

MARM

Nora Radu, Joel Rosenthal and Mary Watson, *Program Chairs*

WEDNESDAY MORNING

Virtual Room

High-Throughput Experimentation to Advance Discoveries in Academia and Industry

Financially supported by GlaxoSmithKline
A. Kelly, *Organizer, Presiding*

8:30 1. High-throughput chemistry: An asset to the modern academic chemist. **M.C. Nicastrì**

8:50 2. HTE in medicinal chemistry. **S. Dreher**

9:10 3. Bigger isn't always better: Efficiency gains through smaller reactions in Discovery High-Throughput Chemistry at GSK. **N.C. Goodwin**

9:30 Intermission.

9:45 4. Development of the High Throughput Experimentation (HTE) core facility at the University of Delaware: Design, implementation, applications, and innovations. **D.A. Watson**

10:05 5. Enabling medicinal chemistry through high-throughput experimentation. **S. Berritt**

Virtual Room

Innovations in Chemistry Education

S. A. Habay, *Organizer*

S. Compton, *Organizer, Presiding*

8:30 6. Multiple ways to virtually engage students in chemistry labs. **A.S. Smeltzer Schwab**

8:50 7. PubChem and its application for cheminformatics education. **S. Kim, E. Bolton**

9:10 8. Secondary chemistry teaching: Do you know the facts?. T.M. Chambers, **J. Breakall, E.C. Gravely, W. Hunter, J.B. Nielson, E.J. Yeziarski**

9:30 9. Changing the sequence kinetics material for general chemistry: Introducing mechanisms first to help students develop a conceptual understanding of reactions. **C.R. Pulliam, D. Rieck**

9:50 Intermission.

10:05 10. Cookie challenge: A unique way to encourage office visits. **D.B. King**

10:25 11. Toward equitable assessment of English Language Learners in chemistry: Identifying helpful features in assessment items. **E. Lee**

10:45 12. Teaching single crystal x-ray crystallography in the undergraduate classroom with common household chemicals. **A. Beauparlant, C.T. Eagle, R. Mohseni**

11:05 13. Video introduction to single crystal x-ray crystallography starring pyrite (fool's gold). **A. Beauparlant, C.T. Eagle**

11:25 14. Efficiently visualizing implicit hydrogens with the prime method. **D.L. Silverio, A. Sam, M. Mistretta, S. Buzzolani**

Virtual Room

Innovations in Inorganic and Organometallic Chemistry

W. Farrell, *Organizer, Presiding*

8:30 15. Activity studies of pentamethylcyclopentadienyl chromium complexes in N₂ activation. **F. Ahmadi Darani**, K.H. Theopold

8:50 16. Optical properties of cesium bismuth bromide perovskites. **M.N. Tran**, I. Cleveland, E.S. Aydil

9:10 17. Palladium biladiene complexes bearing alkynyl-aryl groups for sensitization of ¹O₂ and photodynamic therapy. **A. Rice**

9:30 18. High near-infrared photoluminescence quantum yield in Yb-doped cesium lead halide perovskites. **I. Cleveland**, M.N. Tran, E.S. Aydil

9:50 Intermission.

10:00 19. Improvement of electron transport in cathodes via integration of nanostructured carbons with layered oxides for high power Li-ion batteries. **T. Averianov**, E. Pomerantseva

10:20 20. Improving electrochemical behavior of layered oxides through the intercalation and heat treatment of carbon precursors for next generation cathodes. **R. Andris**, E. Pomerantseva

10:40 21. Why is the product of the reaction (first done by Dr Frankenstein) of green vitriol with the lye of blood one of the ingredients in the table salt that I brought at Wegman's last month. **S.A. Koch**

11:00 22. Bifunctional nickel and copper electrocatalysts for CO₂ reduction and the oxygen evolution reaction. **H. Pan**, C. Barile

11:20 23. Reactivity of zinc oxide clusters supported on mesoporous silica sieve (SBA-15) towards thiophene hydrodesulfurization. A. Chakradhar, **C. Wagner**, R.T. Koodali, B. Selvaratnam

Virtual Room

Innovations in Physical Chemistry

A. V. Teplyakov, *Organizer, Presiding*

8:30 24. Unveiling the genetic fragility of HIV-1 through deep learning. **J.S. Rey**, W. Li, H. Beatson, C. Lantz, A. Bryer, A.N. Engelman, J.R. Perilla

8:50 25. Combining time-resolved spectroscopy and computer simulations to reexamine our picture of bimolecular electron transfer. **C. Rumble**, E. Vauthey

9:10 26. Understanding the charge transfer mechanism in protic ionic liquids. **C. Arntsen**

9:30 27. Fabrication of thermoresponsive bilayer hydrogels through vat photopolymerization additive manufacturing. **F. Klinecicz**, J. Thomas, C.B. Thompson, S. Alfieri, L. Korley

9:50 Intermission.

10:05 28. Blackbody enhanced selective emitter for solar thermophotovoltaics. **J.F. Varner**, J.J. Foley

10:25 29. Enhanced light scattering and absorption by soot aerosols with different coating distributions. **E. Demidov**, A. Khalizov

10:45 30. Mercury cycle: Oxidation, deposition, reduction and diffusion in the arctic. **A. Asaduzzaman**

11:05 31. Atomic-resolution structure of C_{ACTD}-SP1 crystalline arrays in complex with maturation inhibitors by solid state MAS NMR. **S. Sarkar**, K. Zadrozny, R. Zadorozhnyi, R. Russell, C. Quinn, C. Xu, C. Wild, T.J. Nitz, J.R. Perilla, E. Freed, B. Ganser-Pornillos, O. Pornillos, A.M. Gronenborn, T.E. Polenova

11:25 32. Atomic-resolution structures of protein assemblies by integrating magic-angle-spinning NMR distance restraints and low-to-medium resolution cryo-EM density maps. **R.W. Russell**, C. Zhang, C. Guo, M. Lu, C. Quinn, A.M. Gronenborn, T.E. Polenova

WEDNESDAY AFTERNOON

Virtual Room

Plenary: Donna Huryn

Financially supported by Amgen
M. P. Watson, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 33. Academic drug discovery: Playing to the strengths to address challenging targets and unmet medical needs. **D.M. Huryn**

1:50 Discussion.

