CERM 2023 Program Schedule

June 20-23, 2023

Program Chair Daniel Lawson

WEDNESDAY MORNING

S1. Salon I

Circular Economy for Plastics: Challenges and Opportunities

M. Bouguettaya, L. Wang, *Organizers, Presiding*

8:30 Introductory Remarks.

8:40 1. Enabling novel circular economy processes utilizing mass balance in chemical processes. **T. McKay**

9:10 2. Microscopy supports on circular economy in BASF North America. **K. Fa**

9:40 Break.

9:50 3. Evolving industrial analytics for the plastics circular economy. **J. Hankett**

10:20 4. Circular upcycling approach to sustainable silicone polymers. **J.C. Furgal**, K.D. Edirisinghe, H. Espitia Armenta, E. Chandler, C.B. Sims, B. Rupasinghe

S2. Salon II

Education in Chemistry

D. N. Maxwell, *Organizer, Presiding*

8:30 Opening Remarks.

8:35 5. Sense of belonging of students from historically excluded groups in general chemistry courses. **N.M. Karn**, J. Collins, L. Medvedovic, M. Berhe, S. Ogrin-Cotarlan

8:55 6. Implementation of a vertical and interdisciplinary curriculum-based research experience in organic chemistry courses. **M. Abdel Latif**, **M. Livezey**, **S. Scribner**, E. Geragosian, M. Yousif, C. Profley

9:15 7. Navigating the hidden curriculum of academia: Critical approach to understanding the racial and science identity formation of Latine undergraduate students. **D.N. Maxwell**, J.L. Rivera-Colon, K. Hosbein, P. Vincent-Ruz, G.V. Szymczak Shultz

9:35 Intermission.

9:50 8. Student perspectives to transform the general chemistry learning environment at predominantly white institutions. **J. Collins**, N.M. Karn, M. Berhe, S. Ogrin-Cotarlan, L. Medvedovic

10:10 9. Utilizing student-generated Mathematica demonstrations in general chemistry courses. **H.P. Hendrickson**, T. Chua, V. Venkatesh, T. Addy

10:30 10. Utilizing the 'Student Interaction Discourse Moves' (SIDM) framework to characterize student discourse in a chemistry POGIL session. **A. Harrold**, D.N. Maxwell

S3. Salon V

Expanding Green Chemistry in the Undergraduate Curriculum and Research Experiences

N. Kingsley, J. L. Tischler, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 11. Development and assessing the impact of student-generated videos, infographics, and open education resources related to sustainability and green chemistry. **A. Leontyev**, K.D. Grieger

8:55 12. Undergraduate research and green chemistry: Exploring applications within analytical chemistry. **M.J. Fhaner**

9:15 13. Using environmental justice to explore scientific ethics, chemical literature, and presentation skills in a seminar course. **J.L. Tischler**

9:35 Break.

9:45 14. What do our students need to know about green and sustainable chemistry? Panel discussion with industrial chemists. **J.L. Tischler**

10:05 15. Seed to oil, bench and beyond: Medicinal and aromatic plant course. **m.A. Benore**, S. Marincean

10:25 30-minute panel discussion.

S4. Salon VI

f-Block Extravaganza: The Best Symposium at CERM

M. Rashid, S. White, *Organizers, Presiding*

8:30 Opening Remarks.

8:40 16. Controlling the kinetics of oxidation of Eu^{II} relevant to imaging hypoxia in vivo with magnetic resonance imaging. M. Rashid, A. Batchev, M. Samee, R. Pautler, **M.J. Allen**

9:05 17. Investigating the influence of alkyl substituents on the ability of β-carbonylphopshine oxide compounds to sensitize lanthanide luminescence. **S.M. Biros**

9:30 18. Density functional study of binding mechanism of rare-earth elements with Bis(ethylhexyl)amido diethylenetriaminepentaacetic acid. **T. Quainoo**, Z. Liu

9:55 Break.

10:05 19. MR responsive and theranostic probes: Where are we headed?. **T.J. Meade**

S5. Salon VII

Materials and Surface Chemistry

D. B. Lawson, *Organizer, Presiding*

8:30 20. Do functional coatings work for solar panel dust mitigation?. **T.T. Isimjan**, D. West

8:50 21. Laser-induced graphene interdigitated electrodes modified with gold nanoparticles for non-faradaic impedimetric detection of cortisol. **K. Duke**, P. Dhungana, K. Preusser, B. Park

9:10 22. Ligand-associated adsorbents for selective recovery/extraction of rare-earth elements: Role of solid supports. **S. Praneeth**, P. Roy, M. Dardona, A. Sakr, C. Tummala, M.J. Allen, T.M. Dittrich

9:30 Break.

9:45 23. Self-assembly controlled at the level of individual functional groups. **B. Heiner**, S. Kandel, A.M. Pittsford

10:05 24. Iron-coated waste nutshells to recycle the lost phosphate and its potential application as a slow-release fertilizer for agriculture. **C. Tummala**, S.K. Mohanty, T.M. Dittrich

10:25 25. STM investigations into the role of chirality on molecular self-assembly. **A. Pittsford**, B.R. Heiner, A.L. Walter, K. Handy, J. Soucek

S6. Salon III

Organic -- Cosponsored by ORGN

D. B. Lawson, *Organizer, Presiding*

8:30 26. Macrocyclic resorcinarene salts as sensors for bioanalytes. **N.K. Beyeh**

8:50 27. Formal cross-coupling of amines and carboxylic acids to form sp3–sp2 carbon–carbon bonds. **J.L. Douthwaite**, R. Zhao, E. Shim, B.A. Mahjour, P.M. Zimmerman, T. Cernak

9:10 28. Carbenes and carbazoles: Elucidating solution-state behavior with non-traditional hydrogen bonding. **Z. Kinney**

9:30 Break.

9:40 29. New developments in interrupted carbonyl-olefin metathesis reactions. **S. Burns**

10:00 30. Kinetics of chlorine reactions with RNA: A step toward predicting viral inactivation during water treatment. **A. Szczuka**

10:20 31. Alkene aminoarylation via N-centered radical reactivity of sulfinamides. **M. Glossbrenner**

WEDNESDAY AFTERNOON

S7. Salon V

DEI Initiatives Including Social Media Usage in Industry and Academia: TikTok and Tweet Your Way to a Diverse Workforce

S. P. Hickey, *Organizer, Presiding*

2:00 Introductory Remarks.

