

MWRM 2022

WEDNESDAY AFTERNOON

Graduate Iowa City
Benson Room B

Younger Chemists Research Symposium

T. Feldman, N. C. Stumme, A. Van Wyk, *Organizers*
E. Landgreen, B. Neupane, *Presiding*

1:30 Introductory remarks.

1:35 36. Zwitterionic cocrystals: 2,4-pyridinedicarboxylic acid as a cofomer. **C.I. Ezekiel**

1:55 37. Peroxide mediated oxidation of phosphonates in extractants relevant to spent nuclear fuel reprocessing. **G. Benthin**, T. Forbes, K. Carter

2:15 38. Multicomponent solids with components that possess multiple C=C double bonds. **N.A. Samarathne Muhandirange**, L. MacGillivray

2:35 Break.

2:50 39. Polymorphism involving a binary cocrystal of anticancer 5-fluorouracil. **C. Stuedemann**, C. Ortiz de Leon, L. MacGillivray

3:10 40. Spectroscopic identification of uranium within Wind Cave National Park. **J. Heinen**, J. Sebree

3:30 41. Assessing classroom materials for structure using Marzano's Taxonomy. **A. Kreps, R.S. Cole**

3:50 Closing Remarks.

Graduate Iowa City
Benson Room C

Analytical Chemistry

R. S. Anareddy, *Organizer*

A. Gundlach-Graham, *Organizer, Presiding*

1:30 10. Toward fingerprint age determination: Exploring fingerprint chemical complexity and degradation processes with high-resolution mass spectrometry. **A. Paulson, Y. Lee**

1:50 11. Verification of chlorine exposure via analysis of chlorotyrosine-albumin adducts by base hydrolysis to form chlorophenols with analysis via LC-MS/MS. **S. Sultana, S. Christenson, M. Basiouny, J. Rioux, L. Veress, B.A. Logue**

2:10 12. Assessment of potential traumatic brain injury biomarkers in blast-induced rats using LC-MS/MS. **O.P. Adetunji, J. Wu, A. Pfaff, A. Sigler, M. Bose, C. Johnson, N. Ercal, H. Shi, P.K. Nam**

2:30 13. Peptidomics analysis reveals changes in small urinary peptides in patients with interstitial cystitis/bladder pain syndrome. **M. ABID**

2:50 Break.

3:10 14. The use of NMR in food authenticity testing and food adulteration: A case study of pre-grated bovine hard cheeses. **C. Ray, M. Bylo, J. Pescaglia, J. Gawenis, C.M. Greenlief**

3:30 15. Development and validation of an analytical method to identify and quantitate novel modafinil analogs in dietary supplements. **E. Bakota, S. Ford**

3:50 16. Confident metabolite annotation using hydrogen-deuterium exchange in MALDI-mass spectrometry imaging. **J. Rensner**, Y. Lee

4:10 17. How analytical chemistry provides new knowledge about the Earth's climate, past and present, that will help gain needed understanding of the likely future climate. **R.F. Hirsch**

Graduate Iowa City
Benson Room A

Organic Chemistry

C. K. Arnatt, *Organizer*
D. Martin, *Organizer, Presiding*

1:30 28. Phytochemical constituents and anxiolytic property of *R. australis* pulp extract. **M. Arisekola**, O. Oyedeji

1:50 29. Molecular modelling and computational analysis to describe structure activity relationships in a class of compounds effective against *Cryptosporidium parvum*. **T. Schubert**, E. Oboh, H. Peek, M.J. Meyers, C. Huston

2:10 30. Triazole-estradiol analogs: A potential cancer therapeutic for drug resistance. **T. Ostlund**, F. Alotaibi, J. Kyeremateng, H. Halaweish, A. Kasten, S. Iram, F.T. Halaweish

2:30 31. Progress towards the total synthesis of Bastimolide A. **L.W. Howell**, J.N. Hackbarth, G. Friestad

2:50 Break.

3:10 32. Synthesis of salinaphthoquinones via benzoquinones. **D. Finley**, G.A. Kraus

3:30 33. New symmetrical diamide from a leaf litter isolate of *Eupenicillium* sp.. **D.I. Ekanayake**, D.C. Swenson, G.F. Bills, J.B. Gloer

3:50 34. Limonoids as chemical tools to investigate neurodegenerative diseases. **C. Peiris**, D. Martin

4:10 35. Discovery of selective estrogen receptor beta agonists as potential therapeutics to treat hot flashes and memory dysfunction in menopausal women. **W. Donaldson**, K.S. Perera, E. Wetzel, S. Chaudhury, A.M. Hanson, K.J. Marks, S. Brown-Ford, D.S. Sem, J. Kim, A.W. Fleischer, J.C. Schalk, K.M. Frick

Graduate Iowa City
Hoak Room

Atmospheric Chemistry

E. A. Stone, A. V. Tivanski, *Organizers, Presiding*

1:30 Opening Remarks.

1:35 18. Emissions and impacts of sea salt aerosols from sea ice leads in the Arctic: Constraints from observations and modeling. **H.M. Horowitz**, H. Hunter, E. Emme

1:55 19. Quantifying the viscosity of individual submicrometer particles using atomic force microscopy. **C. Madawala**, A.V. Tivanski

2:10 20. Organosulfates in nascent and aged sea spray aerosol. **D. Kirindigoda Gamage**, E.S. Hasenecz, G. Dorcé, K.J. Mayer, J.S. Sauer, C. Lee, K.A. Prather, E.A. Stone

2:25 Break.

2:45 21. Environmental films chemistry in and around Iowa City. **S.K. Shaw**, J. DeYoung, J.S. Grant, G. Akporere

3:05 22. Atmospheric measurement of volatile methyl siloxanes in New York City. **C. Brunet**, R.F. Marek, K.C. Hornbuckle

3:20 23. Method development for quantification of oxidized volatile methyl siloxanes using liquid chromatography-tandem mass spectrometry. **J.N. Meepage**, C.M. Meyer, D.K. Gamage, E.A. Stone

3:35 24. Polychlorinated biphenyls in building materials and school air. **J. Hua**, K.C. Hornbuckle

3:50 Break.

4:10 25. Characterization of pollen fragments, fungal spores, and bacterial endotoxins in the atmosphere during rain events. **C.B. Mampage**, D. Hughes, L.M. Jones, N. Metwali, P.S. Thorne, E.A. Stone

4:30 26. Plastic burning impacts on atmospheric fine particulate matter at urban and rural sites in the USA and Bangladesh. M. Islam, **J. Welker**, A. Salam, E.A. Stone

4:45 27. Impact assessment study of lockdown on air quality amid Covid-19 in Delhi NCR, India. **Y. Srivastava**, A. Chauhan, S. Singh, L. Singh, T. Jindal

Graduate Iowa City
Wayne Ballroom B

Chemical Innovations To Facilitate a Circular Economy and the Remediation of Persistent Pollutants

D. M. Cwiertny, F. J. Williams, *Organizers, Presiding*

1:00 1. Lignin as a source of chemical feedstocks: Boron trihalide mediated preparation of low-crosslinked lignin from White Pine sawdust. **T. Leventis**, M.H. Kazmi, F.J. Williams

1:20 2. Lignin valorization for chemical production. **M.B. Foston**

1:50 3. Implanting molecular decoys to initiate a selective and rapid depolymerization cascade of Polyethylene terephthalate. **D. Dileep**, T. Lee, A.V. Ananin, M.J. Forrester, J. Bonde, L. Burton, V. Camelo Vega, G.A. Kraus, E.W. Cochran

2:10 4. Upcycling polyolefins via selective catalytic conversions. **A.D. Sadow**, W. Huang, F. Perras

2:40 20 minute break.

3:00 5. Development of electrode materials for PFAS destruction. **B.P. Chaplin**

3:30 6. Thermo-responsive hydrogel for PFAS remediation and sampling. M. Ezazi, B. Shrestha, **G. KWON**

3:50 7. Groundwater cleanup by green rust and biochar. **L. Chelsvig**, M. Scherer, H. Bruun Hansen, D. Tobler, K. Dideriksen, D. Latta

4:10 8. Recycled paper-sheet feedstock for composite-based additive manufacturing. **a.W. Bangel**, X. Song

4:30 9. Tales from the entrepreneurial dark side: When sustainability is not really 'sustainable'. **L. Haverhals**

THURSDAY MORNING

Graduate Iowa City
Benson Room B

Biochemistry

R. S. Cole, *Organizer*
B. Stromer, *Presiding*

8:30 Introductory Remarks.

8:35 84. Design and synthesis of small molecules that target UNC119 for the treatment of diabetes mellitus. **A. Moore**, A. Graham, R.J. Kerns, J. Sebag

8:55 85. SARS-CoV-2 Omicron variant spike mutation Q954H enhances fusion core stability relative to previous variants. **V. Outlaw**, N. Vithanage, R. Apurba, C. Bair

9:15 86. Novel interaction between proteins involved in gene silencing: structural studies of PCNA and CAF-1. **M. Dolan**, J. Lovelace, G. Borgstahl, D. Dieckman

9:35 Break.

9:50 87. Sorption of common livestock antibiotics to diatomaceous earth. **Z. Alberto**, B. Stromer

10:10 88. Functional magnetic nanosensors for the ultrasensitive detection of Ebola. **C. Sutton**, S. Ramanujam, C. Soard, N. Koti, S. Santra, T. Banerjee

10:30 89. Tyrosinase substrate binding: A computational chemistry study. **L. Bullock**, M. Sinton

Graduate Iowa City
Wayne Ballroom B

Advances in Crystal Engineering and Solid-State Supramolecular Chemistry

T. Friscic, K. M. Hutchins, *Organizers*
G. Campillo-Alvarado, *Presiding*

8:30 Opening remarks.

