyrimidine Enzymes by Tryptophan. A. N. Broadway, M. F. Santiago

1016. Expression and purification of the bovine leukemia virus (BLV) polyprotein Gag. B. L. Boleratz, D. F. Qualley

1017. Towards the synthesis of a tripyrromethane derivative mimicking the active site of coenzyme F430. C. M. Crooks, N. Klann, A. E. Gorden

1018. Tat-specific factor 1's role in insulin signaling. J. Pearson, L. Fritts, M. Zupp, H. Miller

1019. Mechanistic insights into small-molecule inhibitors of amyloid-β aggregation. K. Carden, J. M. Hanna, Jr., R. K. Lammi

1020. Synthesis and characterization of disulfonated Bis[4-(3-aminophenoxy)phenyl] sulfone polyamide copolymers for proton exchange membrane fuel cells. K. Luitel, J. Poland, A. Aaron, N. Y. Arnett


1023. Geometric Shifts in the Zn^{2+} Chelating Pocket of the ZN-1 Domain within E. coli LeuRS Contribute to the Stabilization of Adenylate. K. E. Polivka, R. A. Whitaker

1024. Study of RNA binding to Matrix Domain of Gag protein in Bovine Leukemia Virus. A. Rimer, D. F. Qualley

1025. OGA, the O-GlcNAc cleaving enzyme, displays concentration dependent specific activity. K. A. Brown, G. L. Crawford
1026. Investigating growth conditions for a biosurfactant producing *Bacillus* strain. **M. P. Fanning**, K. D. Kloeppe, G. L. Crawford

1027. Tetrahydrodipicolinate N-succinyltransferase (DapD) from *Mycobacterium Bovis*: Overexpression and purification. **D. Osula**, C. M. Johnson


1030. Biocatalytic reduction of a non-aromatic nitro group by a nitroreductase from *Salmonella typhimurium*. T. Reams, R. Oliff, J. Park, A. Bommarius, B. D. Feske


1032. Synthesis of citric acid cycle intermediaries from diketopiperazines. **J. Crowetipton**, G. Springsteen

1033. Characterizing Substrate-Specificity in the Aldo-keto Reductases, YHR104w and YOR120w. **C. Poole**, S. C. Mateer

1034. Withdrawn.


1037. Structural and energetic characterization of an ethidium-DNA adduct. **M. K. Longmire**, D. Graves


**Posters: Chemical Education**

Loews Atlanta Hotel
Over Look/Exhibit Hall

D. Sherrill, *Organizer*

4:00 - 5:30


1041. Students as Enzymes: An interactive activity to introduce enzyme kinetics. E. A. Shugart, P. L. Colasurd, **J. H. Shugart**

1042. Organic chemistry students' knowledge structures of fundamental general chemistry topics: Lewis structure and bonding. **N. L. Burrows**, S. Mooring

1043. A model for a sophomore level research class. **H. V. Clontz**, K. R. Wilson, C. E. Dahm
1044. Peer-Led Tutoring for Principles of Chemistry II at Georgia Perimeter College. A. Cook


1046. Using short focused research projects to engage science majors at a two year institution. M. Trani, V. Mativo, P. Pedroso

1047. Guided inquiry experiments for physical chemistry: The POGIL-PCL project. R. M. Whitnell, S. S. Hunnicutt, A. Grushow

1048. Preliminary Assessment of Changes in Quantitative Chemistry Knowledge and Attitudes Following a Summer STEM Enrichment Program for College Freshman at a Liberal Arts College. A. D. Gibson, M. Siopsis


1050. Sol-gel Encapsulated Horseradish Peroxidase. B. Ottoson

1051. Customizing the synthesis of aspirin: An inquiry study into the esterification reaction requirements. F. M. Burke, D. Patel

1052. Direct perspective: Undergraduate participation in experiment development. L. Mandeltort, J. D. Gorden

1053. Computational investigation of a biomimetic model of acireductone dioxygenase. M. Ownbey, K. Smith, J. K. Padden Metzker

1054. Get involved with the ACS Division of Chemical Education. M. B. McGinnis

1055. Fundamentals of Chemistry: Course impact and retention. A. H. Shelton

1056. Chlorine Dioxide-Phenol Reaction: A Kinetic Laboratory Experiment. A. T. Pratt, E. Grimley, D. W. Wright

1057. Analysis of food coloring in introductory chemistry. S. K. Hutchison, M. T. Griffin, K. R. Wilson, J. W. Hall


1060. Enhancing engagement in undergraduate education. D. W. Dixon


Posters: Undergraduate Research

Physical/Computational/General Chemistry

Loews Atlanta Hotel
Over Look/Exhibit Hall
V. Singh, Organizer

4:00 - 5:30


1064. Computational investigations of the borohydride reduction of ketones: The mechanistic source of the stereoselectivity of the reduction of benzil. B. Sauls, D. A. Clabo, Jr.