Virtual Room

Undergraduate Poster Session: Chemical Biology

Financially supported by J-Star Research
J. Fox, *Organizer*

2:30 - 4:30

34. Adsorptive removal of hair dye BB99 from solution using agricultural waste. **G. Mascagni**, M. Nassar, S.A. Shahrear, A. Ulay, A.E. Navarro

35. Optimization of drug-like quinoline based pharmacophore for irreversible inhibition of Nek2 kinase. **L.K. Hauter**, A.I. Bhuiyan, R. Musayev, C. Sweeney, A. Dickson, S. Tabassum, D. Hernandez, A.J. Finkelstein, D. Dana, T.T. Talele, T.K. Das, S.K. Pathak

36. Synthesis of isatin-thiazolidine-2-thione hybrids for acetylcholinesterase inhibition. **S. Davis**, T.J. Eckroat

37. How do lipids bind to the vanilloid site of TRPV1? Insights from molecular docking. **A. Wilson**, V. Carnevale, E. Gianti

38. Thermodynamic measurements of the oxidation-reduction (Fe³⁺/Fe²⁺) reactions of heme-fluoride complexes of hemoglobin and myoglobin: Insights into oxygen binding. **K.G. Flanders**, S.M. Klumpp, J. Cerda

39. Synthesis of m-DAP crosslinked muramyl dimers. **J.R. Ramsey**, S. Mashayekh, C.L. Grimes
40. Importance of MAS-R in inflammation, inflammatory disease, and COVID-19 therapeutics. **Z. Sessions**
41. Using bioinformatic approaches to investigate neisseria meningitidis serogroup W enzyme. **M. Balogun**, N. Johnson, P.C. McCarthy
42. Optimizing conditions to maximize algae growth for biodiesel production. **W.T. Jacoby**, D.D. Zhogina, L.H. Saggese, P. Ananov, S. Ross
43. Identifying small organic molecules that induce an alternative structure in precursor miRNA-92b. **S. Hurwitz**, C.M. Connelly
44. Optimization and characterization of novel formulations for hydrophilic biological drug encapsulation. A. Sanders, J.T. Zangaro, N.K. Webber, S. Ricci, H. Work, **A. Rajan**, K. Casey, B. Carone, N.V. Nucci
45. Green chemistry/bioremediation: Converting SmFixL from an oxygen sensor into a dye-decolorizing peroxidase. **S. Pogash**, M. Reynolds, D. Barry
46. Encapsulation in reverse micelles reveals the thermodynamic impacts of confinement versus interfacial interactions in the unfolding of myoglobin. **C. Stackhouse**, **L. Staman**, **C. Mejia**, N.V. Nucci
47. Fatty Acid Amide Hydrolase (FAAH) inhibitors designed for reduced permeability Bailey Mims, Julianna Young, So Jung Kim, Grace Roe, Dr. Lazenka, Dr. Fulp*. **B.J. Mims**, J. Young, S. Kim, G. Roe, A. Fulp, M. Lazenka
48. Catalysis by sol-gel encapsulated enzymes: Hb/Mb and H₂O₂ dismutation. **N. Shohet**, J. Haidery, H. Ariel, J. Ramos, U. Samuni
49. Investigating the effects of DNA base substitution on DNA structure and dynamics with high-affinity Fis-DNA complex. S. Hancock, **H.E. Little**
50. Separating the effects of confinement and interfacial interactions for the model protein cytochrome c using reverse micelle encapsulation. **B. Berry-White**, **K. Fennimore**, N.V. Nucci
51. Overexpression and purification of alexphander gp94: A predicted MerR-like transcriptional regulator. **e. Chong Qui**, S. Hancock

52. Harnessing green chemistry in the search for agricultural sustainability. **A.B. Saul,** U. Rao

53. In vitro effect of Bee Propolis on Human Tongue Cancer cell death. **E. Asani**

54. Elimination of organosulfur compounds from model fuels with biological wastes: Tackling the acid rain. **A.O. Efunnuga,** A.E. Navarro

55. Uptake of Co(II) ions from aqueous solutions by low-cost biopolymers and their hybrid. **S. Cime,** M. Nassar, A.E. Navarro

56. Effects of annona muricata on a breast cancer cell line. **J. Leon**

57. Triticain- α : An enzymatic approach to managing celiac disease. **J.S. Clem,** S. Grau, H.N. Currie, D. Puthoff

58. Adsorption of heavy metals using chemically-modified tea leaves. **R.A. Ulay**

59. Milk stretches the non-toxic range for curcumin-induced NRF2-activation. **G. Fardella,** E. Chang, I. Gazaryan

Virtual Room

Undergraduate Poster Session: Inorganic and Organometallic Chemistry

N. S. Radu, *Organizer*

2:30 - 4:30

60. Synthesis of mixed bi-icosahedron nanoclusters with increased fluorescence. **S. Topka,** N. Stevens, N. Hondrogiannis, **M. Devadas**

61. Solar degradation of toxic colorants in polluted water by thermally tuned ceria nanocrystal-based nanofibers. **w. wei,** E. Rooney, C. Beck, K. Xu, P. Lu

62. Growth mechanism study and emulsion-templated self-assembly of semiconducting cadmium selenide nanoplatelets. **Z. Jiang,** E. Marino, S. Yang, C.B. Murray

63. Profiling trace element contaminants of toxicological interest in commercially available hemp derived CBD tincture oils. **M.Z. Walton**, T. Gluodenis, R. Thomas
64. Crystallographic effects of doping early transition metals (V, Nb, Mo) into MnO₂ (2x2 tunnel, OMS-2). **T. Praisner**, A.C. Mirich, M. Pickett, S.L. Suib
65. Design and characterization of a novel enzymatic immobilization structure. **M. Pickett**, A. Mirich, S. Pierce, S. March, A.M. Angeles Boza, J.L. Rouge, S.L. Suib
66. Systematic analysis of nanoparticle synthesis in reverse micelles using CdS quantum dots as a model system. C.L. Johnson, A.V. Scorzo, N.K. Webber, **A.R. Calabrese**, A. Weyhmiller, T.V. Douglas, N.V. Nucci
67. Heme model compound peripheral group interactions in low dielectric medium. **K.A. Moulton**, J. Cerda
68. Thin layer chromatography and column chromatography in the advanced inorganic laboratory. **A. Chandra**, L. My, M. Chernys, M. Kim, G. Paniconi
69. Ruthenium(II) based water-oxidation catalyst supported on graphene oxide composites. **C. Amaya**, Y.M. Badiei, W. Li
70. *In vitro* evaluation of a potential Ruthenium-based chemotherapeutic agent for triple negative breast cancer. **A. Yeasmin**, **N. Nayeem**, **M. Contel**
71. Organometallic MRI contrast agents. **M. Izykowicz**, **M. Staszewski**
72. Development of a colorimetric assay for the carcinoembryonic antigen. **B. Berger**, J. Smith
73. Synthesis of meso-Tetraphenylporphyrin (H₂TPP): A quest for better yield and purification. **M. Chernys**, A. Chandra, M. Kim, L. My, G. Paniconi