8:35 62. Anti-crystal engineering as a design approach for the synthesis of ionic liquids. **A.V. Mudring**

9:05 63. Host-guest chemistry between chalcogen bond driven cavitand assembly. **V. De Silva**, B. Averkiev, C.B. Aakeroy

9:25 64. Crystalline plug-in assemblies: U-shaped bipyridines and boronic ester catecholates. **C.J. Hartwick**, L. MacGillivray

9:45 65. Design of experiments for dissolution robustness of late-stage pharmaceuticals. **S.M. Oburn**

10:15 Break.

10:30 66. NMR crystallography and crystal structure prediction using quadrupolar nuclei. A.A. Peach, C.H. Fleischer, K. Levin, S.T. Holmes, J.E. Sanchez, **R.W. Schurko**

11:00 67. The curious case of iodoperchlorobenzene as a halogen-bond donor that templates a [2 + 2] cycloaddition reaction. **R.H. Groeneman**

Graduate Iowa City
Benson Room C

Analytical Chemistry

R. S. Anareddy, *Organizer*

A. Gundlach-Graham, *Organizer, Presiding*

8:30 68. Facile fabrication of hierarchically nanostructured gold electrode for bio-electrochemical applications. **P. Sondhi**, D. Neupane, J.K. Bhattarai, A. Demchenko, K.J. Stine

8:50 69. Fabrication of 3D printed metal superhydrophobic surfaces. **R. Ordikhani Seyedlar**, W. Huang, S.K. Shaw, H. Ding

9:10 70. Fabrication of colloidal nanoporous gold nanoparticles. **D. Lingden**, J.K. Bhattarai, K.J. Stine

9:30 71. Investigating glioblastoma: Utilizing 3D-printed microfluidics to study cell migration in controllable chemical gradients. **A.F. Kreznor**, C.T. Culbertson, S.H. Bossmann

9:50 Break.

10:10 72. Temperature-dependent characterization of eutectogels composed of natural deep eutectic solvents. **N. Stephens**, E.A. Smith

10:30 73. Variable-area fluorescence correlation spectroscopy studies of probe molecule diffusion in nanostructured hexagonally ordered C12EO10 lyotropic liquid crystals. **O. Shafiee**, H. Rashidi, S. Jenkins, T. Ito, D.A. Higgins

10:50 74. Identification of positive correlations between lipidic aldehydes and protein carbonyls in solvent extracted, extruded, and expeller soybean meals through chemometric analysis. **J. Zhang**, P.E. Urriola, S. Naeve, G. Shurson, C. Chen

11:10 75. Study of organic dye nanoconfinement within nanoporous anodic aluminum oxide membranes by fluorescence correlation spectroscopy. **H. Rashidi**, K.J. Howard, O. Shafiee, L. Xue, T. Ito, D.A. Higgins

Graduate Iowa City
Wayne Ballroom C

Applied Learning in the Teaching Laboratory: Engaging students through real world context within the laboratory curriculum.

M. W. Ducey, *Organizer, Presiding*

8:30 Opening Remarks.

8:35 76. Integrating applied learning into the chemical instrumentation curriculum: A natural products themed experimental sequence. **M.W. Ducey**

8:55 77. Incorporating a service-learning component in an organic chemistry laboratory course of a small liberal arts college. **P.P. Bugayong**, M. Doyle

9:15 78. Semester length research projects in the biochemistry laboratory. **M. Sinton**

9:35 79. Lessons learned from the design and implementation of an analytical chemistry cure investigating indoor films. **A.L. Van Wyk**, L. Andrews, A. Julius, B. Shrestha, R.S. Cole, S.K. Shaw

9:55 Intermission.

10:10 80. Making protein crystallography accessible to undergraduates in an introduction to biochemistry lab course. **N.M. DeVore**

10:30 81. Real-world inorganic testing: The spectrophotometric determination of phosphate in local water. **S. Harris**

10:50 82. A polymer entropy lab exercise for undergraduates. **L.E. Prevette**

11:10 83. Chance and chemistry: Using dice to illustrate the role of probability in kinetics and equilibrium in preparation for lab. **P. Colombo**

Graduate Iowa City
Wayne Ballroom A

Environmental Photochemistry

D. M. Cwiertny, K. H. Wammer, *Organizers, Presiding*

8:00 Opening Remarks.

8:05 52. Applying a mechanistic understanding of virus inactivation by UVC to build predictive models. **K. Wigginton**, N. Rockey, Z. Qiao

8:30 53. Predicting dissolved organic matter photoreactivity by its molecular composition, optical properties, and redox activity. **C.K. Remucal**, S.M. Berg, K.H. Wammer

8:55 54. Photochemical reactivity and contaminant transformation in a diverse set of natural waters. **K.H. Wammer**, C.K. Remucal, S.M. Berg, I.M. Kelly, C.D. Knellwolf, C.J. Larson

9:15 55. Photochemical reactions with nucleophiles: Implications for pollutant fate and transport. **D.M. Cwiertny**

9:35 56. Photo-transformation of methionine in the presence of surrogate and standard dissolved organic matters under sunlit irradiation. B. Mohrhardt, B. Barrios Cerda, P. Doskey, R. Kibler, **D. Minakata**

9:55 Break.

10:10 57. Fluorine beyond PFAS: Tracking fluorine during photolysis of fluorinated pesticides and pharmaceuticals. A.P. Bhat, T.F. Mundhenke, W.C. Pomerantz, **W. Arnold**

10:35 58. Determining the fate of lampricides in aquatic systems using a multi-tracer approach. **L.D. Angell**, C.K. Remucal

10:55 59. Photochemical reactions alter dissolved organic matter composition in a stratified, eutrophic lake. **S.M. Berg**, B.D. Peterson, K. McMahan, C.K. Remucal

11:15 60. Dissolved organic matter composition influences its susceptibility to complete and partial photooxidation within lakes. **R. Milstead**, C.K. Remucal

11:35 61. Singlet oxygen, fluorescence quantum yield, and photodegradation of wildfire ashes in solution. **S. Fischer**, F. Leresche, L. Rivera, F.L. Rosario

Graduate Iowa City
Benson Room A

Inorganic Chemistry

E. M. Villa, *Organizer, Presiding*

8:30 90. Three easy and tunable steps from CdTe to Te. **M. Uible**, J. Kieser, S.C. Bart

8:50 91. Synthesis, crystal structure and properties of KV₆Sb₆. **A. Mantravadi**, V. Gvozdetskyi, Y. Mudryk, A. Sarkar, Y.V. Zaikina

9:10 92. Ruthenium phosphinimine complexes as fast initiating olefin metathesis catalysts. S. Saha, **P.E. Sues**

9:30 93. β -FeOOH nanoneedles as a precursor for the synthesis of Fe₃O₄ and FeS₂ nanoparticles. **Y. Vasquez**

9:50 Intermission.

10:10 94. Investigations of one-dimensional “molecular slinky” fluorescent platinum cyanoximates. **M. Dragoi**

10:30 95. Vanadium alkylidene catalysts for olefin metathesis. **S.A. Fosu**, E.R. Saucerman, W. Farrell, B. Vlasisavljevich

10:50 96. Applications of germanes and germanium amides as reagents for hydrodefluorination and amidation of acid fluorides. **C.S. Weinert**, A. Hayatifar, V.A. Fortney

11:10 97. Metal organic frameworks functionalized with Cr(III) metal complexes for selective trimerization and tetramerization of ethylene. **V. Yempally**, w. Chen, H. Zhou, S. Madrahimov

Graduate Iowa City
Hoak Room

Chemoselective Functionalization of Strong Bonds

D. Martin, F. J. Williams, *Organizers, Presiding*

8:00 Introductory remarks.

8:05 42. New methods for iron-catalyzed C–N and C–C bond formation with terminal alkynes. **J. Neely**

8:25 43. Selective C–H functionalization of diamondoids using visible-light photoredox catalysis. **H. Dang**, D. Martin

8:45 44. Atom-swapping reaction sequences enabled by nickel-catalyzed decarbonylation of lactones. **J. Li**

9:05 45. Direct deoxygenative transformations of carboxylic acids and related C–O bond activations. **S.B. Munoz**

9:25 46. Photochemical strategies for the generation of alkyl and aryl radicals from carbon–chlorine bonds. **S. Pitre**

9:45 Break.

9:55 47. Continuous process for the safe preparation of aryldiazoacetates and direct use in an enantioselective cyclopropanation reaction. **S. Lathrop**

10:15 48. Organic transformations enabled by d0 metals and redox-active ligands. **C. Roberts**, R. Belli, V. Tafuri, J. Gavin, C. Seong

10:35 49. Single atom logic for skeletal editing. **M.D. Levin**

10:55 50. C–X bond activation (X = H, C, O, F) using electron-rich anionic aluminium(I) compounds. **S. Aldridge**

11:15 51. Cobalt-catalyzed decarboxylative coupling. **J.A. Tunge**

THURSDAY AFTERNOON

Graduate Iowa City
Benson Room C

Chemistry Education: Translating Theory Into Practice

N. M. Becker, *Organizer*

T. B. Higgins, *Organizer, Presiding*

1:30 Opening Remarks.

1:35 106. Exploring the role of journal special issues in translating theory into practice. **T. Holme**

1:55 107. OrganicERs: Building a community of practice for organic chemistry instructors through workshops on active learning. **A. Leontyev**

2:15 108. Efficacy of meaningful learning opportunities through incorporating local research into chemistry classroom discussion activities. **N.E. States**, R.S. Cole, E.A. Stone

2:35 109. Promoting conceptual understanding of chemical equilibrium through algorithmic problem-solving. **N.C. Ulrich**, E.M. Kowalski, T. Spudich

2:55 110. Approaches to systems thinking in the analytical chemistry classroom. **G. Clark**

3:15 Concluding Remarks.