2:05 32. Chemists with disabilities and inclusion: ACS efforts and resources. **J. Landis**

2:30 33. Investing in the bigger picture: Importance of incorporating diversity, equity, and inclusion into research. **B. Simms**

2:55 Break.

3:05 34. Understanding diversity, equity, and inclusion in chemistry through National Diversity Equity Workshops (NDEWs). **V. Chandra Saman**

3:30 35. Fostering diversity, equity, inclusion, and respect across the chemistry enterprise. **R. Joseph**

S8. Salon II

Education in Chemistry

D. N. Maxwell, *Organizer, Presiding*

2:00 36. Identifying the relevance of organic chemistry through writing. **S. Milne**, S. Finkenstaedt-Quinn, N. Garza, S.C. Zimmerman, G.V. Szymczak Shultz

2:20 37. Polymer and organometallic systems thinking activities for second semester organic chemistry. **A. Anderson-Wile**, S. Madsen

2:40 Break.

2:50 38. Eliciting student understanding of the relationship between energy and interactions in the context of effects of solvation in organic reactions by engaging them in causal mechanistic reasoning. **K. Seth**, E.L. Day, M. Cooper

3:10 39. Case study on post-secondary chemistry instructors' resources for planning instruction. **R. Fantone**, G.V. Szymczak Shultz

3:30 40. Analysis of silylated polyphenols found in banana peels. **B. Miburo**

3:50 Break.

4:00 41. Investigating how organic chemistry faculty structure their knowledge and their beliefs about student learning. **S. Abeywardana**, M. Cooper

4:20 42. Analysis of the ashes of the peels of bananas grown in South Georgia. **B. Miburo**

S9. Salon VI

f-Block Extravaganza: The Best Symposium at CERM

M. Rashid, S. White, *Organizers, Presiding*

2:00 43. Ligand-Associated Sorbents and Extraction Systems for Rare-Earth Element Recovery from Coal Fly Ash. **T. Dittrich**

2:25 44. Employing radicals and bismuth in lanthanide single-molecule magnet design. **S. Demir**

2:50 45. Cadmium Schiff base complexes that glow: Unexpected structures and room temp phosphorescence. M. Deal, M. Zeller, **E.R. Trivedi**

3:15 Break.

3:25 46. Coordination chemistry studies for ion flotation to selectively remove nickel(II) and cobalt(III) using amine-based ligands. **E. Mwakazi**

3:50 47. Multi-electron redox chemistry with thorium(IV) iminoquinone complexes. **S.C. Bart**

S10. Salon VII

Materials and Surface Chemistry

D. B. Lawson, *Organizer, Presiding*

2:00 48. Electropolymerization of organometallic cyclopentadienyl pyridazines for advanced electronics. V. Mattern Mondragon, **D.J. Little**, N.C. Tice, S.T. King

2:20 49. Morphology-controlled vapor-phase nanowire growth with Ruddlesden-Popper Lead Bromide Perovskite. **P. Yadav**, K. Moon, A. Biswas, S. Kim

2:40 50. Ultrafast excited-state interactions between carbon dots and luminescent materials. **S. Saha**

3:00 Break.

3:15 51. CdS ultrasmall quantum dots: Synthesis and gelation kinetics. **I. Ahmed**, V. Alevato Neves, S.L. Brock

3:35 52. Photoluminescence enhancement of quantum-sized gold nanoclusters by Chemiluminescence-resonance-energy-transfer. **S. Saxena**, A. Alharbi, R. Guda

S11. Salon III

Organic

D. B. Lawson, *Organizer, Presiding*

2:00 53. Riboflavin binding protein: Vitamin interactions in the binding pocket. **S. Marincean**, D. Nichols, M. Benore

2:20 54. Reliable C-3 substitution in pentadiynyl Nicholas reactions and the preparation of dichlorodimethoxy analogues of hinokiresinol and nyasol. **B. St. Onge**, M. Muresan, J.R. Green

2:40 Break.

2:55 55. New developments in visible light-mediated aza Paternò-Büchi reactions. **S. Parikh**

3:15 56. Photo and catalytic desulfurizations: Application to organic molecules, peptides and proteins. **V. Naresh Murty**, G. Samala, R. Morsy, L. Mendoza, J.L. Stockdill

3:35 57. Investigating coupling reagents for the synthesis of ferrocene hybrids from ferrocenecarboxylic acid in organic laboratories. **M. Abdel Latif**, **S. Scribner**, **M. Livezey**, **E. Geragosian**

P1. Salon IV

Physical/Inorganic & Biochemistry Poster Session

D. B. Lawson, *Organizer, Presiding*

4:00 - 6:00

58. Effect of PRIMA-1^{MET} and vitamin D on triple negative breast cancer cell lines. **S. Kotob**, **A. Savoie**, **J. Kelts**

59. Characterization of an exact electron correlation symmetry in AHCs using MO Theory at the single CI level of approximation. **C.A. Farwick**, M. Masthay

60. Photo-responsive Cr(III)-supramolecular siloxane polymers with self-healing potential. **H. Espitia Armenta**, J.C. Furgal

61. Single-molecule human nucleosome spontaneously ruptures under the stress of compressive force: New perspective on gene stability and epigenetic pathways. **l. shahu**

62. Synthesis and characterization of cadmium valen complexes with tunable room temperature phosphorescence. M. Deal, M. Zeller, **E.R. Trivedi**

63. CO_2 deprivation and oxidative stress delay the production of cyanophages and lysis of infected cyanobacteria. **S. Badshah**

64. Modulation of multiple signaling pathways by spinosyn A induces anti-tumorigenic effects on ERα-positive breast cancer cells sensitive to progesterone: Evidence from RNA sequencing analysis. B. Xhabija, **A. Kaniski**, D. Matti

65. Targeting multiple signaling pathways, baicalein suppresses tumorigenesis in ERα-positive breast cancer cells. B. Xhabija, **A.J. McLaughlin**, **E. Ujeniuc**

66. Disrupting bacterial homeostasis: Stealth manganese carrier for killing multidrug-resistant *Staphylococcus aureus*. **K. Mudarmah**, S. Huang