Virtual Room

Undergraduate Poster Session: Measurement and Data Science

K. S. Booksh, S. L. Neal, *Organizers*

2:30 - 4:30

74. Random forest model prediction of compound oral exposure in the mouse. **H. Mughal**, H. Wang, M. Zimmerman, M. Paradis, J.S. Freundlich
75. Mechanistic investigation of fragmentation of protonated of nitroanisoles by mass spectrometry. **D. Ju**, A.B. Attygalle
76. Evaluate the effectiveness of washing strategies on pesticide removal from skin and flesh of strawberries, apples, and grapes using QuEChERS and LC-MS/MS analysis. **V. Tran**, J.A. Palkendo
77. Development of a method for the quantitation of carbohydrates in aquatic systems. **M.H. Schuch**, W.R. Lacourse
78. Analysis of benzodiazepines used in drug facilitated crimes. **M. Gysbers**, **T. Maslin**, S. Haddadi, V. Niri
79. Tongue cancer viability in organic tea tree and alma treatments. **R. Gonzalez**

Virtual Room

Undergraduate Poster Session: Organic Chemistry

Financially supported by PharmaBlock
M. P. Watson, *Organizer*

2:30 - 4:30

80. Synthesis of phenyl pyridines, pyridazines and pyrimidines to test for their inhibition on the enzyme Uridine Nucleoside Ribohydrolase (UNH). **E. Ajmal**
81. Investigation of pyridine-based bis-benzimidazoles as potential chemotherapeutic lead compounds. **A. Alagaratnam**, L. Barasa, S. Yoganathan
82. Greener synthesis of pterostilbene derivatives as drug candidates for the treatment of Alzheimer's. **V. You**, K. Bhat
83. Ni-catalyzed oxidative esterification of allylic sp³-carbon. **I. Hicks**, **E. Sehovic**, P. Kaur

- 84.** Novel conversion of 1,3-thiaza-4-ones to dimeric thioacetals. **M.W. Russell**, L.J. Silverberg
- 85.** Synthesis of 2-(2-methylpyridin-3-yl)phenol derivatives as uridine nucleoside ribohydrolase inhibitors. **D. Vanegas**
- 86.** Synthesis of phenyl pyrazoles for the inhibition of unH in trichomonas vaginalis. **K. Nelson**
- 87.** C-glycosides synthesis by coupling C-linked glycosyl crotylboronates with simple aldehyde. **A. Anous**
- 88.** Use of heme proteins in bioremediation efforts: Turning heme green. **D. Barry**, M. Reynolds, S. Pogash
- 89.** Desolvation pathways of four niclosamide solvates. **R. Gao**, J.E. Werner, J.A. Swift
- 90.** Non-precious metal-based MOFs as catalysts for decarboxylative coupling reactions. **C.B. Aristil**
- 91.** From natural to synthetic: Photophysical improved cyanine dyes and their bright future. **Y. Liang**, Z. Zhou
- 92.** Synthesis of sulfoxides from 2,3-diphenyl-2,3-dihydro-1,3-thiaza-4-ones. **G. Muench**
- 93.** Synthesis of 1(benzotriazolyl)ethyl ferrocene: A potential cancer growth inhibitor. **A. Aryal**, M. Squires, D. Aucoin
- 94.** Benzylic functionalization electrochemical oxidation. **K. Lee**, Y. Xing

Virtual Room

Undergraduate Poster Session: Physical Chemistry

M. P. Watson, *Organizer*

2:30 - 4:30

- 95.** Using NMR titrations to assess halogen-bonding strength as a function of molecular structure towards sensor development. **Q. Dang**, L.B. Hughes, M.C. Leopold
- 96.** Design of ionic liquids bearing thioether side chains. **M. Mughal**, J.F. Wishart, E.W. Castner, Jr., S.I. Lall-Ramnarine
- 97.** Preparation and characterization of ionic liquid–polymer gels. **S. Nembhard**, N. Zmich, J.D. Ramdihal, J.F. Wishart, E.W. Castner, Jr., S.I. Lall-Ramnarine
- 98.** Determination of asymmetrical viral capsid morphology through computational modelling of cryo-EM data. **T. Nesterova**
- 99.** Enhanced ionic liquid- single-walled carbon nanotubes mixtures for energy storage applications. **Z. Piao**, T. Hemraj-Benny
- 100.** Assessing the long-term effects of the cellular environment on HIV-1 pNL4-3 capsid. **C.A. Sheopurkar**
- 101.** Antibacterial activity of sulfur-doped carbon/g-C₃ N₄ composite under visible light. **M. Mirza**, A. Daoud, W. Li
- 102.** Single-particle tracking measurements in poly(ethylene glycol) hydrogels: Does size matter?. **K. Foreman**, K. Tran-Ba
- 103.** Absorption IR spectroscopy tracks the effect of gold nanoparticles on the ordering of phospholipids. **K. Kalloo**, S. Finn, N. Escoffery, Q. Lu, **R. Helburn**

Virtual Room

Undergraduate Poster Sessions: Polymers & Soft Materials

M. P. Watson, *Organizer*

2:30 - 4:30

- 104.** Solvent-assisted nanochannel encapsulation of a natural phase change material in polystyrene hollow fibers for high-performance thermal energy storage. **D.K. Patel**, H.S. Singh, P. Lu

- 105.** In-air polymerization and crosslinking of monomers during electrospray deposition. **C. Nachtigal**, J. Singer
- 106.** Study of nanocomposites of PolyRhodanine/Palladium/Cobalt: Synthesis and application. **M. Chauhan**, A. Sharma, S. Jaser, S. Nieves, Q.R. Johnson, G.K. Longia
- 107.** G3-G5 PAMAM dendrimer demulsification studies of known oil compositions in water emulsions. **M.A. Salah**
- 108.** Interactions of CO₂ with polymer surfaces for sequestration: A computational study. **R.B. Komma**, L. Tribe
- 109.** Polyaniline nanofiber-metal nanoparticle composites for the catalytic degradation of congo red and other targets: A mini-review. **D. Mahabir**, D.M. Sarno
- 110.** Porous microspheres of polyaniline and its derivatives as a material for cargo loading and delivery: A mini-review. **M. Chen Weng**, D.M. Sarno

WEDNESDAY EVENING

Virtual Room

BILL Talk: Barbara Morgan

Cosponsored by BMGT
M. P. Watson, *Organizer*
J. Cohen, *Presiding*

6:00 Introductory Remarks.