Graduate Iowa City
Wayne Ballroom B

Advances in Crystal Engineering and Solid-State Supramolecular Chemistry

T. Friscic, K. M. Hutchins, *Organizers*
K. T. Holman, J. Stojakovic, *Presiding*

1:00 98. Crystal engineering to liquid engineering: Salts, cocrystals, deep eutectics, crystals, liquids...it's about the interactions and effects. **R.D. Rogers**

1:30 99. Modular and hierarchical supramolecular chemistry: A tricky balancing act. V. Panikkattu, **C.B. Aakeroy**

2:00 100. Cocrystals based on 5-fluorouracil. **C. Li**, **C. Ortiz de Leon**, L. MacGillivray

2:20 101. Use of cycloaddition reactions to control thermal expansion in organic materials. **G. George**, D. Unruh, K.M. Hutchins

2:40 Break.

3:00 102. Recent outcomes of using linear templates to control reactivity in Iowa. **K.M. Hutchins, T. Friscie**

3:20 103. Leonard R. MacGillivray as a graduate student. **J.L. Atwood**

3:50 104. Crystal engineering: Then and now. **M.J. Zaworotko**

4:20 105. Building molecules in crystals. **L. MacGillivray**

Graduate Iowa City
Benson Room B

Chemistry Research at Primarily Undergraduate Institutions-Session 1

N. B. Bowden, J. W. Wackerly, *Organizers*
M. T. Wentzel, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 111. Mössbauer spectroscopy of iron-sulfur proteins in whole cells. **C.V. Popescu, S.A. Elmi, J.C. Tran, C. Fontenot, H. Ding**

1:55 112. UV modification of polyethersulfone membranes using fractionated natural organic matter (NOM). **C. Johnson-Edler**

2:15 113. Green(er) one-pot synthesis of substituted isoindolinones. **A. Baer, B.J. Andersh, U. Schnupf, R. O'Connor**

2:15 114. Drug and gene delivery systems and their mechanisms. **L.E. Prevet**

2:35 Discussion Panel.

2:50 Break.

3:05 115. Exploration of endophytic species from Wisconsin towards the discovery of new natural product antibiotic scaffolds. **K.C. Garber**

3:25 116. Centering identities, interests, and backgrounds of students in their undergraduate research projects. **L. Gentile**

3:45 117. Undergraduate research experiences: What works and what does not. **A. Ayella, A. Bajracharya, S. Shrestha**

4:05 Discussion Panel.

4:20 Closing Remarks.

Graduate Iowa City
Benson Room A

Inorganic Chemistry

E. M. Villa, *Organizer, Presiding*

1:30 118. Solvent uptake dependence on surface adsorption in metal-organic nanotubular (MONT) systems. **L. Applegate, J. Leddy, T. Forbes**

1:50 119. Investigation of solid-state metathesis as a rapid and convenient synthetic method to the formation of cobalt-iron boride solid-solutions and the effect of chemical composition on electrocatalytic activity. **J.P. Abeysinghe, E.G. Gillan**

2:10 120. Single crystal proton conduction study in uranium metal organic nanotubes. **T.H. Jahinge, T. Forbes**

2:30 121. Relating the structures and aqueous solution reactivities of two Anderson-type polyoxometalate ions. **E.M. Villa**

2:50 Intermission.

3:10 122. Unsymmetrical functionalization of 2-isocyanoazulene and 2-isocyano-6,2'-biazulene ligand platforms. **G. Griaznov, K. Reddish, A. Gideon, J.J. Meyers, M.V. Barybin**

3:30 123. Homoleptic complexes of isocyano- and diisocyanobiazulenes with a 12-electron, ligand-based redox capacity. **P. Connelly**, D.A. Maldonado, J.C. Applegate, M.V. Barybin

3:50 124. Synthesis of tetraaza and tetraamido macrocyclic ligands and their metal complexes: Potential catalysts in nitrene transfer chemistry. **H. BHATIA**, L. Adams, I. Winter, P. Stavropoulos

Graduate Iowa City
Hoak Room

Organic Chemistry

C. K. Arnatt, D. Martin, *Organizers*

1:30 125. Structural landscape of 2-aminopyridines: Chains or dimers?. **N. Marasinghe Prins**, B. Averkiev, C.B. Aakeroy

1:50 126. Structural landscape of pharmaceutically relevant 1,3,4-chalcogenadiazole derivatives. **L.J. Handlos**, V. De Silva, B. Averkiev, C.B. Aakeroy

2:10 127. Rotation-inversion of tertiary carbamates. Synergy of VT NMR measurements and computational analysis of multi-paths isomerization. **B.M. Jameson**, R. Glaser

2:30 128. Dithiophosphates to release hydrogen sulfide to increase the harvest yield of crops. **N.B. Bowden**, E.M. Brown, N. Pasan, a. paudel

2:50 Break.

3:10 129. BODIPY based photocages for glycan synthesis. **K. DISSANAYAKE**, S. Lechnitz, A. Winter, P.H. Seeberger

3:30 130. Metal-catalyzed halogen exchange of trifluoromethyl arenes. **A. Schneider**, A. Dorian, F.J. Williams

3:50 131. Photocatalytic activation of alcohols to carbon centered radicals using cobalt complexes. **C. Ludwig**

4:10 132. Optimization of MMV665917 to identify new lead compounds for treatment of cryptosporidiosis. **E. Oboh**, M.J. Meyers, T. Schubert

Graduate Iowa City
Wayne Ballroom A

Sustainable Electrochemistry: Saving the World, One Electron at a Time

J. Coduto, N. C. Stumme, *Organizers, Presiding*

1:30 133. Electrochemistry of organic redox-active systems using ionic liquid supporting electrolytes. **N.C. Stumme**, S.K. Shaw

1:50 134. Tailoring of a reinforcing and artificial self-assembled alkyl sulfonic acid layer electrolyte interphase on silicon as anode for high-energy-density lithium-ion batteries. **A. Hailu**, F. Wang

2:10 135. Organosilyl ester and sulfone electrolytes for applications in lithium-ion batteries. **L.J. Lyons**, K. Dixon-Anderson, R. Nieto, C.J. Sabah, S. Sharpe

2:30 136. 190 proof ethanol as a substitute for acetonitrile in electrochemical analysis. **A. Lazicki**

2:50 Intermission.

3:10 137. Facile and flexible, solvent-free synthesis of carbon black supported Cop3 for hydrogen evolution reaction (her) electrocatalysis. **I.A. Liyanage**, E.G. Gillan

3:30 138. ORR and OER catalysts based on thin-film $\text{La}_x\text{Sr}_{1-x}\text{Co}_y\text{Fe}_{1-y}\text{O}_3$ materials produced by spray pyrolysis. **L.R. Sharpe**, D. Dervishogullari, J. Rebelsky, C. Sharpe

3:50 139. TafFit: An algorithm for fitting tafel data and determining kinetic parameters. **J. Coduto**, J. Leddy

4:10 140. Redox potentials of magnetite suspensions under reducing conditions. **M. Scherer**, T.C. Robinson, D. Latta, J. Leddy

4:30 141. ++Electrochemical hydrogen generation by magnetoelectrocatalysis. **J. Leddy**

Graduate Iowa City
Wayne Ballroom D

Symposium in Honor of the 2022 Midwest Award Winner

R. S. Cole, *Organizer*
M. S. Gordon, *Presiding*

3:00 Opening Remarks.

3:05 142. Improving critical materials recovery with computational chemistry and machine learning. **M. Pérez García**, F. Zahariev, T. Ash, E. Stender, M.S. Gordon, T.L. Windus

3:35 143. Software design for the exascale era: The NWChemEx perspective. **R. Richard**

4:05 144. Award Address: Sustainable computational chemistry software and applications. **T.L. Windus**

4:50 Closing Remarks.

FRIDAY MORNING

Graduate Iowa City
Wayne Ballroom A

Chemistry Education Posters

R. S. Cole, *Organizer*

8:00 - 9:45

145. Analysis of evolution of students' learning approaches in the first semester of organic chemistry. **H. Malinakova**

146. Molecules meet materials NSF-REU site. **P. Miro**, J.D. Hoefelmeyer

147. Development of selected chemical indicators for breweries in North America to improve employee safety and health through education and workplace orientation. **J. Thissen**

148. Protein centric research in undergraduate Labs: The malate dehydrogenase cure community (MCC) supports faculty and promotes student collaborations. **B.M. Martinez-Vaz, L. Gentile**, K. Callahan, C.N. Peterson, K. Huisinga, J. Provost, J.K. Bell, J.E. Bell

Graduate Iowa City
Benson Room A

Computational Simulations for Sustainable Chemistry

M. R. Siebert, *Organizer, Presiding*

8:00 Opening remarks.