67. Chemical tools to identify substrate motifs of a kinase enzyme for characterization of cell signaling. **H. Bremer**, M. Pflum

68. Application of nanosecond excitation in light-induced cellular processes. **J. Leone**

69. Investigating novel structural and functional binding interactions of UHRF2 with H3. **J.R. Kean**, R.C. Trievel, B. Albaugh

70. Use of entangled two photon microscopy for imaging of brain tissue. **P.R. Johnson**, O. Varnavski, T. Liu, C. Fields, D. Pal, G. Mashour, T.G. Goodson

71. Cellular investigation of UHRF1 interactions with a novel histone modification. **P. Khuansanguan**

72. $Cu_xFe_yP_z$ nanoparticles synthesis and characterization for overall water splitting reaction. **F. Sultana**

73. *Cannabis sativa* may play a role in the phytoremediation of PFAS: Hemp seedlings can take up PFAS from a hydroponic solution and from soil. **E.F. Wells**, **K. Schick**, D. Dotson, L.J. Putman

74. Investigating the ground and several excited states of late 3D and 4D transition metals through multireference calculations. **M. Khorrami**, N. Almeida, A.K. Wilson

75. Characterizing the energy levels of early 3d and 4d transition metals by multireference techniques. **E.M. Telb**, N. Almeida, A.K. Wilson

76. Effect of PFAS on proteins: Computational investigation. **R. Massoud**

77. Making and adjusting Galinstan in the teaching laboratory: An example of some fascinating, low-melting alloys. P. Lee, A. Fei, M. Golden, H. Obeid, H. Rice, L. Romeo, M. Yousef, O. Ammoun, J. Jakubczak, **M.A. Benvenuto**

78. Boiling and freezing point adjustment experiments for the general chemistry laboratory: Elevating the boiling point and depressing the freezing point of water to extremes, using high molality salt solutions. **B. Gheorghila**, Z. Arrington, K. Yeldo, S. Arment, J. Crandall, L. Jeki, P. Anton, C. Cole, G. Crocker, J. Kusiak, E. Rihacek, C. Spitzer, C. Tayler, O. Ammoun, J. Jakubczak, N. Ka, M.A. Benvenuto

79. Regulation of the amyloid precursor protein (APP) by acetylcholinesterase and brain-derived neurotrophic factor in lung cancer cells. **H. Al khashali**, R. Ray, K. Coleman, B. Haddad, B. Darweesh, J. Guthrie, D. Heyl-Clegg, H. Evans

80. Modeling the elusive element astatine. **V. Casetti**, J. MacLean, A. Rusakov

81. Exploring the signaling pathways involved in controlling the levels of soluble Amyloid Precursor Protein α (sAPPα) levels in lung cancer cell culture media. H. Al khashali, R. Ray, **K.E. Coleman**, B. Haddad, **B. Darweesh**, J. Guthrie, D. Heyl-Clegg, H. Evans

82. Exploring the magnetic properties of coupled di-blatter radicals. **G. Flores**, D.B. Lawson, C.P. Constantinides

83. Design and synthesis of the lanthanide-based host-guest systems. **M. Boraghi**

84. Effects of mutated DBD2 on BRCA1 function. **V. Salib**, C. Wu, K. Lowran

85. BioBricks® platform for engineering of diverse anthracyclinone core scaffolds. **N.E. Schwartz**, J. Hecht, E. Nybo

86. Theoretical interpretations of ESi-MS experiments of melamine and cyanuric acid. **K.M. Handy**, A.L. Walter, B. Heiner, S. Kandel

87. ESI investigation of melamine and cyanuric acid for future pulse-deposited STM studies. **A.L. Walter**, K.M. Handy, J. Soucek, A.M. Pittsford, B. Heiner, S. Kandel

88. Study of electric fields in conductor and dielectric layers and surface plasmon resonances using theoretical calculation and computational simulations. **R. Kyung**, H. Jing

89. Establishing histone deacetylase 7 as an epigenetic reader. **I. Kodikara**, M. Pflum

90. Photoactivatable glycolipid probes for identifying outer membrane proteins in mycobacteria. **K. Biegas**, H.W. Kavunja, N. Banahene, B.M. Swarts

91. Targeting mycobacterial persistence: Trehalosamines inhibit the trehalose catalytic shift in *Mycobacterium tuberculosis*. **K. Kalera**, J. Lee, D.H. Swanson, U. Johnson, A. Stothard, A.W. Poston, H. Eoh, B.M. Swarts

92. Synthesis and study of frustrated magnet KHoSe2. **M. Boswell**, H. Wang, W. Xie

93. Synthesis and characterization of lipid-based cubosomes loaded with siRNA. **M.M. Hossain** , M. Bayachou

94. Synthesis of mycolic acid analogue for probing mycolic acid recycling pathways in mycobacteria. **A. Kruskamp**, K. Agu, N. Banahene, B.M. Swarts

95. Facile approach for preparing clickable platinum-based anticancer agents. **W. Jogadi**, Y. Zheng

96. Synthesis of carbonate-free nanojars by depolymerization of copper(II)-hydroxide/pyrazolate polymers. **P. Singh**, G. Mezei

97. Electron and energy transfer dynamics in 2D PbS nanomaterials. **A.J. Roach**

98. PFAS adsorption and transport in soils. **C.E. Schumm**, N. Loganathan, A.K. Wilson

99. Metal hydride hydrogen compression. **K. Karkare**

100. Investigation of the impact of PFAS on nuclear receptors via computational methods. **D. James**, N. Almeida, S. Bali, C. Wang, A.K. Wilson

101. Studies of bacillithiol transferases: Enzymes involved in cellular detoxification in gram-positive organisms. **M. Buchman**, P.D. Cook

102. Purification and structural analysis of UHRF2 bound to H3K9me3. **W. Jones**

103. Coumarin-functionalized near infrared emitting metallacrowns for red-shifted excitation. **T. Lathion**, S. Eliseeva, M. Zeller, S. Petoud, V.L. Pecoraro

104. Copper-mediated coupling of dodecaborates with phenols. **M.G. Pirie**, J.A. Dopke, R.J. Staples

105. Heck couplings of aldehydes with dodecaborates. **W.J. Kidder**, J.A. Dopke, R.J. Staples

106. Experimental and computational approach to redox mediator design: Exploring the role of molecular structure in controlling bioelectrocatalysis. **L. Mtemeri**