6:05 111. Transition from chemist to business director: Leadership lessons. **B. Morgan**

6:25 Discussion.

THURSDAY MORNING

Virtual Room

Advances in Chemistry in Pharmaceutical and Agriculture Industry

Financially supported by Adesis Inc.

Z. Dong, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 112. Recent success stories from the women of Merck small molecule process research and development. **J. McCabe Dunn**

9:05 113. Chemical process development innovations to expand patient access to transformative medicines: Recent examples from the Janssen pipeline. **J. Balsells, S. Wagschall, D. Brogini, R. Panish, S.L. Plunkett**

9:35 114. Flavonids revisit. **V.J. Lee**

10:05 Intermission.

10:15 115. Second Harmonic Generation (SHG): A powerful platform screening technology to detect protein conformational change and its application in drug discovery. **H. Lin**

10:45 116. Development of a scalable process for insecticide Tyclopyrazoflor. **X. Li, Q. Yang, B.A. Lorsbach, K. Gray**

11:15 117. Overview of agricultural discovery at FMC. **T. McMahon**

11:45 Concluding Remarks.

Virtual Room

Empowering Chemists with Disabilities

K. S. Booksh, *Organizer, Presiding*

8:30 118. Communicating chemistry content effectively to the blind. **C.A. Supalo**

8:50 119. Computational biophysical chemistry for researchers who are visually-impaired. O.R. Shaw, **J.A. Hadden-Perilla**

9:10 120. Voice control of a raman microscope with Commercial Off the Shelf (COTS) software. **K.S. Booksh**, R. McCormick, D. Greco

9:30 121. Well succeed experience in teaching chemistry to deaf students in Brazil. **H.V. Silva**

9:50 122. Panel discussion: Making career decisions during the pandemic. **K.S. Booksh**

Virtual Room

Inorganic and Organometallic Young Investigator Symposium

Cosponsored by INOR

Financially supported by DuPont

W. Farrell, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 123. Design and synthesis of highly porous coordination cages. **E.D. Bloch**

9:10 124. Molecular strategies to modulate the electrode-electrolyte interface in heterogeneous electrocatalysis. **V. Thoi**

9:45 125. Photoswitchable extended network materials. **K.M. Waldie**

10:20 Intermission.

10:35 126. Developing hydrolytic mini-metalloenzymes using *de novo* proteins. **K. Buettner**

11:10 127. Olefin metathesis with vanadium(V) alkylidenes: Current possibilities and limitations. **W. Farrell**

Virtual Room

Protein Quality Control

Financially supported by Purisys

K. R. Schmitz, *Organizer*

K. R. Schmitz, *Presiding*

8:30 128. Systematic discovery of terminal sequences that mark proteins for proteolysis in *E. coli*. P.C. Beardslee, **K.R. Schmitz**

8:55 129. Co-translational protein quality control is a target for new antibiotics. **K. Keiler**, J.N. Alumasa, M. Cabrera, Z. Aron, C. Dunham

9:20 Intermission.

9:30 130. Proteasomal conformation controls unfolding ability. J. Cresti, A. Manfredonia, C. Bragança, J. Boscia IV, C. Hurley, M. Cundiff, **D. Kraut**

9:55 131. Countering deleterious phase transitions in ALS/FTD. **J. Shorter**

Virtual Room

Spectroscopy: From Molecules to Macrostructures

Cosponsored by COLL

A. V. Teplyakov, *Organizer, Presiding*

8:30 132. Properties of solar energy and spintronic materials from DFT. **L. Bendavid**, O.T. Fauth, A.O. Atsango, R.W. Smith

9:00 133. Surface supportive metal-organic framework as a drug delivery system. S.G. Guillen, A. Bui, **F. Tian**

9:30 134. Time-resolved X-ray spectroscopy studies of long lived photoinduced charge separation in redox active metal organic frameworks. **J.V. Lockard**, L. Hanna

10:00 Intermission.

10:15 135. Imaging partially ordered molecular materials through vibrational nano-spectroscopy. **E.A. Muller**, B.T. O'Callahan, J. Joseph, T. Cigeroglu

10:45 136. High-resolution, rotationally-resolved spectroscopy of the 3300 cm⁻¹ band of astrochemically-relevant HCN. J. Palko, T. Howard, **L.G. Dodson**

11:15 137. Gas-surface interactions of Hg(II) compounds probed by mass spectrometry. **A. Khalizov**, N. Mao

THURSDAY AFTERNOON

Virtual Room

Plenary: Dan Nocera

Financially supported by Chemours
J. Rosenthal, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 138. Complete artificial photosynthesis: Sustainable and renewable carbon, nitrogen and phosphorus cycles for fuel and crop production. **D.G. Nocera**

1:50 Discussion.

Virtual Room

Biophysical Chemistry

Cosponsored by COMP
J. R. Perilla, *Organizer*
G. Brannigan, E. R. May, *Presiding*

2:00 139. Atomistic dynamics of a viral infection process: Release of membrane lytic peptides from a non-enveloped virus. **E.R. May**

2:20 140. Differential thermodynamics and kinetics of prefusion spike proteins of SARS-CoV-1 and 2. V. Govind Kumar, D. Ogden, U. Isu, A. Polasa, J. Losey, **M. Moradi**

2:40 141. Protein interface flexibility in pleomorphic viral assemblies via solid-state NMR spectroscopy. G. Michel, J. Gonzalez-Roman, C.A. Figueroa Morales, N. Rodriguez-Marino, **M.J. Bayro**

3:00 142. All-Atom MD simulations of the HBV capsid: Revealing mechanisms of function and disruption. **J.A. Hadden-Perilla**

3:20 Intermission.