8:05 149. Kinetic modeling of unconventional catalysts for CO₂ utilization. **B. Liu**, N. Manavi

8:25 150. Theoretical investigation of CO₂ activation and dissociation on corrugated graphitic carbon nitride surface decorated with dispersed single atoms (Fe, Co and PD). **G.D. Fao**, J. Jiang

8:45 151. Unraveling the telomerization of δ -lactones from CO₂ and 1,3-dienes. **J. Barroso**, S.A. Fosu, R.M. Rapagnani, I.A. Tonks, B. Vlasisavljevich

Graduate Iowa City
Wayne Ballroom A

Organic Chemistry Posters

C. K. Arnatt, *Organizer*

8:00 - 9:45

152. Electrostatic loading and photoredox-driven release of functional cargo from oligoviologen-crosslinked materials. **M. Palmquist**, J. Dorsainvil, A. Delawder, J. Yang, M. Danielson, M. Gruschka, T. Saak, X. Kong, T.A. Wencewicz, J.C. Barnes

153. Theoretical pyrolysis of methyl linoleate for renewable energy production. **E.O. Eguaosa**, M.R. Siebert

154. Meta-aerogels: Auxetic shape-memory polyurethane aerogels. **A. Doulah**, S. Malakooti, R.U. Soni, V.A. Edlabadkar, R. Zhang, S.L. Vivod, N. Leventis, C. Sotiriou-Leventis, H. Lu

155. Detection of microbial metabolite using structure-switching signaling aptamers. **Y. Chang**, K.D. Moeller

156. Poly[N,N'-(phenylamine)sulfides] derivatives: Synthesis, isolation, characterization, and application. **a. paudel**, N.B. Bowden

157. Antibacterial properties of N-heterocyclic carbene-silver complexes. H. Palencia, **J. Gutschenritter**, **A. Ahmed**, V. Lo, S. Chandra, **O.A. Lozano-Ramos**

- 158.** Fabrication of auxochromic polymers via step growth polymerization of diamine derivatives with sulfur monochloride. **S.M. Rathnayake Wickremasinghage**, M.A. Breuer, N.B. Bowden
- 159.** Correlation of nanomorphology with drug uptake and in vitro release profiles using polyurea aerogels as the model system. **S. Adom**, C. Sotiriou-Leventis
- 160.** Withdrawn
- 161.** Organic and organometallic luminophores for detection of amyloid oligomers. **Z. Li**, F. Pigge
- 162.** Imidazolidine hydride donors in palladium-catalyzed intramolecular reductive Heck-type reactions. **S.L. Tun**, S. Mariappan, F. Pigge
- 163.** Polymerization and physical properties of cyclic and linear (m)PEG benzyl methacrylate analogues. **A. Freedman**, C.R. Pugh
- 164.** Synthesis of palladium(II) complexes bearing phosphorous ylides as ligands and evaluation of their utility as cross-coupling catalysts. **A. Poddar**, F. Pigge
- 165.** Highly effective separation of fatty acid esters derived from vegetable oils using chemically stable-covalent organic framework (COF) incorporated epoxy membranes. **N. Ranasinghe Arachchige**, N.B. Bowden
- 166.** Carbon aerogels derived from polybenzoxazine and polybenzodiazine aerogels as high-capacity desiccants. **V.A. Edlabadkar**, A. Doulah, R.U. Soni, N. Leventis, C. Sotiriou-Leventis
- 167.** Preparation of chalcogenophenecarboxylic acids for metal-organic framework synthesis. A.S. Brown, **M.R. Hulce**
- 168.** Synthesis of butyrolactones by intramolecular cyclization of cinnamaldehydes, promoted by N-heterocyclic carbenes.. **H. Palencia**, M. Pattabiraman, O.A. Lozano-Ramos, J. Gutschenritter, S.A. Moteki
- 169.** Synthesis of novel DNA-binding polyamides to prevent cancer-related gene expression. **H.Q. Nguyen**, A. Paul, M. Georgiadis, W. Wilson, B.K. James
- 170.** Design and synthesis of estrone analogues towards treatment of hepatocellular carcinoma. **N. Aparicio**, T. Ostlund, K. SutraDhar, F.T. Halaweish

- 171.** Polar and non-polar stacking of perfectly aligned parallel belowamphiphile monolayers (PBAMs) of (PhO, F)-azine. Importance of non-covalent interlayer interactions. **H. Bhoday**, S.P. Kelley, R. Glaser
- 172.** Synthetic efforts towards brocazine family of natural products and proposed stereochemical structure activity relationship studies. **A.L. Fernando**, W. Hulangamuwa, R. Rafferty
- 173.** Lagunamide family: total synthesis efforts, final structural determination, biological evaluation, and new family identification. **S. Perera**, A. Fatino, R. Rafferty
- 174.** Synthesis and characterization of biodegradable hyperbranched polymers for the targeted delivery of therapeutic drugs to treat lung cancers. **N. Koti**, A. Worsley, T. Banarjee, S. Santra
- 175.** Microwave-assisted synthesis of hydrogenation catalysts based on hyperbranched polyester polymer templated gold nanoparticles. **F. Kajal**, C. Worsley, C. Sutton, T. Banerjee, S. Santra
- 176.** Iodination of trifluoromethyl arenes using metal catalysis. **T. Chiarella**
- 177.** Synthesis and structure-activity relationship of antagonists for G protein-coupled receptor linked with neuropathic pain. **I.I. Olayide**, K. Braden, N. Latzo, D. Salvemini, C.K. Arnatt
- 178.** Boron-mediated halogen exchange. **A. Corkovic**, A. Dorian, H. Koska, F.J. Williams
- 179.** Synthesis and characterization of novel donor-acceptor substituted 1,4-diphenyl-1,3-butadienes: Potential dipole-parallel aligned NLO active materials. **J.D. Nulsen**, H. Bhoday, R. Glaser
- 180.** Direct detection of DHT diradicals. **U. Banerjee**, M. Austin, Y. Qiu, D.L. Phillips, A. Winter
- 181.** Polymorph control and solubility enhancement in salts of trimethoprim. **L. Ma**, Q. Zheng, D. Unruh, K.M. Hutchins
- 182.** Synthesis of radioactive hydrogen sulfide donors for use in biological systems. **E.M. Brown**, N.B. Bowden

183. Cavitand-mediated photocycloaddition (PCA) optimizing reaction parameters for yield maximization. M. Pattabiraman, **P. Puntambekar**, M. Hoover

184. Synthesis and evaluation of potential LPS antagonists. **S. Kafle**, K. Dhami, M.R. Nichols, C.D. Spilling

185. Design, Synthesis, and biological evaluation of fluorinated Estrone analogues targeting Prostate Cancer. **K. SutraDhar**, A. Irianni, m. carson, F.T. Halaweish

186. Progress towards the synthesis of (Z)-2-amino- α -hydroxyimino-4-thiazole esters. **G.P. Nora**

187. Comparative study on synthesis of bio-degradable aliphatic polyester via melt-polycondensation. **A.L. Yadav**, T. Dawsey, R.K. Gupta

188. Synthesis of derivatives of the antifungal drug ciclopirox for evaluation against herpes simplex virus 2. **M. Zangi**, L. Morrison, M.J. Meyers

189. Cyclic voltammetry and spectroelectrochemical studies of ferrocenium and Ferrocenophanium cations to understand the catalytic activation of propargylic alcohols. **S. Bezawada**

190. Synthesis and degradation of aliphatic polyester carbonate copolymers using novel chloroformates. **M. Moradi**

191. Selective photocatalytic functionalization of diamantane. **M.M. Wymore**, D. Martin

192. Progress towards a catalytic functionalization of formate esters. **L. Evans**, C. Ludwig, D. Martin

193. Synthesis and reactivity of enol ester epoxides: From hydrocarbons to 1,2-difunctional compounds. **J.N. Hackbarth**, G. Friestad

194. Characterization of pyrolysis oils for asphalt fortification. **R. Herndon**, Z. Mayes, G. Riddle, K.H. Woelk, M. Abdelrahman, M. Ismail

195. Theoretical exploration of possible mechanisms of the bromic acid oxidation of malonic acid via tartronic acid to mesoxalic acid. **E. Hay**, R. Glaser

196. Synthesis of triazole bisphosphonates with modified isoprenoid tails. **M. Maalouf**, N.R. Gehrke, **D.F. Wiemer**

197. Total synthesis of the trikentrins and herbindoies via indole aryne cycloaddition and cycloaddition/rearrangement methodologies. N.L. Chandrasoma, A. Nerurkar, D. Luo, **K.R. Buszek**

198. Synthesis of Ferrocenophanium catalysts and their application as catalysts in propargylic substitution reactions. **N. Ušto**, E.B. Bauer

199. Substituted *N*-vinylpyridinium tetrafluoroborate salts: Improved electrophilic coupling partners for Pd(0)-catalyzed cross-coupling reactions. **T. Domingos**, K.R. Buszek

200. Design and synthesis of Estrone analogs targeting pancreatic cancer. **A. Irianni**, T. Ostlund, K. SutraDhar, F.T. Halaweish

201. Synthesis of neuroprotective limonoids and analogs. **Z. Banarjee**, **E.Y. Bonsu**, D. Martin

202. Sunflower-oil-based polyurethane/ graphene nanoribbons composite film: Synthesis and properties. **v.d. suthar**, m. Asare, R.K. Gupta

Graduate Iowa City
Wayne Ballroom B

Advances in Crystal Engineering and Solid-State Supramolecular Chemistry

T. Friscic, K. M. Hutchins, *Organizers*
Q. R. Chu, *Presiding*

8:30 214. Intercalation, oxidation, and bond formation in 1D and 2D iron chalcogenides. **K. Kovnir**

8:50 215. 2D Coordination networks based on pyrogallol[4]arene stabilized with cation- π interactions. **K. Sikligar**, S.P. Kelley, G.A. Baker, J.L. Atwood

9:10 216. Structural modification and chemical functionalization of metal-organic supercontainers for anion binding. **K. Chitrakar**, Z. Wang

9:30 Break.

9:50 . Crystal engineering boron-based molecular materials: Use of the hydrogen bonding of boronic acids and the dative b←n bond to direct reactivity in the organic solid state. **M. Vasquez-Rios**, G. Campillo-Alvarado, C. Li, H. Höpfl, D.C. Swenson, L. MacGillivray

10:10 218. Modulating thermal expansion by fine-tuning the molecular dimensions and number of functional groups in selected alkyl carbamates. **K. Shunje**, B. Averkiev, C.B. Aakeroy

10:30 219. Chemistry of Illumina's SBS technology. **J. Stojakovic**

11:00 220. Crystal engineering construction of renewable cyclobutane-containing polymers (CBPs). **Q.R. Chu**

Graduate Iowa City
Benson Room B

Chemistry Research at Primarily Undergraduate Institutions-Session 2

N. B. Bowden, M. T. Wentzel, *Organizers*
J. W. Wackerly, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 221. Synthesis and applications of cambiarene macrocycles. **J.W. Wackerly**

8:55 222. Aromatic (di)hydrazide electron acceptors. **D.D. Cao**, J. Amundson

9:15 223. Extended arenes containing 1,2,3-triazole subunits from a click/coupling approach. **J.T. Fletcher**

9:35 224. Turning on the light: Developing next generation agrochemicals via organic photochemistry. B. Steeno, A. Metz, N. Haen, **I. MacKenzie**

9:55 Discussion Panel.