107. Synergistic effect of cocatalyst and S-scheme heterojunction over 2D/2D g-C_3N_4/MoS_2 heterostructure coupled Cu nanoparticles for selective photocatalytic CO_2 reduction to CO. **M. Al-Ghorbani**

108. Tri-cure hybrid organo-silicon coatings. **C.B. Sims**, C.U. Lenora, J.C. Furgal

109. Regulation of Cisplatin resistance in lung cancer cells by Nicotine, BDNF, and adrenaline. **R. Ray**, B. Haddad, H. Al Khashali, K. Coleman, J. Guthrie, D. Heyl-Clegg, H. Evans

THURSDAY MORNING

S12. Salon V

Biochemistry

I. Muqbil, *Organizer, Presiding*

8:30 110. Revving up a designed copper nitrite reductase using non-coded heterocycles. **W. Pitts**, A. Deb, J.E. Penner-Hahn, V.L. Pecoraro

8:50 111. Determination of tautomerase product profile via structural feature elucidation. **K. Silva**, A. Sirinimal, J. Geiger, K. Draths

9:10 112. Finding the perfect prodrug: Modifying platinum (IV) prodrug ligands to exploit cisplatin-resistant ovarian cancer mutations. **M. Cheline**, Y. Zheng

9:30 Break.

9:40 113. Chemical remodelling of the mycomembrane with chain-truncated lipids sensitizes mycobacteria to antibiotics. **I. Gaidhane**, K. Biegas, B. Swarts

10:00 114. Characterization of trehalose analogues' hydrolytic resistance and their potential use as inhibitors of trehalose utilization in microorganisms. **U. Johnson**, B. Swarts

10:20 115. Analysis of cell-surface associated biomolecules of *Pseudomonas aeruginosa* planktonic and biofilm cell subpopulations using MALDI-TOF MS. **C.N. Morse**, T.A. Dodson, N. Wamer, E.A. Carlson, J. Gadient, E.G. Prestwich

S13. Salon VI

Computational Chemistry from Electrons to Macromolecules

A. Walker, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 116. SlaterRKS method: Exchange correlation potential from slater FCI densities. **S. Tribedi**

8:55 117. Multiconfiguration pair-density functional theory beyond single-point calculations. **P.B. Calio**, M. Hermes, J. Bao, I.F. Galván, R. Lindh, D.G. Truhlar, L. Gagliardi

9:15 118. Developing novel adhesives for microplastic remediation: How composition and environment impact selectivity. **E.M. Jugovic**, P.M. Zimmerman

9:35 Break.

9:45 119. Monte Carlo framework for molecularly doped organic semiconductors. **A. Verma**, N. Jackson

10:05 120. Application of the semi-stochastic CC(*P*;*Q*) approach for electronic excitations in molecules and singlet–triplet gaps in biradicals. **A. Chakraborty**, S.H. Yuwono, J. Deustua, J. Shen, P. Piecuch

10:25 121. From atoms to proteins and quantum mechanics to molecular dynamics. **N. Almeida**, S.C. North, T. Melin, S. Bali, A.K. Wilson

S14. Salon II

Education in Chemistry

D. N. Maxwell, *Organizer, Presiding*

8:30 Opening Remarks.

8:35 122. Grading gets in the way of my students' learning: Alternative grading strategies. **M.J. Mio**

8:55 123. Storytelling in chemical education. **S.N. Collins**, M. Nelson, T. Steele

9:15 124. Investigating the use of ChatGPT with chemistry exam questions. **T.M. Clark**

9:35 Intermission.

9:50 125. Isolation of microplastics and student perceptions of their environmental footprint. **K. Hall**, A. Anderson-Wile

10:10 126. Organic chemistry students' engagement in mechanistic reasoning about the role of adenosine triphosphate (ATP) in reaction coupling. **C.G. Franovic**, **D. Losinski**, K. Noyes, M. Cooper

10:30 127. "Mostly I just copy what my chemist colleagues tell me": An investigation of molecular biology instructors' experiences teaching about adenosine triphosphate (ATP) and chemical bond energy. **C.G. Franovic**, K. Noyes, N.R. Williams, M. Klymkowsky, M. Cooper

S15. Salon III

Organic

D. B. Lawson, *Organizer, Presiding*

8:30 128. New developments in catalytic carbonyl-olefin metathesis. **T. McClure**

8:50 129. Photocaged R-alkoxysilanes for on-demand functionalization and polymerization control. **M.R. Rashed**, J.C. Furgal

9:10 Break.

9:20 130. Insights into the mechanism of Boyland-Sims oxidation reaction. **J. Joseph**

9:40 131. Acetylene dicarboxylic acid: C4 bridge between C1 feedstocks and commodity chemicals. B. Amaniampong, H. Nayebi Gavgani, A. Mathes Hewage, **K. Draths**

S16. Salon VII

Pharmaceutical Chemistry and Drug Discovery

S. C. Timmons, *Organizer, Presiding*

8:30 132. Crosslinked polyethylenimine: Novel drug delivery system for acidic drugs. **K.N. Kelsall**, L.M. Foroughi, D.S. Frank, L. Schenck, A. LaBuda, A.J. Matzger

8:50 133. Michigan drug discovery: Partnering a portfolio of projects. **P.L. Toogood**

9:10 134. Design, synthesis, and biological evaluation of PF543 analogs as two pore channel blockers. **A. Hamzah**, G.A. Soares, T.F. Walseth, K.A. Wall, J.T. Slama

9:30 Break.

9:45 135. Structure-based drug design of novel therapeutics against an inflammatory cytokine. **D.L. Warner**

10:05 136. Revealing weak sports in cancer viability through GLUT-targeting molecular probes. **M. Tanasova**

10:25 137. Dynamics and energetics of the transport cycle for small multidrug resistance transporters. **D. Sarkar**, J.L. Egleston, J.V. Vermaas

S17. Salon I

Sustainability in Automobiles: How Chemistry Is Enabling the Environmental Transition of An Industry

M. Bouguettaya, L. Wang, *Organizers, Presiding*

8:30 Opening Remarks.