3:40 143. Updating the CHARMM lipid force field and modeling membrane leaflet composition asymmetry. Y. Yu, M. Hsieh, **J.B. Klauda**

4:00 144. Identifying structurally-resolved lipid fragments through molecular simulation. T.T. Joseph, M. Arcario, J. Petroff, W. Cheng, J. Henin, **G. Brannigan**

4:20 145. Plasma membranes are asymmetric in lipid unsaturation, packing and protein shape. **I. Levental**

4:40 Concluding Remarks.

Virtual Room

Energy Catalysis

Financially supported by Strem
J. Rosenthal, *Organizer, Presiding*
H. Shirley, *Presiding*

2:00 Introductory Remarks.

2:05 146. Coordination chemistry flow battery. **S. Reece**

2:35 147. Anti-catalysis: Applications of the kinetic inhibition of water splitting. **M.P. Marshak**

3:00 148. Sustainable and efficient energy storage using a flow battery assembly based on iron, air, and water. **L. Tran**, J. Rosenthal

3:20 Intermission.

3:30 149. Insights into electrocatalytic oxidation reactions using first-row transition metal complexes. **K.M. Waldie**

3:55 150. Recent developments in the application of oxazoline-containing ligands in CO₂ reduction catalysis. **A.M. Angeles Boza**, J.K. Nganga, K.A. Grice, M.Z. Ertem

4:20 151. Anion induced surface structuring of copper cathodes as a means to control the selectivity and activity of electrochemical CO₂ reduction. **L. Xiong**, T. Kunene, J. Rosenthal

4:40 152. Approaches to the catalytic synthesis of weak bonds. **P.J. Chirik**

5:10 Concluding Remarks.

Virtual Room

Frontiers in New Methods for Organic Synthesis

Cosponsored by ORGN

M. P. Watson, *Organizer, Presiding*

2:00 Introductory Remarks.

2:05 153. Umpolung approaches to aryl ether synthesis via electrophilic oxygen species. **S. Wengryniuk**

2:35 154. Fe-catalyzed multicomponent Radical cascades/cross-coupling accelerated by a computational and experimental approach. **O. Gutierrez**

3:05 155. New methods for the development of novel ingredients. **K. Steward**

3:35 Intermission.

3:45 156. New reactions for installing heteroatoms in complex molecules. **D.A. Watson**

4:15 157. Oxygen driven fragment coupling for the synthesis of natural products and antibacterials. **M. Kozlowski**

4:45 158. Innovation in the synthesis of complex pharmaceutical agents. **M.D. Eastgate**

Virtual Room

Innovations in Chemical Biology

Financially supported by Merck Sharpe Dohme

J. Fox, *Organizer, Presiding*

2:00 159. Salt bridge between a conserved arginine and a heme propionate plays a key role in the oxygen sensing mechanism of the FixL protein from *Sinorhizobium meliloti*. **M. Reynolds**

2:20 160. PubChem for drug discovery in the age of big data and artificial intelligence. **S. Kim**, E. Bolton

2:40 161. Theranosis of liver fibrosis in non-alcoholic fatty liver disease (NAFLD) with collagen-targeted thermoresponsive assembled protein. **A. Wang**, E. Fisher, J.K. Montclare

2:55 162. Engineering fluorinated thermo-responsive assembled protein (F-TRAP) for theranostic applications in glioblastoma multiforme. **A. Bhattacharya**, Y.Z. Wadghiri, D. Placantanokis, J.K. Montclare

3:10 163. Potential muscarinic antagonist antidepressants that lack cognitive deficits in rodents. **C.R. Johnson**, B. Kangas, E. Jutkiewicz, G. Winger, J. Bergman, A. Coop, J. Woods

3:25 164. Chemical approaches for understanding the landscape of RNA modifications. **E. Arguello**, R. Kleiner

3:40 Intermission.

3:50 165. Fluorescent probe design for targeting and imaging carbonylation in live cells. H. Erkan, D. Telci, **O. Dilek**

4:10 166. Sponge Mimetic Tubules (SMT) to explore biomorph templated evolution of animal life. **K.S. Raja**

4:30 167. Visible light promoted tryptophan photoconjugation using donor-acceptor pyridinium salts. **C. Hoopes**, A. Sarkar, N. Kuehl, N. Collins, M. Taylor

4:45 168. Post-polymerization modification of hydrogel microfibers synthesized via interfacial tetrazine ligation. **P. Ramaraj**

5:00 169. Electro-genetic control and regulation of a synthetic *Escherichia coli* consortia. **E. VanArsdale**, J. Pitzer, S. Wang, K. Stephens, G.F. Payne, W.E. Bentley

Virtual Room

Spectroscopy: From Molecules to Macrostructures

Cosponsored by COLL

A. V. Teplyakov, *Organizer, Presiding*

2:00 170. Oxidation of Cu₂O(111) by NO₂ : An ambient pressure x-ray photoelectron spectroscopy study. **B. Karagoz**, M. Blum, A.R. Head

2:20 171. Investigating plasmonic resonances in metal-semiconductor heterostructures. **J.P. Avenoso**, M. Jia, O.E. Babawale, L. Gundlach

2:40 172. Reactions of boric acid and 4-fluorophenylboronic acid with H- and Cl-terminated Si(100) surfaces. **D. Silva Quiñones**, A.V. Teplyakov

3:00 Intermission.

3:15 173. Pump-degenerate four wave mixing spectroscopy of the interfacial electron transfer on perylene-sensitized TiO₂ surfaces. **H. Yan**, J.P. Avenoso, S. Doble, L. Gundlach, E. Glaoppini, L. Rego

3:35 174. Comparison of spectral unmixing algorithms applied to simulated and measured frequency domain dynamic fluorescence reaction monitoring of semiconductor quantum dot surface passivation. **D.B. Sanap**, M. Murray, S.L. Neal

3:55 175. Mapping preferential adsorbate interactions at electrodeposited Cu interfaces via shell-isolated nanoparticle enhanced raman spectroscopy. **D. Raciti**, A.R. Hight Walker, T.P. Moffat

THURSDAY EVENING

Virtual Room

Innovations in Chemical Biology

J. Fox, *Organizer*

5:30 - 7:30

176. Toward a mechanistic understanding of ferrous iron transport: Deciphering the function of FeoA. **A. Sestok**, J. Brown, J. Obi, S. O'Sullivan, D. Deredge, A.T. Smith