10:15 Break.

10:30 225. Hydroamination of aryl-alkynes: Discovery, mechanistic insights, and applications. **E.H. Fort**, M. Le, M. Marron, A. Stokka

10:50 226. Controlling thermal expansion properties within organic solids. **R.H. Groeneman**

11:10 227. Indirubin: A platform for a successful undergraduate research project.. **J.A. Shriver**

11:30 Discussion Panel.

11:45 Closing Remarks.

Graduate Iowa City
Wayne Ballroom D

Sustainable materials and energy for a brighter future

R. K. Gupta, *Organizer, Presiding*

8:30 228. Make selenium reactive again: Activating elemental selenium for synthetic optimization of various selenium-containing compounds. **Y. Abusa**, P.A. Yox, S. Cady, F. Perras, J. Opare - Addo, E.A. Smith, K. Kovnir

8:50 229. Greening the synthesis of poly(phenylene oxides). **E.H. Fort**, S. Ramaswamy, M. Guino-O

9:10 230. Chicken fat-based polyols for high-performance polyurethane foams. **A. Perera**, **K. Madhushani**, F. de Souza, T. Dawsey, R.K. Gupta

9:30 232. Optimization of nickel and cobalt-based metal-organic framework via different techniques for application in energy storage devices. **M. Chaudhari**, **s. bhardwaj**, S. Chaudhary, R.K. Gupta

9:50 Break.

10:10 231. Highly efficient cobalt-iron-based electrocatalysts for overall water-splitting reactions.. **s. bhardwaj**, M. Chaudhari, R.K. Gupta

10:30 233. Manufacturing of polyurethane wood adhesive through bio-based castor oil polyol and crosslinking additive.. **Y.N. DESAI**, R.K. Gupta

10:50 234. Green synthesis of cobalt oxide nanoparticles by using waste Citrus reticulata for applications in electrochemical energy storage. **R. Srivastava**, s. bhardwaj, R.K. Gupta

11:10 235. Ternary NiSi_{1-x}P_x electrocatalysts for hydrogen evolution reaction (HER). **S. Kong**, K. Kovnir

Graduate Iowa City
Hoak Room

The Good, The Bad, and The Ugly: Showcasing DEI Efforts Across Institutions

E. Belzer, H. Dang, C. Hartwick, C. Ortiz de Leon, *Organizers*
K. Hunter, L. J. Scharlott, *Organizers, Presiding*

8:30 Opening Remarks.

8:35 236. Living in the borderlands: The navigation of STEM and racial identities within graduate students. **K. Hosbein**, W. Feng, M. Gillis, P. Vincent-Ruz

9:00 237. The Midwest retreat for diversity in chemistry: Purpose, planning, and problems. **K. Rahn**, G. Viswanathan, E. Soto, R.K. Anand

9:25 Break.

9:30 238. How AIMS (Alverno initiatives in math and science) supports DEI designation at Alverno College, a HSI and women's college. **L. Guilbault**

9:55 239. Lessons learned: Inclusive mentoring practices and forming a sustainable departmental DEI committee. **L. Adams**

10:20 240. Using DEI Moments to promote an inclusive culture in research and teaching. **E.A. Arriaga**

10:45 Break.

10:55 DEI Discussion.

11:25 Closing Remarks.

Graduate Iowa City
Wayne Ballroom C

Radiochemistry and f-block chemistry

T. Forbes, *Organizer*

K. Carter, *Organizer, Presiding*

8:00 Introduction.

8:05 204. Electronic structure and bonding in uranium-arene complexes. **R.R. Bhowmick**

8:25 205. Paired synthetic and computational efforts exploring hydrogen bonding effects on bonding, electronic structure and spectroscopic signals of uranyl halides. **H. Rajapaksha**, L. Augustine, M. Pynch, T. Forbes, S.E. Mason

8:45 206. Tuning the electrodeposition of f-elements in molten alkali halide salts. **M.M. MacInnes**, K.A. Pace, N.H. Anderson, S.A. Kozimor, Z.R. Jones, E.R. Batista, M.Y. Livshits, K.E. Knope, I.M. DiMucci, B.W. Stein, F.R. Rocha, V. Mocko, C. Eiroa-Lledo, J.N. Wacker, P. Yang

9:05 207. Geochemical and mineral controls on the speciation of uranium in the subsurface. **D. Latta**, T.C. Robinson, M. Scherer, E.J. O'Loughlin, K.M. Kemner, M. Boyanov

9:25 208. Design, synthesis, and evaluation of bio-inspired ligands for uranyl chelation relevant to targeted radiotherapy. **A. Katuwana Arachchige**, V. Karapala, K. Carter

9:45 Break.

9:55 203. Aqueous speciation and nucleation of tetravalent actinides in the presence of chloride and nitrate ligands. **P. Miro**

10:20 209. Preorganization of diglycolamide ligands for the improved separation of trivalent lanthanide and actinide elements. **J.A. Nakath Durage**, K. Carter

10:40 210. Discovery of new topological features in a hydrothermally synthesized uranyl peroxide cluster. **B. Lottes**

11:00 211. Designing lanthanide and actinide polyoxometalate to access atomic clock transition for application in quantum information sciences(QISs). **P.J. Subintoro**, K. Carter

11:20 212. Speciation and nucleation of an(iv) ions in presence of zwitterionic glycine. **S. Mazumder**, P. Miro

11:40 213. Surface effects and uptake of water within metal organic nanotubes. **V.S. Samarasiri**, T. Forbes

Graduate Iowa City
Benson Room A

Computational Methods and Applications

P. Miro, *Organizer*

B. Vlasisavljevich, *Organizer, Presiding*

9:20 Opening remarks.

9:25 241. Using electronic structure calculations to understand the metal ligand cooperative binding of carbon dioxide to Manganese PNP pincer complexes. **E. Landgreen**, H.R. Petras, S. Ramadugu, S. Country, C. Sindt, S.R. Daly, J.J. Shepherd

9:45 242. Cooperative and anticooperative effects in the hydrogen bonds within ethylammonium nitrate. **S. Kim**, M.S. Gordon

10:05 445. Using machine learning to find the correlation among structural features about controlling metal dissolution process. **Y. Chen**, B. Hudson, S.E. Mason

10:25 Break.

10:45 244. Designing a spectroscopic map for 'alkynes' of vibrational probes. **K. Streu**, T. Haupt, S. Hunsberger, C.A. Daly

11:05 245. Computational studies of mNeonGreen: As a sulphate sensor. **V.N. Parthiranaige**, W.S. Ong, K. Ji, S. Dodani, A. Walker

Graduate Iowa City
Wayne Ballroom A

Analytical Chemistry Posters

R. S. Anareddy, A. Gundlach-Graham, *Organizers*

10:15 - 12:00

246. Isco samplers and PFAS applications: Study on tubing material and vacuum sampler. **P.B. Liescheski**, I. Vestalo, K. Belt

247. Studying the binding affinity of LPS antagonist AM-12 with membrane proteins and LPS binding protein. **P. Sondhi**, A. Demchenko, K.J. Stine

248. Effects of dietary docosahexaenoic acid on lipid peroxidation products in offspring mice. **K. Nyarko**, B. Fisher, M. Appenteng, C.M. Greenlief

249. Breaking down space rocks for oxygen. **R. Arnold**, D.W. Welsh, N.L. Netzer

- 250.** Utilizing ionic liquids for the extraction of oxygen and metals from lunar regolith. **N.L. Netzer**, D.W. Welsh, R. Arnold
- 251.** Characterizing proteinase K in the enzymatic hydrolysis of photodegraded polylactic acid. **M. Brown**, M.A. Maurer-Jones
- 252.** Monolayer study of DMPC and cholesterol, and their interactions with LPS and a potential LPS-antagonist; AM-12. **D. Lingden**, G. Shrestha, A. Demchenko, K.J. Stine
- 253.** Utilizing DNA photoproducts as intrinsic probes for G-quadruplexes in vivo. **S. Scruggs**, . Yang, N. Gutierrez-Bayona, J.S. Taylor, M.L. Gross
- 254.** Measuring the mobility of YOYO-1 stained DNA at different temperatures. **E. Mendez-Ortiz**, E. Baxter, **B. Menke**, **K. Kounovsky-Shafer**
- 255.** Concentrating lambda concatemer DNA utilizing an acrylamide roadblock. **T. Huynh**, S. Rau, **K. Kounovsky-Shafer**
- 256.** Developing an insert to protect large DNA molecules during cell lysis. **C. Polen**, T. Huynh, A. White, **K. Kounovsky-Shafer**
- 257.** Morphological changes of environmental films with elevation. **U.G. AKPORE**, A.p. Julius, j.L. deyoung, S.K. Shaw
- 258.** Influences of convective storms on bioaerosols in a semi-arid grassland environment. **T.K. Feldman**, C.B. Mampage, R. Perkins, T.C. Hill, L.D. Grant, S.C. van den Heever, P.J. Demott, S. Kreidenweis, E.A. Stone
- 259.** Characterization of airborne particles released by birch and timothy grass. **J.C. Fernando**, L.M. Jones, E.A. Stone
- 260.** Development of a dynamic headspace gas-chromatography mass-spectrometry method for the determination of methyl mercaptan protein adducts. **K. BILKIS**, B.A. Logue
- 261.** Identification of cell-cell signaling peptides within the central nervous system of thirteen-lined ground squirrels during hibernation by mass spectrometry-based peptidomics. **S. Mousavi**, H. Qiu, E. Tom, F. Heinis, M. ABID, M. Andrews, J.W. Checco