8:35 138. Chemistry challenges in the automotive industry: OEM perspective. **M. Nichols**

9:20 139. Developing structural natural fiber parts using Spray Transfer Molding (STM) process for automotive applications. **E. Shakour**

9:50 Break.

10:00 140. Sustainable solutions for automotive OEM coatings. **K. Hartlieb**

10:30 141. Modeling solid electrolyte interphase formation and growth in Li-ion batteries using reactive molecular dynamics simulations. **A. Ojha**

THURSDAY AFTERNOON

S18. Salon VI

Computational Chemistry from Electrons to Macromolecules

A. Walker, *Organizer, Presiding*

2:00 142. Understanding PFAS toxicity through computational approaches. **S. Bali**, N. Almeida, D. James, C. Wang, R. Martin, K. Hall, A. Nair, A.K. Wilson

2:20 143. From the astatine's quantum chemistry to the development of new heavy-element computational infrastructure. **A. Rusakov**

2:40 144. Computational insights to sulfate sensing in mNeonGreen via flexible loop engineering. **V. Pathiranage**, K. Ji, W.S. Ong, S. Dodani, A. Walker

3:00 Break.

3:10 145. Computational insights into *minima remodeling* using myoglobin in organic solvents for pharmaceutical applications. **H. Palomino**, S. Liu, M.A. Hix, A. Walker, N. Lehnert

3:30 146. Potential energy curves and the singlet-triplet gap of cyclobutadiene: CIPSI-driven CC(*P*;*Q*) study. **S. Priyadarsini**, K. Gururangan, J. Shen, P. Piecuch

3:50 147. Advances in time-dependent spin-orbit configuration interaction: Spin-flip and pulse optimization. **B. Peyton**, A.K. Wilson

S19. Salon II

Education in Chemistry

D. N. Maxwell, *Organizer, Presiding*

2:00 148. How the analysis of publication practices during the Coronavirus pandemic informs teaching the information literacy in chemistry. **Y. Sevryugina**

2:20 149. Active learning in the general chemistry lab using the 5E Instructional Model. **J. Nagy**

2:40 150. Can the organic chemistry laboratory be green ? . **M. Zhang**, E.L. Day, S. Petritis, H. Mcfall-Boegeman, M. Cooper

3:00 Break.

3:10 151. Framing our teaching: Exploring graduate teaching assistants' enactment of a collaborative activity in an organic chemistry laboratory. **D. Haas**, I. Zaimi, G.V. Szymczak Shultz

3:30 152. Is scientific reproducibility a fallacy, a misunderstanding or sign of poorly designed experiments?. **A.L. Ekstrom**

3:50 Break.

4:00 153. Exploring how graduate teaching assistants enacted an active-, cooperative-learning activity in a second-semester organic chemistry course. **I. Zaimi**, D. Haas, G.V. Szymczak Shultz

4:20 154. Characterizing resources students use to understand chemical equilibrium via mathematical thinking and mechanistic reasoning. **V. Scammahorn**, M. Cooper

4:40 155. OrganicERs: Active learning workshops to build a community of practice for organic chemistry instructors. **A. Leontyev**

S20. Salon VII

Energy in Chemistry: Fuel Cells, Bioenergy and Energy Storage

I. Ahmad, *Organizer, Presiding*

2:00 156. Design of transition metal phosphide nanoparticles for energy conversion: Electrocatalytic water splitting. **S.L. Brock**

2:25 157. Additive carbon dots nanocrystals for enhancement of the efficiency of dye-sensitized solar cells in energy applications technology. **G.K. WATIRO**

2:50 Break.

3:00 158. Solubility trends in pyridinium salts for non-aqueous organic redox flow batteries. **S. Samaroo**, C. Hengesbach, C. Bruggeman, N.G. Carducci, L. Mtemeri, R.J. Staples, T.F. Guarr, D.P. Hickey

3:25 159. Fundamental insights to the motional narrowing of organic exciton polaritons. **S.T. Wanasinghe**, A. Rury

S21. Salon V

Paramagnetic Materials: Synthesis, Properties and Applications

P. Constantinides, *Organizer, Presiding*

S. R. Smith, *Presiding*

2:00 Introduction.

2:05 160. 1-(2-Ethoxyphenyl)-3-phenyl-1,4-dihydrobenzo[e][1,2,4]triazin-4-yl as a spin source in organic spintronic devices. **C.P. Constantinides**

2:25 161. Towards molecular alloys: Computational and experimental studies on *p*-NCC_6F_4CNEEN (E = S/Se). **A. Wehelie**, L. Watanabe, B. Zhang, S. Nikoo

2:45 162. Synthesis, characterization, and reactivity of paramagnetic (PNNP)Co complexes. **J. Miller**, C.M. Thomas

3:05 Break.

3:20 163. Synthesis and magnetic properties of large Fe^{III} based coordination clusters. **D.J. Cutler**, E.K. Brechin, J. Schnack, H. Nojiri

3:40 164. Exploring the cluster chemistry of pyridyl alkoxide ligands for the discovery of 3d/4f single molecule magnets. **G. Delle Monache**, M. Pilkington

4:00 165. Strong coupling and magnetic blocking in organometallic Lanthanide single-molecule magnets. **S. Demir**

S22. Salon I

Sustainability in Automobiles: How Chemistry Is Enabling the Environmental Transition of An Industry

M. Bouguettaya, L. Wang, *Organizers, Presiding*

2:00 166. Building sustainable cathode material production in North America and globally. **W. Mays**

2:30 167. Mitigating the hazards of battery thermal runaway events. **C. Gorin**

3:00 168. eMobility Material Analysis solutions Platform (e-MAP) in BASF. **Y. Zhang**

P2. Salon IV

Analytical/Organic Poster Session

D. B. Lawson, *Organizer, Presiding*

4:00 - 6:00

169. Considerations for developing a greener chromatographic method. B.A. Alden, K.D. Berthelette, K. Haynes, **N. Santiago**

170. Efficient synthesis of the *N*-Boc-Adda amino acid. **M. Yadab**, J.L. Stockdill

171. Towards a polyethylene terephthalate (PET) degradation scheme. **E. Grim**

172. Dimerization kinetics of NAD^+ biomimetics: Alternating current voltammetry as an analytical tool. **C. Bruggeman**, D.P. Hickey