177. Withdrawn

178. Study of dopamine-induced functional adaptations in astrocytes. **S.P. Aryal**, C.I. Richards

179. Aptamer based label-free and sensitive detection of miRNA. **M. ISLAM**

180. Epigenetic modifications of histones in a yeast amyloid-beta overexpression model. **M. Hugais**, S. Cobos, S. Bennett, G. Foran, J. Paredes, M. Torrente

181. Indirect downregulation of MCL-1 via targeted PROTACs. **A. Chan**, S. Fletcher

182. PROTAC strategy to rescue venetoclax sensitivity in AML-resistant cells. **C.C. Goodis**, I.L. Conlon, A. Cottingham, S. Fletcher

183. Structure-activity relationship studies of ketamine. **A. Abelian**, M. Dybek, J. Wallach, A. Adejare

184. Identification of diverse targets of arginine phosphorylation in *Mycobacterium smegmatis* by shotgun proteomics. **E.C. Ogbonna**, K.R. Schmitz

185. Mapping out histone post-translational modifications in a yeast prion model. **S. Cobos**, E. Son, J. Paredes, N. Rana, A. Olivera, H. Ibrahim, B. Salib, S. Bennett, M. Torrente

186. Functional characterization of undenatured type II collagen supplements : Are they interchangeable?. R.B. Harris, F. Fonseca, C. Ottinger, **M. Sharp**

187. Development and application of methods to classify Clp protease protein paralogs in actinobacteria. **J. Jiang**, K.R. Schmitz

- 188.** Targeted, catalytic, near-IR light-triggered release from dihydrotetrazine precursors. **J. Rosenberger**, Y. Xie, Y. Fang, A. Tallon, J. Fox
- 189.** Exploring the relationship between temperature activated hydrogen-deuterium exchange and protein stability with SANS. **R. Donnelly**, Y. Liu, N.J. Wagner
- 190.** Blood-brain barrier permeability and AChE inhibition of ionophoric polyphenols. **A. Martinez**, M. Zahran, M. Gomez, J. Guevara, R. Pichardo-Bueno
- 191.** High-throughput discovery of sequences that promote proteolysis in bacteria. **P. Beardslee**
- 192.** Activation of tetrazines by a genetically encodable catalyst for intracellular spatially controlled bioorthogonal chemistry. **A. Tallon**, Y. Xie, J. Fox
- 193.** Application of Fundator's multidimensional time model to finding trace of fractional multidimensional Fokker-Plank equation dynamics in DNA replication in formation of CpG islands, analog bases, and repeats of G-quadruplexes. **M. Fundator**
- 194.** Novel application of qPCR melt analysis following BRED. S. Hancock, **F. Habtehyimer**
- 195.** Identification of a secondary binding site for acyldepsipeptide fragments within the bacterial Clp protease. **M. Prorok**, J. Husdon, K.R. Schmitz
- 196.** Nipamovir: Synthesis and preclinical evaluation of an anti-HIV thiobenzamide prodrug. **M. Robello**, H. Nikolayevskiy, M.T. Scerba, R. Nahui Palomino, V. Mercurio, T.L. Hartman, R.W. Buckheit, L. Margolis, D.H. Appella
- 197.** New electron transport and biomedical applications for peptide amphiphile materials. **L.A. Solomon**

Virtual Room

Innovations in Chemistry Education

S. Compton, S. A. Habay, *Organizers*

5:30 - 7:30

198. Case for case studies when teaching biochemistry. **D. Bassolino**, D.A. Barr, K. Schroeder

199. Sustainability and safety in chemistry: An upper level undergraduate elective. **C.A. Dougherty**, K.E. Kristian

200. Impact of recitation timing on student performance in undergraduate general chemistry. **A. Howcroft**, D. King

201. Hybridization of C-H bonds is directly related to electronegativity of substituents. **D.D. Clarke**

202. Teaching hands on chemistry labs to the visually impaired. **T. Ladogana**

Virtual Room

Innovations in Inorganic and Organometallic Chemistry

E. A. Hernandez-Pagan, *Organizer*

5:30 - 7:30

203. Strategies for the photoreduction of Tc-99 pertechnetate to low valent Tc by Keggin polyoxometalates. **I. Radivojevic Jovanovic**, C.M. Gallagher, R. Salcedo, W.W. Lukens, B.P. Burton-Pye, D.M. McGregor, L.C. Francesconi

204. Mathematical aspects of application of fractional multidimensional Fokker-Plank equation to the theory of rate of chemical reactions based on spectroscopy experiments with examples. **M. Fundator**

205. Optimizing the properties of sol-gel based silica nanoparticles. A. Fried, H. Ariel, J. Ramos, J. Lam, **U. Samuni**

206. Electron microscopy of platinum-based anti-cancer drugs: Cisplatin, oxaliplatin, and carboplatin. **V. Galemba**, G. Paniconi

207. Development of heterometallic platinum(IV)-gold(I) compounds as potential chemotherapeutics against specific genitourinary cancers. **J. Lopez-Hernandez**, H. Karim, R. DeGregorio, M. Contel

208. Two-dimensional materials based photocatalysts for light-induced H₂ production. **J. Ran**

209. Designing silicon substrates for area-selective deposition of TiO₂. **T. Parke,**
A.V. Teplyakov

210. Interplay between mesoscale architecture and catalytic output in CO₂ gas-diffusion electrolyzers. **D. Raciti,** T. Braun, B. Tackett, H. Xu, M. Cruz, B.J. Wiley, T.P. Moffat

211. Immobilization of water-oxidation catalysts on plasma grafted poly(acrylic) acid modified anodes. **Y.M. Badiei,** C. Traba, C. Amaya

212. Mechanism and kinetics of the MAX etching reaction for MXene synthesis. **M. Anayee,** A. Goad, D. Dogias, Y. Gogotsi

213. Flexible approach to fabricate a well-ordered array of Metal/Semiconductor hemispherical nano-heterostructures. **O.E. Babawale,** J.P. Avenoso

214. *In situ* adsorption studies of anisole on NiMo oxide catalysts under hydrodeoxygenation reaction conditions. **T. Hu,** S. Blomberg, A.R. Head

215. C-N bond formation by nitride migratory insertion into Cr-C bond. **L. Zhang,** K.H. Theopold

Virtual Room

Innovations in Measurement and Data Science

L. Gundlach, S. L. Neal, *Organizers*

5:30 - 7:30

216. Fluorescence reaction progress monitoring of solid-phase asymmetric ionic nanoscale probe synthesis. **C. Von Suskil,** S.L. Neal