1066. Electrochemical analysis of symmetric 1,4-fluorenylenes functionalized with electron donating and electron withdrawing groups. B. E. Levy, B. J. Laughlin, Y. Htet, R. C. Smith, A. G. Tennyson

1067. Theoretical studies of hydrogen abstraction reactions from hydrofluoroethanes. T. A. Dray, T. V. Albu

1068. Comparison of the reaction rates between tetramethyl orthosilicate and various carboxylic acids. C. R. Garrett, C. E. Dahm


1070. Modeling studies of binding of gingerol to Bcl-2 protein. L. A. Sharpe, D. A. Abramovitch, F. A. Norris

1071. Determination of the release rate of two antibiotics embedded in a nanofiber mesh applicable to limb salvage. C. Quinn, P. O'Brien, S. Symes


1074. Modeling of pulsatile Nonnewtonian blood flow as a Bingham fluid in a branched artery. A. Vanlandingham, R. Wilcox

1075. Computational study on the electronic structures of functionalized cyclosilanes. D. C. Yost, S. Kilina

1076. Presence of pharmaceuticals and personal care products in treated wastewater from a small college community. A. Bray, E. M. White

1077. Approach toward 1,2,3-triazoles sensors for the detection of heavy transition metal cation. K. V. Hawkins, N. Ballantyne, K. Afeku, K. S. Aiken, S. M. Landge


1079. How sweet it is: Developing an undergraduate laboratory experiment on the spectroscopy of sweet tea. C. C. Rogers, B. B. Fenn, J. L. Armstrong, K. D. Kloeppep


1081. Photodegradation Mechanisms of Vardenafil and Sildenafil. L. Herbert, W. Cory


1084. Using DNA Computational Design to Construct and Image Nanostructures. J. Waller, R. Wadkins

1085. Protein similarity networks reveal relationships among sequence, structure, and function within the cupin superfamily. R. Uberto, E. Moomaw


1087. Progress Towards Sideband Cooling of Atomic Ion-Molecular Ion Coulomb Crystals. J. Gray

1088. Computational studies of paradifluorobenzene cations with two HCN molecules. J. C. Rowe

1089. Engaging rural students in place-based chemistry: Development and implementation of contextualized experiments for agricultural regions. L. S. Fitts, S. R. Fulgham

1090. Effect of ultrasounds on alpha-amylase. A. Rizzo, A. Gaquere-Parker

1091. Iron competition: Protein vs. synthetic drug. A. Laufer, R. M. Majors, C. M. Davis McGibony

1092. Can cosmetic surfactants be benignly precipitated from aqueous solutions? E. D. Keith, M. N. Richardson, K. A. Sands, H. S. Leach, J. M. Carr

1093. Solvent effects on the absorption maxima of conjugated dyes: Testing the applicability of the particle-in-the-box model. A. Brislinger, C. Williamson, M. Kendrick-Murphy


1095. Simulating the quantitative effect of glucose on post-mortem ethanol production by Candida albicans. T. Vasiljevic, S. E. Hooper Marosek


1097. Computational simulation of the binding of deltorphin I to the δ-opioid receptor. M. A. Tapia, K. S. Kroeger

1098. An investigation of W438 as a route of misguided electron transfer for KatG. E. McCurdy, O. Njuma, E. Ndonsta, D. Goodwin

1099. UV damage recognition by UV-DNA damage binding protein. A. L. Hughes, G. M. Gray, A. van der Vaart

1100. Revealing the binding affinity of β-glucuronidase/ligand complexes via computational chemistry. J. D. Mace, D. S. McKnight, T. J. Fuhrer

1101. Degradation of estrogen by lignolytic enzymes from Oak Mountain State Park fungi. C. Farmer, A. Hampton, C. M. Johnson, D. Gregory

1102. A focus on focusing proteins. M. Roberson, R. Montgomery

1103. Synthesis, NMR assignments, mass spec, and NCI cell line studies and a proposal as a treatment for autism, research with byrostatin. R. Robertson, T. McGregor, H. Franklin, J. L. Perry, T. Manning, G. Wylie, D. Phillips, B.
Bythell, F. Zhang

1104. Alternative approach to confirming precipitation reactions in aqueous solutions. S. Brigham, P. Walters, M. Han


1106. Reliability of fire debris analysis evidence storage containers. A. Noble


1108. Implementation of a new graphical multiscale modeling interface into the CHARMMing web-portal. V. Schalk, F. C. Pickard, Y. Pevzner, B. T. Miller, H. L. Woodcock

1109. In vitro selection with stem loop DNA. M. Harrell, A. C. Spencer

SATURDAY MORNING

Posters: High-School

Loews Atlanta Hotel
Over Look/Exhibit Hall

N. Kirk, Organizer

11:00 - 12:00


1111. Synthesis of Silver Nanoparticles using Domestic Microwave. S. S. Kim, L. Kim, S. Kang, G. Paniconi

1112. Improved performance in microbial fuel cells. M. Shin, S. Kang, S. Woo, S. Chung

Symposium for Undergraduates on Careers in Chemistry

Loews Atlanta Hotel
Salon H

N. Kirk, Organizer

11:00 1113. Chemistry in art conservation. R. Stein

11:40 1114. Scientific progress: Industry versus Academia. J. MacDonald

12:20 1115. Trace residue analysis for the US Army. K. E. Mooney

SATURDAY AFTERNOON

Undergrad Awards Luncheon

(Ticketed event)

Loews Atlanta Hotel
Salon A

N. Kirk, Organizer

1:00 1116. Science from the International Space Station. L. J. Delucas