173. Quinones as redox electrolytes in pH gradient flow batteries. **C. Jiang**, A.W. Lantz

174. 'Nitrogen effect': Complexation with macrocycles potentiates fused heterocycles to form halogen bonds in competitive solvents. **F.B. Osei**, K. Twum, S. Nadimi, R. Puttreddy, Y.B. Ojong, J.J. Hayward, K.T. Rissanen, J. Trant, N.K. Beyeh

175. Synthesis of a series of ligands, in the freshman chemistry laboratory, to be used as complexing agents. **A. Ivanciu**, G. Brown, M. Caruso, Y. Park, P. Bedi, R. Nistor, H. Song, M. Naddaf, N. Alkhareef, F. Abdulrahim, A. Al-Wakeel, A. Alduis, J. Fettohy, N. Kheirbek, F. Siddique, A. Mousaad, R. Hamo, R. Virk, E. Koneva, G. Mihalopoulos, Z. Shouman, R. Trotman, L. Jeki, J. Crandall, M.A. Benvenuto

176. Regioselective and functional divergent azidation of olefins for the preparation of biomolecular probes. **J. Truong**, **M. Huynh**

177. Synthesis of bisphenol A analogs for reproductive toxicity testing: A search for safer plastics. W.S. Shall, J. Clore, **S.C. Timmons**

178. Monitoring and quantitation of bacterial growth via capillary isotachophoresisi. **J. Gibbons**, A.W. Lantz

179. Pi-stacking interactions between lumiflavin, tryptophane and tyrosine via density functional theory. **M. Al-Modhafir**, D.B. Lawson, S. Marincean

180. Nuclear magnetic resonance spectroscopy as a tool for identification of varietal honey. **T. Mac**, J. Norris, G. Wilmes, M. Goodrich, **C.D. Emal**

181. Tracking bitterness units in beer throughout the brewing process using a streamlined spectroscopic method. **K. Kean**, **C.D. Emal**

182. Diaminoanthracene dicarboxylic acid as a bis-aryne building block for polycyclic hydrocarbon synthesis. **G. Rudebusch**

183. Self-assembly of pyridyl-coinage metallo-macrocycles: Synthesis and applications. **C. Goldsmith**, E. Adusei, Z. Kinney

184. Flavor component profiling of American whiskeys by direct analysis in real time mass spectrometry. H.A. Lindsay, R. Armitage, **J. Zhu**

185. Synthesis and examination of the influence of a fluorine atom at various positions in the tail of alkoxy cyanobiphenyl mesogens. **K. Agrahari**

186. Assessment of seasonal variations of major chemical elements in water samples collected from Rouge River. Y. Deng, **S. Stanton**, **A. Benson**

187. Diaryl selenides motifs as catalytic sites on electrode surface for peroxynitrite sensing. **m.a. ibrahim**, **H. Kalil**, F. Fouad, M. Bayachou

188. Dynamic assembly of photoactive naphthodithiophene-based materials. **E.B. ADUSEI**, M. Caswell, C. Goldsmith, L. Haddad, D. Alinj, J. Park, Z. Kinney

189. Synthesis of phenanthridine: Establishing a proof of concept for a new approach to the preparation of benzo[2,7]naphthyridines. **S. Dorn**, **A. Martin**

190. Atmospheric dry and wet deposition of total phosphorus to the Great Lakes. **M.M. Lynam**, L. Oriol, A. Steiner

191. Investigating the effect of phenolic compound concentrations in staghorn sumac seeds on the winter foraging behaviors of birds. **J. Hiebert**, M. Cleland, S. Krebs, M. Schummer, V. Niri

192. Synthesis of diazirine all in one click NAADP for isolation and purification of the NAADP receptor in sea urchin egg homogeenates. **Y. Zhang**, T.F. Walseth, J.T. Slama

193. Mid-Michigan technician group (MMTG). **L.J. Brissette**

194. Paramagnetic ionic liquids for extraction and forensic analysis of textile dyes. **J. Moss**, **D. Bwambok**

195. Design and synthesis of platinum ligands for cancer treatment. **K.J. Friedrich**, **M. Iwu**, **J. Sinani**, D. Nguyen, S. Hakim, H. Kizy, J. Zdankowski

196. Evaluation of antibacterial activity of compounds extracted from stem bark of *Alafia multiflora*. **C. Kuedukey**, **D. Anum**, J. Borgia, J. Mckillip, D. Bwambok

197. Classification of biodegradable chemicals based on their structures and physicochemical properties using computational simulations. **R. Kyung**, E. Cho

198. Synthesis and characterization of a novel set of RM734-CN(2F) variant ferronematic liquid crystals. **P. Guragain**

199. Functionalization of commercial hydrophilic-lipophilic balanced copolymer for automatic magnetic dispersive micro-solid phase extraction of surface water contaminants. **C. Gemuh**, B. Horstkotte, P. Solich

200. Computational insights on the structure of transition states and intermediates of the Boyland-Sims oxidation reaction. **I. Hall**, A.L. Pumford, E.J. Behrman, J. Joseph

P3. Salon IV

Chemical Education Poster Session

D. B. Lawson, *Organizer, Presiding*

4:00 - 6:00

201. To the rescue of our K-12 schools, please!. **N. Saab**

202. Is the NGSS curriculum sufficient to promote proficiency in high school chemistry?. **L.H. Kolopajlo**

203. Exploring the Tyndall Effect: Blending the chemistry and math with easy-to-use, inexpensive materials. **B. Gheorghila**, Z. Arrington, K. Yeldo, S. Arment, S. Cacanindin, R. Seklauoi, Z. Kanji, L. White, E. Aeck, A. Alexander, L. Weisend, D. Hamze, J. McKenzie, R. Kesto, A. Khosho, A. Ramirez, A. Spahiu, A. Naeem, L. Murshed, E. Ely, T. Johnson, Z. Madden, E. Koneva, M. Caruso, G. Brown, Y. Park, C. Shouman, J. Page, L. Sabra, Z. Shouman, R. Trotman, E. DeVito, X. Sterling, O. Agholor, A. Bosah, L. Adamczyk, K. Moroz, N. Shabil, Z. Albdair, J. Kroha, J. Whitener, K. Strnad, J. Crandall, L. Jeki, N. Ka, M.A. Benvenuto