217. Photodegradation of semiconductor quantum dots in microheterogeneous media using wavelength- and frequency-resolved fluorescence decay measurements. **M.J. Murray,** S.L. Neal

Virtual Room

Innovations in Organic Chemistry

M. P. Watson, *Organizer*

5:30 - 7:30

218. Deaminative reductive methylation of alkylpyridinium salts. **O. Bercher**, S.L. Plunkett, T. Mortimer, M.P. Watson

219. Synthesis and evaluation of biaryl compounds as inhibitors of nucleoside hydrolases to treat trichomoniasis. **M.A. Vanalstine-Parris**, V. Abrego, E. Ajmal, A. Gil, K. Nelson, R. Shin, D. Vanegas, E. Saljanin, C. Ventura, B.J. Stockman

220. Reactions of isocyanates and isothiocyanates with 2-bromoallylamines: Investigations into the synthesis of 1,3-dihydro-2*H*-imidazol-2-ones and 4-imidazoline-2-thiones. **T.J. Eckroat**

221. One-pot chemoenzymatic reactions in water enabled by micellar encapsulation. **C. Hastings**

222. Photochemical and photophysical study of *bis*-alkylated lumazine and pterin photosensitizers. M. Sosa, M. Vignoni, M. Urrutia, M.I. Quindt, S. Bonesi, D. Denburg, A. Greer, A.H. Thomas, **E. Greer**

223. Adjuvant compound analysis for mechanistic insight to promote photodynamic action. **S. Jabeen**, **L. Lapoot**, R.M. O'Connor, M. Zatulovski, A. Greer

224. Superhydrophobic antimicrobial photodynamic inactivation of bacterial biofilm with airborne singlet oxygen. **C. Tonon**, S. Ashraf, A. Rastelli, G. Ghosh, T. Hasan, Q. Xu, **A. Greer**, A.M. Lyons

225. Deaminative nickel-catalyzed one-carbon homologation of alkyl amines. **C. Twitty**, J. Xu, M.P. Watson

226. Development of a hiyama cross-coupling of highly substituted vinylsilanes. D.A. Watson, S.B. Krause, H. Omar, **A. Conner**

Virtual Room

Innovations in Physical Chemistry

J. R. Perilla, *Organizer*

5:30 - 7:30

227. Computational design of foldamer based water channels. **S. Houshyar Azar**, Z. Liu, V. Pophristic

228. Development of ^{19}F fast magic-angle-spinning NMR spectroscopy for structural characterization of protein assemblies. **B.R. Runge**, C. Quinn, R. Zadorozhnyi, M. Fritz, J. Struppe, I.L. Byeon, A.M. Gronenborn, T.E. Polenova

229. ^{19}F magic angle spinning NMR spectroscopy to probe protein-ligand interactions. **R. Kalabekova**, C. Quinn, M. Akke, A.M. Gronenborn, T.E. Polenova

230. Determination of histidine protonation states in proteins by fast magic angle spinning NMR. **R. Zadorozhnyi**, B.R. Runge, S. Sarkar, C. Quinn, K. Zadrozny, B. Ganser-Pornillos, A.M. Gronenborn, T.E. Polenova

231. Towards the atomic resolution structure of a novel disulfide-rich biomaterial. **S. Zeinalilathori**, C. Zhang, T.E. Polenova, C. Thorpe

232. Thermal dry etching of CoFeB alloy thin films using chlorine and acetylacetone (acacH). **M. Konh**, A.V. Teplyakov

233. Realistic SARS-CoV-2 liposomes via *VesGen*: an efficient tool for modeling large and complex lipid membranes. **A.J. Bryer**, J.R. Perilla

234. Molecular determinants of Ebola nucleocapsid stability from molecular dynamics simulations. **C. Xu**, N. Katyal, T. Nesterova, J.R. Perilla

235. Impact of cavity losses on nonadiabatic couplings and dynamics for many molecules coupled to a single photon in polaritonic chemistry. **F. Suchanek**, J. Foley

236. All-atom MD simulations of CpAM-bound HBV capsids reveal allosteric mechanisms relevant to assembly regulation and inhibitor binding. **C. Perez Segura**, B.C. Goh, J.A. Hadden-Perilla

237. Development of novel xanthate-modified and unmodified exchangers for remediation of effluent in contaminated water within Enugu State metropolis. **E. Agboeze**, J.C. Attah

238. Three conformationally distinct models of the full-length SARS-CoV-2 spike protein with representative post-translational modifications. **P. Jones**, J.A. Hadden-Perilla

Virtual Room

Innovations in Polymers & Soft Materials

L. Kayser, *Organizer*

5:30 - 7:30

239. Conductive hydrogels based on a water-soluble EDOT derivative. **D. Nguyen**, L. Kayser

240. Degradable multiblock copolymers as scaffolds for conductive polymers. **E. Awuyah**, L. Kayser

241. Synthesis of stimuli-responsive and conducting polyelectrolyte complexes. **V. Damani**, L. Kayser

242. Tunable microfibers via interfacial tetrazine ligation. **O.J. George**, H. Zhang, A. Ravikrishnan, S. Liu, H. Zhang, J. Fox, X. Jia

243. 3-D cytocompatible network construction mediated by long wavelength photocatalytic activatable bioorthogonal reactions. **H. Zhang**, C. Wang, J. Fox, X. Jia

244. Impact of the molecular structure of poly(styrene sulfonate) on the mixed ionic-electronic conduction of PEDOT:PSS. **C. Lo**

245. Celebrating the 100th Anniversary of the Delaware ACS Section. **N.W. Henry**

246. Electrochemical behaviour of polymer nanocomposite on different electrode substrates. **F. SALIH**, A. OUARZANE, K. Lafdi, M. EL RHAZI

Virtual Room

Carothers Award Symposium

Financially supported by Incyte

M. P. Watson, *Organizer*

J. Qu, N. Radu, *Presiding*

7:00 Introductory Remarks.

7:30 247. Lessons learned from nature: From biomineralization to biomaterials. **A. Campbell**

8:15 Discussion.