- 262.** Successive exposure of cereal crops to CeO₂ nanoparticles and perfluorooctanesulfonic acid (PFOS): Wheat and barley studies. **N. Kirwa**, D.C. Wagner, P. Ofoegbu, P. Clubb, K. Coates, E. Horn, C. Rico
- 263.** Spatiotemporal variation of ambient air pollution particulate matter elemental composition at tuberculosis clinics in Hanoi, Vietnam.. **M. Zavala**, H. Phan, T. Trinh, R. McLaughlin, J. Balmes, N.V. Nhung, P. Nahid, R. Blount
- 264.** In-situ tracking of surface reactivity during lead-acid battery refurbishment via chelation treatment. **A. Baby**, A. Asserghine, J. Rodriguez Lopez
- 265.** Neucode tags for highly multiplexed metabolomics. **S. Grady**, M. Armbruster, J. Edwards, C.K. Arnatt
- 266.** Performance of daughter plants of wheat previously exposed to perfluorooctanesulfonic acid (PFOS). **O.R. Ogundele**, N. Kirwa, P. Clubb, C. Rico

Graduate Iowa City
Wayne Ballroom A

Biochemistry Posters

R. S. Cole, *Organizer*

10:15 - 12:00

- 267.** Effect of polymer architecture on chromobacterium viscosum lipase activity in reverse micelles. **A. Freedman**, A. Gabriele, C.R. Pugh
- 268.** Single molecule kinetics study of two proteins involved in gene silencing. **E. Hebert**, O. Nicholson, D. Dieckman
- 269.** Bioconversion of lignin and plastic-derived aromatic compounds by rewiring aromatic catabolism in *E. aphidicola* LJJ01. **L. Dissanayake**, S. Kayastha, R. Ligon, A. Sparks, A. Zatar, S. Jayasekara, L. Becker, L. Jayakody

- 270.** CRISPR/Cas9 Ribonucleoprotein Editing for Lactate Dehydrogenase gene knockout in SW480 cells.. **S. Shrestha**
- 271.** Evaluation of quantum dot-aptamer bioconjugate binding to target proteins in cells. **W. Peschel, B. Thong Sing-Yi, B. Eichler**
- 272.** The quantum yield of fluorescent proteins. **C. Padgett, N.M. DeVore**
- 273.** Structural engineering of thermal stable fluorescent proteins TGP and YTP. **M. Anderson, C. Padgett, N.M. DeVore**
- 274.** Characterization and crystallation of the canine p53 protein. **D. Sitapara, N.M. DeVore**
- 275.** Development and continued optimization of a cyan thermal protein (CTP). **D. Sitapara, C. Padgett, N.M. DeVore**
- 276.** Testing some unique nitrogen containing molecules for their in vitro effect using the parasitic protozoan *Leishmania tarentolae*. **K. Wallace, Z. Zelaya, C. Hamaker, M.A. Jones**
- 277.** Toward enzyme-responsive polymeric micelles with hydrolysable cores for targeted therapeutic delivery. **D.D. Wallace, A.M. Keller, S.A. Innes, A.J. Luthi, M.P. Thompson, N.C. Gianneschi**
- 278.** Interactions between Anti-HER2/neu peptide (AHNP) conjugates and HER2+ breast cancer cells. **K.D. Gomel, L.E. Prevette**
- 279.** Triazole-estrone analogs: A potential drug treatment for triple negative breast cancer. **E. Hedge, T. Ostlund, F. Alotaibi, J. Laddusaw, F.T. Halaweish**
- 280.** Inhibitory potential of gold nanoparticles on the amyloid fibrillation of human insulin. **H. Grannemann**
- 281.** Exploring the potential role of glyco-curcumin analogs as MD-2 inhibitors in the inhibition of response to LPS. **D. Talasila, P. Sondhi, E. Bauer, K. Stine**
- 282.** Development of a pyruvate dehydrogenase kinase inhibitory assay. **N. Fancher, M. Moxley**
- 283.** Rapid detection of food-borne pathogens using lateral flow assay. **E.E. Arogunyo, S. Santra**

Graduate Iowa City
Wayne Ballroom A

Inorganic Chemistry Posters

E. M. Villa, *Organizer*

10:15 - 12:10

284. New transition metal chemistry for atomic layer deposition of thin films. **W. Waduge**, S. Sundrani

285. Development and characterization of a family of MnIII-alkylperoxo complexes. **S.A. Brunclik**

286. Directing anisotropic growth of gold nanoparticles through a green, one-pot, LED-mediated synthesis utilizing pre-nucleation gold salt structures. **A. Siegel**

287. First dimercapto-terminated biazulenenic π -linker. **S. Kelsey**, J.C. Applegate, P. Connelly, M.V. Barybin

288. Synthesis, characterization, and electrochemical comparison of nickel complexes containing new redox-active tetradentate ligands derived from o-phenylenediamine. **D. Duffy**, M. Skaria, K.D. Spielvogel, N.C. Stumme, S.R. Daly, S.K. Shaw

289. Nickel and copper complexes of SNS Schiff base ligands for photocatalytic degradation of methylene blue. **T.O. Falola**, C. Hamaker

290. Reactivity of a uranyl superoxide catalyst for direct air carbon dioxide separations. **S. Scherrer**, D.V. Kravchuk, T. Forbes

291. First diisocyano-terminated terazulenenic π -linker and its chemically reversible polyelectrochromism. **J.A. Mandigo**, N.R. Erickson, M.V. Barybin

292. Synthesis and characterization of Dipyrazolylpyridine ruthenium complexes for water splitting reactions. **P. Mofle**, A. Hussain, K. Mariappan

293. Flexible carbon cloth modified cobalt telluride for sensitive and selective detection of dopamine. **K. Lagemann**, H. Singh, M. Nath

294. Metal complexation with macrocyclic supramolecular constructs for bioavailable radionuclide delivery. **S. Kruse**, T. Forbes, L. MacGillivray

Graduate Iowa City
Wayne Ballroom A

Physical Chemistry Posters

A. Bhattacharjee, A. V. Tivanski, *Organizers*

10:15 - 12:00

295. NMR analysis of an 8mer non-palindromic DNA sequence containing a U:G mismatch. **A.C. Pilarski**, N.M. DeVore, G.A. Meints

296. Electronic structure and dynamics of bisphosphonate polyoxovanadates in noble metal surfaces. **M. Mahama**, B. Vlasisavljevich, P. Miro

297. Computational insights into pairing induced quorum quenching in lactone autoinducers. **P. Miro**, **B. Vlasisavljevich**

298. Binary phase TiO₂-NiO hybrid nanocrystal for photocatalytic water splitting. **N. Muttakin**, R. Mia, J.D. Hoefelmeyer

299. Recycled face masks for electrochemical energy storage devices. **A. Gupta**, **C. Allison**, **M. Chaudhari**, **P. Zalavadiya**, F. de Souza, R.K. Gupta, T. Dawsey

300. A facile approach to synthesize cobalt phosphide as an efficient electrocatalyst. **P. Neely**, **H. Oferrell**, W. Lin, R.K. Gupta

301. How to reach the thermodynamic limit faster in periodic coupled cluster theory using the transition structure factor. **T. Mihm**, T. Schäfer, L. Weiler, S. Ramadugu, A. Grüneis, J.J. Shepherd

302. Effect of temperature on the potential energy surfaces of homonuclear diatomics. **H.R. Petras**, W.Z. Van Benschoten, J.J. Shepherd

303. Microwave synthesis of metal oxides for water splitting applications. **C. Allison**, **A. Gupta**, **M. Ellis**, **A. Jones**, W. Lin, **R.K. Gupta**, T. Dawsey

304. Development and analysis of ringdown-free T1 relaxation methods. **Z. Mayes**, K.H. Woelk

305. Electrochemical synthesis of cobalt nickel phosphides for high-performance energy storage devices. **Y. Ma**, **W. Lin**, R.K. Gupta

306. Using the structure factor to investigate the Wigner crystallization in a finite three-dimensional electron gas. W. Van Benschoten, **T. DeMello**, T. Mihm, J.J. Shepherd

307. Analysis of the a $4\pi\tau - x$ 4σ - electronic transition of molybdenum nitride (MoN). **N. Woods**, L.C. O'Brien, K. Bales, G. Hotz, S. Tadakamalla, J.J. Obrien

FRIDAY AFTERNOON

Graduate Iowa City
Wayne Ballroom A

Undergraduate Research

R. Harrison, J. A. Schmidt-McCormack, *Organizers*

1:00 - 2:45

314. Assessing substituent position of indole-substituted tryptophan derivatives for designing LAT1 inhibitors. **J. Bohlke**, C. Clausen, D.B. Silva, K. Hutchinson, A. Schlessinger, A.A. Thomas

315. Synthesis and activity of carboxylic acid bioisosteres to probe the CoA binding site of serotonin N-acetyltransferase. **K. Lytle**, **J. Bohlke**, M. Hill, N. Fancher, M. Moxley, A.A. Thomas