204. Faculty beliefs on teaching and learning: Potential roadmap towards using evidence-based practices. **J. Starkie**, S. Abeywardana, V. Scammahorn, M. Cooper

205. Green Organic Chemistry lab manual: What's new?. **M. Zhang**, E.L. Day, M. Cooper

206. Bridging the STEM gap in Appalachia: Engaging with students to iteratively improve faculty practices in support of student success. **J. Joseph**, A. Chapman, R. Niichel

207. Process orientated guided inquiry learning in the physical chemistry laboratory. **T.R. Brewer**, K. DeVries

208. Convenient method of esterification of fatty acids: Undergraduate organic lab experiment. **P.R. Di Raddo**

FRIDAY MORNING

S23. Salon VII

Catalysis by Metal Complexes and Nanomaterials

M. Young, M. Zhou, *Organizers*

A. R. Parent, D. Xiao, *Presiding*

8:20 Introduction.

8:25 209. Biomimetic tridentate *cis, cis*-1,3,5-cyclohexane ligands and transition metal complexes. A. Olivelli, L. Wolff, R. Chafin, S. Parkin, **A. Huckaba**

8:45 210. Probing the mechanism for 2,4'-dihydroxyacetophenone dioxygenase (DAD) using biomimetic iron complexes. **F.A. Chavez**

9:05 211. Oxygen gas as a sustainable oxidant for C-H bond activation and drying oil autoxidation. A. Kalbach, **A.R. Parent**

9:25 212. Iron(II)-alkoxide mediated carbene transfer to form cyclopropanes. **L. Kulathungage**, S. Kurup, R.L. Lord, S. Groysman

9:45 Morning Coffee Break.

10:00 213. Cobalt-catalyzed dimerization of terminal alkynes to 1,3-enynes. **N.A. Ward**, J. Prybil, A. Kollar, C.R. Wade

10:20 214. Exploring new approaches for Rh catalysis. **M. Young**, S. Vanaparthi, I. Alahakoon, K.K. Shrestha

10:40 215. C-N bond formation from C1 feedstocks. **M. Zhou**, D. Xiao, Y. Wang, X. Zhou, D. Hanson, E. Washburn, M. Ekmekci, D. Dennis, A. Paripati

S24. Salon II

Analytical

K. C. Lanigan, *Organizer, Presiding*

8:30 216. Evaluation of multiple linear regression statistical methods to predict biodiesel spill composition. **W.H. Shirley**, M. Voisinet, V. McGuffin, R. Smith

8:50 217. Electrochemical analysis of Bovine exhaled breath condensate to detect biomarkers of respiratory disease using nanocarbon electrodes. **A. Jacobs**, S. Peteu, M.C. Prete, A. Lesch, G.M. Swain

9:10 218. Human serum albumin nanoparticles with near infrared ionic dye and chemotherapeutic drug for therapeutic applications. **T. Alonge**, **D. Bwambok**

9:30 Break.

9:40 219. Application of electrochemical sensors to detect nitric oxide and acetylcholine release from mouse myenteric ganglia using an APP/PS1 mouse model. **S.A. Henderson**, J.J. Galligan, G.M. Swain

10:00 220. Environmental estrogens: An analytical challenge. **Y. Zuo**, S. Zhou, F. Albalawi, Y. Deng

10:20 221. The effect of added organic solvent on electron transfer kinetics and molecular diffusion in room temperature ionic liquids. **S.G. Ralahamilage**, G.M. Swain

S25. Salon I

Cellular Signaling/Biochemistry

B. Xhabija, *Organizer, Presiding*

8:30 Opening Remarks.

8:40 222. Excited state simulations of fluorescent proteins for rational design. **A. Walker**

9:00 223. Understanding the role of JPT2 in NAADP-mediated calcium signaling in T cells. **G.A. Soares**, S.E. Nada, K.A. Wall

9:20 224. Molecular and structural characterization of the histone binding domains of the epigenetic regulator UHRF2. **B. Albaugh**, S. Ginnard, A. Winkler, C. Mellado-Fritz, R. Kemmer, T. Bluhm, N. Butkevich, M. Gilliam, S. Abdrabbo, B. Kaitlyn, D. Heyl-Clegg, R.C. Trievel

9:40 Coffee Break.

9:55 225. Role of the dual specificity phosphatase hYVH1 in ribosome dynamics. **P.O. Vacratsis**

10:15 226. Targeted protein degradation from the endoplasmic reticulum. **R. Baldridge**, R. Sharninghausen, J. Hwang, D. Dennison

10:35 227. Unicorn in the garden: Uracils in DNA. **A. Bhagwat**

S26. Salon VI

Computational Chemistry from Electrons to Macromolecules

A. Walker, *Organizer, Presiding*

8:30 228. Mitigating climate change: Atomistic simulations shed light on bromoform-membrane interactions. **K.J. Cheng**, J. Shi, T.V. Pogorelov, S. Capponi

8:50 229. Understanding carbonate formation in aqueous solutions at the atomic level via multi-level quantum mechanics/molecular dynamics simulations. **J. Boyn**, E.A. Carter

9:10 230. Computational study of quantum mechanical protein–ligand binding energies using the Molecules-In-Molecules (MIM) method. **s. maier**, B. Thapa, J.A. Erickson, K. Raghavachari

9:30 Break.

9:40 231. Assessing electrostatic approximation of binding free energy by Wolf summation. **G. Schwing**, B. Crawford, M. Barhaghi, L. Schwiebert, J. Potoff

10:00 232. Quantum electron dynamics: Towards electron control. **Z. Stewart**, A.K. Wilson

10:20 233. Permeability, energetics and mean first passage time of photosynthetic for metabolite transport in synthetic carboxysomes. **D. Sarkar**, C. Maffeo, M. Sutter, A. Aksimentiev, C. Kerfeld, J.V. Vermaas

S27. Salon III

Physical

D. B. Lawson, *Organizer, Presiding*

8:30 234. Multiconfiguration electron-nuclear dynamics on open-shell molecules. **C. Wang**, I. Ulusoy, L. Aebersold, A.K. Wilson

8:55 235. Halogen bonding and electron-transfer processes involving molecular iodine. **E. Adeniyi**, L. Snowden, S.V. Rosokha

9:20 Break.