- 316.** Progress towards a novel protecting-group-free total synthesis of (–)-Quinine: Construction of the quinuclidine moiety. **H.D. Nguyen, Y. Fu, K.A. Robb**
- 317.** Rhodanine-indolinone carboxylic acids as inhibitors of serotonin N-acetyltransferase. **M. Hill, N. Fancher, M. Moxley, A.A. Thomas**
- 318.** Interactions of hydrogen gas with Cu-ZnO/Al₂O₃ catalysts used in industrial methanol synthesis. **H. Bahn, K. Lai, Z. Mayes, K.H. Woelk**
- 319.** Comparison of multiple neural network methods to recognize active SRp40 ESE motif candidates. **K. Kammerer, T. Law, S. Svojanovsky**
- 320.** Synthesis of novel amine-containing oxazolidinone antibiotics. **B. Thomas, J.T. Ippoliti**
- 321.** Acid-labile polymersomes for nanoscale cancer drug delivery systems. **L.J. Hankins, J.A. Queenan, L.E. Prevette**
- 322.** Catalytic generation of cyclobutanes in the solid state: Facile access to TPCBs using mechanochemistry.. K. Putnam, **C.J. Hartwick, L. MacGillivray**
- 323.** Protein engineering of a fluorescent watermelon malate dehydrogenase. **W. Yu, S.J. Hoversten, M. Fiereck, L. Gentile**
- 324.** Synthesis of organic linkers for metal-organic frameworks (MOFs). **C. Friederichs, J.T. Ippoliti**
- 325.** Cobalt-mediated lactonization using visible light. **S. Patterson**
- 326.** Bacterial growth and gene expression in the presence of glmS riboswitch analogs. **K. Timboe, A. Van Cleave, C. Weber, J. Strauss Soukup**
- 327.** Cucurbituril synthesis: Effect of experimental conditions and additives on the reaction characteristics. P. Puntambekar, A. Birthi, **M. Pattabiraman**
- 328.** Identifying SARS-CoV-2 Inhibitors in the ORF8 Protein. **S. Chiu, M. Nguyen, L. Gentile**
- 329.** Synthesis of 7-hydroxy-4-methylcoumarin via the Pechmann condensation reaction using alumina sulfuric acid catalyst. **M. Hall, J.A. Morrill**
- 330.** Preventing rearrangement of antimicrobial ether-containing 1,3,4-trisubstituted-1,2,3-triazolium salts. **D.R. Brown, J.T. Fletcher**

331. Syntheses and crystal structures of novel lanthanide phosphites utilizing organic templating cations. **K. Huisman**, E.M. Villa

332. Toward optimization of additive compositions for cell-free protein synthesis. **J.D. Linhardt**, K. Yoshimatsu

333. Investigation of the efficiencies of cell-free protein systems through use of fluorescent biomolecules. **L.G. Spillman**, K. Yoshimatsu

334. Studying the behavior of recast Nafion® film modified electrodes in various nonaqueous systems using cyclic voltammetry and rotating disk voltammetry. **A.F. Claire**, D. Lehto, P.A. Zacher, K.L. Knoche Gupta

335. Characterization and structural analysis of lactate dehydrogenase: Model for protein structure study. **A. Bajracharya**

336. Comparing the bioelectrochemical activity of methanol dehydrogenases from lanthanum-grown versus calcium-grown *Methylobacterium extorquens*. **M.M. Weiss**, **B.H. Shoberg**, **R.M. Boese**, M.H. Ibrahim, K.L. Knoche Gupta

337. Withdrawn

338. Imaging and analysis of the gallium beating heart oscillating reaction using machine learning. **M. Ramsay**, Y. Guo

339. Characterizing the role of the cell wall in bacterial death caused by treatment with antimicrobial peptides. **K. Lutz**, **A. Schurr**, C. Volle

340. Structural and functional analysis of *Crassostrea gigas* OAZ-PK RNA. **R. McCracken**, S. Thompson, S. Venkatraman, J. Strauss Soukup

341. Solid state synthesis optimization: forming extended uranyl solid materials via mild temperature flux reactions. **H.N. Lightfoot**

342. Online preconcentration and electrophoretic separation of adenine nucleotides using capillary electrophoresis with UV detection. **R. Stegmaier**, G. Bulgakova, S.M. Lunte

343. Mesoporous silica nanoparticles for targeted anticancer drug delivery. **L. Lang**, N. Wellala Wijewantha, G. Sereda

344. Characterization of fractionated natural organic matter used to modify polyethersulfone ultrafiltration membranes. **J. DeLair**, **J. Radtke**

- 345.** Synthetic efforts towards the natural product Lagunamide C. **K. Wildeman, S. Perera, R. Rafferty**
- 346.** Revisiting Benoxacor: Photolysis transformation product validation and new pathway identification. **J. Hoffman, M.E. McFadden, K.P. Reber, J.D. Sivey, D.M. Cwiertny**
- 347.** Polyamine specificity and polyamine-induced conformational changes in human OAZ RNA. **J. Lemke, D. Gomez, S. Venkatraman, R. McCracken, S. Thompson, J. Strauss Soukup**
- 348.** Computational study of small molecules with open and closed states of human STING: Effects on protein conformations and binding free energies. **H. Gates, R.T. Payne, S. Crivelli, M. Watanabe**
- 349.** Hydrogen atom transfer and oxygen activation in polyoxovanadate-alkoxide clusters. **S. Schulz, P. Miro**
- 350.** Stability studies using UV-Visible spectroscopy on neutral and charged TEMPO. **T. Liu, R. Ordikhani Seyedlar, S.K. Shaw**
- 351.** Reactivity of Mn(III)-hydroxo complexes with phenols. **B. Nguyen, P. Singh, T.A. Jackson**
- 352.** Synthesis of aspirin using a Lewis acid. **A. Primrose, L. Baker**
- 353.** Exploring and characterizing the sensitivity of *Bdellovibrio bacteriovorus* against different physiological stressors. **R. Zurick, J. Azenon, C. Volle**
- 354.** Design and development of an affinity proteomics workflow for the discovery of novel cytosine epigenetic readers in non-small cell lung cancer. **J.E. Gann, A. Rajcewski, F. Rodriguez, A. Rahim, N.Y. Tretyakova**
- 355.** Throughout comparison of data independent acquisition processing tools for LC-MS/MS proteomic analyses using an open-sourced HeLa proteomics data set. **D. Kobuzi**
- 356.** Synthesis and characterization of pyrylium dyes for light-driven catalysis. **N. Hayes**

Graduate Iowa City
Wayne Ballroom B

Advances in Crystal Engineering and Solid-State Supramolecular Chemistry

T. Friscic, K. M. Hutchins, *Organizers*
S. Kruse, *Presiding*

1:30 . Stabilization via delocalization: Crystal engineering aromatic organic small molecules for radiation resistant materials. **S. Kruse**, T. Forbes, L. MacGillivray

1:50 358. Cheap porous molecular solids applied to complex chemical separations problems. **K.T. Holman**, P.N. Pandey

2:20 359. Effect of dimensionality on thermal expansion behaviors of cocrystals of carboxylic acids and bipyridines consisting of motion-capable groups. **N. Juneja**, D. Unruh, K.M. Hutchins

2:40 360. Understanding mechanism of direct air capture in metal-organic supercontainers. **L. Spencer**, Z. Wang

3:00 Break.

3:20 361. Unraveling supramolecular features and morphologies of elastic single-crystal electronics. **G. Campillo-Alvarado**

3:50 362. A “Baking powder” for olefination: A halogen-bonded phosphonium salt cage encapsulates and derivatizes small-molecule carbonyl compounds. **J.M. Marrett**, H.M. Titi, T. Friscic

4:10 363. Data science applied to crystal engineering. **A. Sokolov**

4:30 Closing remarks.

Graduate Iowa City
Benson Room B

Chemistry Research at Primarily Undergraduate Institutions-Session 3

N. B. Bowden, M. T. Wentzel, *Organizers*
J. W. Wackerly, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 364. Developing a research-based capstone project for organic chemistry lab. **B. Woods**, C.S. Bagwill

1:55 365. Development of a discovery-based, sophomore-level organic chemistry laboratory experiment exploring the factors that influence the position of substitution in electrophilic aromatic substitution reactions. **S. Stoffregen**, K.P. Peterson, J. Hassing, C. Wizceb, M.P. Maddox, K.E. Norris, A. Hunt

2:15 366. Syntheses of homoallylic allene-containing alcohols by sequential 1,2 – 1,4 hydride additions. **M.R. Hulce**

2:35 Discussion Panel.

2:50 Break.

3:05 367. Development of catalysts for sustainable polymer labs leading to a new collaboration. **M.T. Wentzel**, E. Chapman, J.E. Wissinger

3:25 368. Easier, better, faster, stronger: Collaborating across PUIs for organic chemistry research. **M.T. Wentzel**, **S. Zingales**

3:45 369. A bite-sized approach to medicinal chemistry research at PUIs: Small, directed mini-projects can build to a larger research question. **S. Zingales**

4:05 370. Research for the Common Good: Can we trust lead-free marketing for tableware?. **S. Steigner**, Q. Zhang

4:05 Discussion Panel.

4:20 Closing Remarks.

Graduate Iowa City
Benson Room A

Computational Methods and Applications

P. Miro, B. Vlasisavljević, *Organizers*
M. Momenitaheri, *Presiding*

1:30 Opening remarks.

1:35 371. Adsorption of organic redox-active molecules to the Ag(111) surface. **A.K. Sweet**, S.E. Mason

1:55 372. Crystal features governing oxygen vacancy formation in ABO₃ perovskites. **R.B. Wexler**, G.S. Gautam, E.B. Stechel, E.A. Carter

2:15 373. Molecular level insights on nanoporous materials in condensed phases from atomistic molecular dynamics simulations. **M. Momenitaheri**

2:35 374. Quantitative predictions of experimental behavior of materials for renewable energy applications. **A.V. Mironenko**

2:55 Break.

3:15 375. Non-unitary operators and state preparation on quantum computers using the singular value decomposition. **A. Schlimgen**, K. Head-Marsden

3:35 376. Quantum algorithms for open quantum system dynamics. **K. Head-Marsden**

3:55 377. CASPT2 molecular geometries for transition metal complexes. **B. Vlasisavljević**

4:15 . Nucleation mechanism and redox profiles of functionalized polyoxovanadate-alkoxides clusters. **P. Miro**

Graduate Iowa City
Wayne Ballroom C

Organic Chemistry

C. K. Arnatt, D. Martin, *Organizers*

1:30 379. An unusual Diels–Alder reaction. **S.R. Hussaini**

1:50 380. Nickel-catalyzed formation of α -substituted γ -amino ketones via alkene carboacylation. **A. Moore**, L.M. Stanley

2:10 381. N-Heterocyclic carbene–carbodiimide (NHC-CDI) adducts for latent organocatalysis. **D. Pham**, R.O. Smith-Sweetser, C.E. Dewey, J.R. Lamb

2:30 382. Synthesis of oxaboranes via nickel-catalyzed dearylativative cyclocondensation. **M.T. Koeritz**, H.K. Banovetz, S.A. Prell, L.M. Stanley

2:50 Break.

3:10 383. Structure-based design of bisubstrate tetracycline destructase inhibitors that block flavin redox cycling. **E.E. Williford**, C.M. DeAngelo, K.S. Blake, H. Kumar, K. Lam, K.V. Jones, N. Tolia, G. Dantas, T.A. Wencewicz

3:30 384. Ni(cod)(duroquinone)-catalyzed C-N cross-coupling for the synthesis of N,N-diarylsulfonamides. **T. You**, J. Li

3:50 385. Catalytic enantioselective synthesis of planar chiral macrocycles. **S. Wei**, J. Li

4:10 386. [TMS]FeCl₄ Catalyzed Carbonyl Olefin Metathesis. S. Todtz, **C. Schneider**, C. Anderson

4:30 387. New strategies for photocatalytic metal-catalyzed carbonylation and cyclization. **I. Owolabi**

Graduate Iowa City
Benson Room C

Physical Chemistry

A. Bhattacharjee, A. V. Tivanski, *Organizers, Presiding*

1:30 Opening Remarks.

1:35 388. Modeling the polarized absorption spectra of n-alkyl anilino squaraine thin films: Highlighting the role of intermolecular charge-transfer. **N. Hestand**

1:55 389. Molecular geometries of Mn(III) complexes by multireference methods. **S. Roy Chowdhury**

2:15 390. Computed magnetic properties of lanthanides. **A. Garcia Alejo**

2:35 Break.

2:55 391. Photodissociation of the N₂-NO Complex. **B.F. Parsons**

3:15 392. Designing the designer solvent: investigating structural phase behavior of binary imidazolium-based ionic liquid molecular cosolvent mixtures. **C.B. Lasar**, M.L. Cousineau, K.J. Gudenkauf, D. Duffy, B.J. Bellott, S.K. Shaw

3:35 393. Selective oxidation of alkene in oxygen by hollow Mn₃O₄ nanoparticles. **P. Nandy**, J.D. Hoefelmeyer

3:55 394. Modifying the cooperative effect of composites [Fe(Htrz)₂(trz)](BF₄) plus polyaniline through iron magnetite addition. **W. Chin**

Graduate Iowa City
Wayne Ballroom D

Sustaining Scientific Glassblowing and Chemistry

B. Revis, *Organizer, Presiding*

1:00 Opening Welcome.

1:05 308. Supporting research at the University of Iowa: One hundred years. **B. Revis**

1:35 309. 3D printing glass. **J.F. Destino**

2:05 310. Understanding Glass "length" through its Chemical and Atomic Structure.
D. Sidebottom

2:35 311. Sustaining scientific glassblowing: Is scientific glassblowing at an end?. **B. Revis, K. Paris**

3:05 Pannel Q&A.

3:35 Break.

3:55 312. Glassblowing contributions to biomedical research and patient care at Mayo Clinic. **K. Bennet**

4:25 313. Celebrating the International Year of Glass and its future. **J. Kohl**

Graduate Iowa City
Wayne Ballroom A

Undergraduate Research 2

3:15 - 5:00

395. Groundwater cleanup by ferrous iron minerals. **V. Pardo, L. Chelsvig, D. Latta, M. Scherer**

- 396.** Lead sorption by syringe filters biases drinking water particulate lead measurements. **L. Zepeski**, D. Land, M. Scherer, D.M. Cwiertny, C. Meyer, D. Latta
- 397.** Analysis of heavy metals in sediment collected up and downstream along the Neosho River to Tri-state Mining District. **G. Slabaugh**, B. Preston, A.B. Edmonds, H. Schultz, Q. Zhang
- 398.** Heavy metal accumulation onto sediments in Northeast Iowa. **H. Cronin**, E. Pichelmann, M. Wilker, D. Pfeffer-Kleemann
- 399.** Controls on phosphorus capture in farm ponds: Does internal phosphorus loading limit efficacy of this BMP?. **T. Grindle**, A. Graham
- 400.** Geochemical controls on Hg biogeochemistry at Swamp White Oak (SWO), Eastern Iowa. **F. Getachew**, A. Graham
- 401.** Heavy metal uptake and nutrient composition in hydroponically grown *Lactuca sativa*. **N. Bauer**, **K. Sorenson**, C. Strong
- 402.** Controls on Hg methylation and demethylation rates in wetland sediments as inferred from enriched stable isotope tracer experiments. **A. Szlembarska**, A. Graham
- 403.** Direct air capture via metal-organic supercontainers. **Y. Huang**, H. Li, Z. Wang
- 404.** Determination and comparison of calcium, iron, and magnesium in romaine crops from differing agriculture method. **A. Auclair**
- 405.** GCMS study of lipid composition of fermenting bee bread and common pesticides. **J.J. Becher**, J.L. Duffy-Matzner
- 406.** Method development for the detection and comparison of potential trace level compounds in sources of the herbal supplement Epigallocatechin Gallate using HPLC. **A. Hash**, E. Price
- 407.** Exploration of Wisconsin endophytic species in search of new natural product antibiotic scaffolds. **S.P. Pardini**, **L.M. Shallow**, **C.N. Sylvain**, K.C. Garber
- 408.** Utilizing carbonized local corn husk as anodic material for sustainable batteries. **M. Moorer**, P.P. Bugayong
- 409.** Analysis of strontium content in leaves of *spinacia oleracea* via atomic absorption spectroscopy. **W. Henning**, J.N. Woodford

- 410.** Mössbauer analysis of the iron-sulfur cluster in the Fur protein from E. coli. **S.A. Elmi**, C. Fontenot, H. Ding, C.V. Popescu
- 411.** Biodegradable polymer-derived precision nanomedicine for targeted drug delivery and treatment of prostate cancer. **P. Worsley**, J. Beach, A. Worsley, C. Worsley, S. Santra
- 412.** Quantitative and qualitative analysis of microplastics of the west coast in Chilaw, Sri Lanka. **R. Wijeratne**, A. Jayasundera
- 413.** Analyzing STEM instructor classroom facilitation. **C.C. Lovig**, N.E. States, H.T. Nennig, R.S. Cole
- 414.** Exploring inclusion in undergraduate chemistry for students with a broad spectrum of interests. **S.J. Hoversten**, L. Gentile
- 415.** Characterization of uranyl salts under UV light in alcohol systems. **E.S. Belzer**, D. Kravchuk, T. Forbes
- 416.** What can we learn by adding an artificial band gap to a model metal?. **K. Boyler**, T. Mihm, J.J. Shepherd
- 417.** Density functional theory calculation of barrier heights of bipentacene scaffolded molecules: Understanding singlet fission. **S. Thor**
- 418.** Increasing recyclability of polyethylene terephthalate. **L. Burton**, D. Dileep, M.J. Forrester, E.W. Cochran
- 419.** Exploring the uses of heterogeneous frustrated Lewis pairs. **N.R. Loutsch**, A. Castillo, J.D. Hoefelmeyer
- 420.** Mössbauer analysis of the iron-containing IscA protein from E. coli. **J.C. Tran**, C. Fontenot, H. Ding, C.V. Popescu
- 421.** Computational study of gas-phase ozonolysis of alpha- and beta-pinene. **T. Olguin**, **L. Rolands**, S. Stoffregen
- 422.** Syntheses and structures of mix-metal sulfites: The facile linking of hard and soft metals via sulfite. **W. Swenson**, E.M. Villa
- 423.** Electrochemically assisted deposition of ZIF-8 nanofilms on insulator substrates. **S. Jenkins**, T. Ito

- 424.** Development of inorganic cores for HA/CS layer-by-layer microcapsules for incorporation onto contact lenses. **J. Sanderson, S.A. Knutson, E. Bates,** Z. Schulte, J.L. Duffy-Matzner
- 425.** Studies of zingerone incorporated HA/CS layer-by-layer treated contact lenses. **E. Bates,** J.L. Duffy-Matzner, J. Sanderson, S.A. Knutson
- 426.** Synthesis and characterization of new metal-organic supercontainers for potential anion binding. **A. Thomas,** K. Chitrakar, Z. Wang
- 427.** Lanthanide complexes of tridentate 2,6-bis(1-benzyl-1,2,3-triazol-4-yl)pyrazine. **M.N. Meyer,** J.T. Fletcher
- 428.** One step synthesis of cobalt and iron-based highly efficient electrocatalyst. **H. Reynolds, S. Grana,** W. Lin, R.K. Gupta
- 429.** Colorimetric analysis of lead ions (Pb²⁺) using modified gold nanoparticles. **M. Bhatta,** B. Davies, S.M. Adem
- 430.** Characterization of uranyl salts under ultraviolet light in alcohol systems. **E.S. Belzer,** D. Kravchuk, T. Forbes
- 431.** Understanding HCO₃⁻ binding in metal-organic supercontainers for direct air capture. **Z. Burmood,** L. Spencer, Z. Wang
- 432.** Binding of metal centers to redox-active camphor ligands. **M. Fiori,** J.F. Dunne
- 433.** Single molecule detection using a sandwich assay with quantum dots. **R. Schon,** A.M. Keller
- 434.** Computational study of a naphthaquinone mechanism. F. Burnett, **A.N. Garr**
- 435.** Ruthenium complexes and their applications towards Dye-Sensitized Solar Cells (DSSCs). **B. Brekke,** A. Hussain, K. Mariappan, A.G. Sykes
- 436.** Perturbative corrections for connected triple excitations in multicomponent coupled cluster theory. **D. Fowler,** K. Brorsen
- 437.** Synthesizing and characterizing graphene-based quantum dots for bioimaging applications. **A. Dhimal,** H. Nguyen

438. Development of nano-PDLCs with low haze. **M. Redding**, M. Mostafa, A. Jakli, J. West