9:30 236. Real-time electron dynamics under the influence of strong light-molecule coupling. **J. Weidman**, A.K. Wilson

S28. Salon V

Sustainable and Environmentally Beneficial Polymers

J. C. Furgal, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 237. Increasing sustainability through self-healing and recycling: Extending the lifetime of silicone materials. L.J. Voigt, P. Azadi Namin, K. Tucker, P. Booth, J. Trevino, **P. Zelisko**

8:55 238. Stereolithography with lignin and cellulose: Designing chemistry for 3D printed continuous and aligned fiber composites that mimic plants. **S.C. Chmely**, E. Battisto, M. Rohi, A. Arya, J.M. Catchmark

9:15 239. Silicon-based hybrid photo-responsive network polymers toward reusable environmental sponges. **J.C. Furgal**, C.B. Sims, M. Erfani Jazi

9:35 Break.

9:45 240. Computational investigation of charge transfer in ferrocene-based polymer materials. **H.P. Hendrickson**, T. Chua, L.J. Welch, C. Qian, J. Feldblyum

10:05 241. Self-healing polymers for life cycle management. **A. Pena-Francesch**

10:25 242. Electrochemical upcycling of poly(vinyl chloride). **R.K. Jha**, A.J. McNeil

FRIDAY AFTERNOON

S29. Salon II

Analytical

K. C. Lanigan, *Organizer, Presiding*

2:00 243. MALDI-MS based screening for PFAS uptake by bacteria. **I. Reza**, A.J. Reynolds, H.J. O'Shaughnessy, T. Qiu

2:20 244. Elucidation of fungal cell walls structure and remodeling by antifungal drugs using solid-state NMR. **I. Gautam**, L. Fernando, M. Widanage, A. Lipton, N.M. Washton, F. Vigier, J.P. Latgae, T. Wang

2:40 245. Green approach for extracting per- and poly- fluoroalkyl substances from water. **D. Bwambok**, N. Dominguez

3:00 Break.

3:10 246. Development of a yeast-based assay for bioavailable nutrients. **H. Shepherd**, M. Trentman, J. Tank, J. Praner, A. Cervantes, P. Chaudhary, J. Gezelter, A. Marrs, K. Myers, J. Welsh, Y. Wu

3:30 247. Detection and quantification of poly- and perfluoroalkyl substances using MALDI-TOF with trapped ion mobility–a novel approach to *in-situ* analysis of perfluoroalkyl substances. **A.J. Reynolds**, T.(. Qiu

3:50 248. Optimizing detection of underivatized neurochemicals using MALDI-TIMS-TOF for mass spectrometry imaging applications. **R.E. Jacobson**, T.(. Qiu

S30. Salon VII

Catalysis by Metal Complexes and Nanomaterials

M. Zhou, *Organizer, Presiding*

2:00 249. Metal-catalyzed reactions as undergraduate research topics. **J.P. Lanorio**

2:20 250. Effects of intramolecular interactions on electrocatalytic CO2 reduction. **J. Zhou**, W. Nie, C.C. McCrory

2:40 251. Electropolymerized molecular electrocatalyst films for selective nitrate reduction to ammonia. **M. Askari**, J. Kallick, C.C. McCrory

3:00 Break.

3:10 252. Design nanoalloy catalysts for converting lignin into value-added chemicals guided by inverse molecular design theory. **D. Xiao**

3:30 253. Catalytic applications of diphosphine complexes immobilized in metal-organic frameworks. **J. Hilliard**, C.R. Wade

3:50 254. Development of high-throughput workflows in MOF-catalyzed organic transformations. **J.R. Bour**

S31. Salon I

Cellular Signaling/Biochemistry

B. Xhabija, *Organizer, Presiding*

2:00 255. Rational design of redox mediators for enzymatic bioelectrocatalysis from the ground up. L. Mtemeri, **D. Hickey**

2:20 256. Optogenetic and chemogenetic sensors and tools for studying brain signaling. **W. Wang**

2:40 257. Using small molecule anti-cancer drugs to probe mechanisms of cancer cell death. J. Brooks, F. Gojcaj, M. Harris, D. Proffett, **M.R. Livezey**

3:00 Break.

3:15 258. Chemical tools to study cell biology: Kinase-catalyzed labeling. **M. Pflum**

3:35 259. Structure of the human nuclear pore complex. **S. Mosalaganti**

3:55 260. Cholesterol homeostasis and TCDD-induced, AHR-mediated liver injury. **J.J. LaPres**

S32. Salon VI

Computational Chemistry from Electrons to Macromolecules

A. Walker, *Organizer, Presiding*

2:00 261. Accurate predictions on metal diffusion and metal-water-ligand-protein interactions. **Z. Li**, K.M. Merz

2:20 262. Synthetic models for alkene dioxygenase. **F.A. Chavez**

2:40 Break.

2:50 263. QM/MM spin-restricted ensemble-referenced Kohn–Sham nonadiabatic molecular dynamics via an OpenMolcas-GAMESS-US/Tinker interface. **D. Kaliakin**, M. Huix-Rotllant, N. Ferre, M. Filatov, A. Blanco-González, X. Yang, M. Olivucci

3:10 264. Quantum chemistry explains why cells activate carboxylic acid by converting it to thioester. **M.E. Ayoub**

S33. Salon V

Sustainable and Environmentally Beneficial Polymers

J. C. Furgal, *Organizer, Presiding*

2:00 265. Integrating metal coordination bonding into materials for enhanced stability and photoresponse. **A.D. Ostrowski**

2:20 266. Completing the cycle: Photodegradation as a tool for upcycling polymers. **J. Sivaguru**

2:40 267. Towards enediyne substituted polycaprolactones in an attempt to generate Calicheamicin-like anticancer activity. **A. Bhadran**

3:00 Break.

3:10 268. Probing ion diffusion in plant secondary cell wall models at different relative humidity using molecular simulations and X-ray fluorescence. **D. Sarkar**, L. Bu, J.E. Jakes, J. Zieba, I. Kaufman, M.F. Crowley, P. Ciesielski, J.V. Vermaas

3:30 269. Catalytic transformations between forms of silicon. **K.D. Edirisinghe**, J.C. Furgal