FRIDAY MORNING

Virtual Room

Alternative Grading in the Chemistry Curriculum

S. A. Habay, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 248. Getting started with mastery grading. **A. Deckert**

9:05 249. Implementation and outcomes of mastery-based grading in general chemistry. **E.E. Wilson**

9:35 250. Student-centered grading practices and the journey to (mostly) gradeless chemistry labs/lectures. **C.J. Sobers**

10:05 Intermission.

10:15 251. Bundle up! Using bundled grading in a remote organic chemistry course.
S.A. Habay

10:45 252. Techniques for getting students to meet the “specification” in specifications grading. **W. Hollinsed**

11:15 253. Five year study using specifications grading in an undergraduate chemistry curriculum. **H.J. Fletcher**

Virtual Room

Frontiers in Chemical Biology

Financially supported by Bristol Myers Squibb
J. Fox, C. L. Grimes, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 254. Mapping glycoconjugate interactions in native cellular environments. E. Joeh, W. Li, C. Parker, **M. Huang**

9:15 255. Catalytic activation of bioorthogonal chemistry with light (CABL) enables rapid, spatiotemporally-controlled labeling and no-wash, subcellular 3D-patterning in live cells using long wavelength light. **A.W. Jemas**

9:45 256. Modified *N*-acetyl muramic acid probes for improved bacterial peptidoglycan metabolic incorporation. **A.R. Brown**, K. Wodzanowski, C.C. Santiago, S.N. Hyland, J.L. Follmar, C.L. Grimes

10:00 257. Development of chemical biology probes for applications in drug discovery. **C. Am Ende**

10:15 258. Programmable technologies to retune gene expression at the RNA level. **K. Jones**, Y. Cao, S. Rauch, B.C. Dickinson

10:55 259. Activity-based proteomics: Target and ligand discovery on a global scale. **B.F. Cravatt**

11:35 Concluding Remarks.

Virtual Room

Innovations in Organic Chemistry

Financially supported by Organic Reactions

M. P. Watson, *Organizer, Presiding*

8:30 260. New methods for the synthesis of tetraarylmethanes. **A.J. Catino**, J.D. Selingo, M.J. Fadelici

8:50 261. Deaminative alkyl–alkyl cross-couplings of alkylpyridinium salts and alkenes. **K. Baker**, D. Lucas Baca, S.L. Plunkett, M.E. Daneker, M.P. Watson

9:05 262. Rapid synthesis of diverse imidazoles through microwave-assisted multicomponent reaction. **J.A. Smith**, M. Rotella, M. Osunsanya, I. Nwadike, B. Tankeu, O. Gutierrez

9:25 263. Diastereoselective alkynylations of β -(Bromo)iminium ions via Copper(I) catalysis. **S.O. Santana**, W. Guan, M.P. Watson

9:40 264. Study of the solubility of hypervalent iodine reagents and synthesis of hypervalent iodine reagents with increased solubility in non-polar solvents. **D.L. Silverio**, I.D. Hyatt, V. Seecharan, L. Armand, J. Noorollah, N. Singh, A. Zhang, K. Freddo, N. Spatola, S. Prasad, A. Chaudhry, S. War

10:00 Intermission.

10:10 265. Synthesis of a novel sulfide-modified salicylaldehyde auxiliary for flexible peptide ligation. **B.H. Williamson**

10:30 266. Cyclic sulfones from double conjugate addition of Rongalite. **M. Bebbington**

10:50 267. Practical implementation of predictive retrosynthesis in ReaxysChemistry database. **I. Samkurashvili**, S.E. Dueball

11:10 268. Photoredox catalysis for the synthesis of ambiphilic polymers via decarboxylative fluorination. **M. Talley**, C. Machado, W. Guan, T.H. Epps, M.P. Watson

11:25 269. T3P promoted synthesis of 2,3-diaryl-2,3-dihydro-1,3-thiaza-4-ones. **L.J. Silverberg**

Virtual Room

Nanoparticles: Characterization & Applications

Financially supported by Waters Corp.

L. Gundlach, *Organizer*

S. L. Neal, *Organizer, Presiding*

8:30 270. Plasmonic electricity: Fluorophore-induced plasmonic current. **C.D. Geddes**

9:10 271. Visualizing dynamic changes in metal nanoparticle surface chemistry. **K.A. Willets**

9:40 272. Terahertz camera-less imaging of semiconductors overcoming the Abbe diffraction limit. **A. Rahman**

10:10 Intermission.

10:25 273. Synthesis and characterization of carbon dots and their application in dye sensitized solar cell (DSSC). **J. Uddin**

10:55 274. Enhanced catalytic activity of nickel nanoparticles explained by bimetallic effect on carbon nanotube formation. **C. Byron**, M.S. Ferrandon, G. Celik, R. McCormick, J. Sloppy, K.S. Booksh, M. Delferro, C. Ni, A.V. Teplyakov

11:25 275. Algorithm for soot aggregate restructuring. **D. Singh**, O. Enekwizu, A. Khalizov

Virtual Room

Porous Materials

Financially supported by TA Instruments

E. D. Bloch, *Organizer, Presiding*

C. M. Brown, T. J. Kempa, *Presiding*

8:30 276. Design of functional sites in porous framework materials for energy storage. **V. Thoi**

8:50 277. Adsorption of small molecules in metal-organic frameworks. **C.M. Brown**

9:10 278. Perspective on novel porous materials scale-up: Practical challenges in manufacturing and commercialization. **M. Kapelewski**

9:30 279. Tunable Metal-Organic Framework (MOF) nanoparticles as inhaled drug delivery vehicles. Z. Stillman, B. Jarai, G. Decker, L. Attia, E.D. Bloch, **C. Fromen**

9:50 280. Microporous nanocomposite emulsion thermosets for multi-material, multifunctional porous composites. **Y.K. Patel**, J. Singer

10:10 Intermission.

10:25 281. Kinetic and deactivation mechanisms of isostructural MIL-101 for organic small-molecule oxidations. R. Yang, **M.L. Sarazen**

10:45 282. Stimuli-responsive 2D metal-organic frameworks prepared by chemical vapor deposition. **T.J. Kempa**

11:05 283. Beyond nanostructured supports: Maximizing catalytic centers in metal-organic frameworks. **A.J. Morris**

11:25 284. Metal-organic frameworks at the interface of medicinal and materials chemistry. M. Zick, R. Mandel, F. Chen, J. Woods, J. Lee, M. Gonzalez, E. Velasquez, A. Uliana, J. Hsu, J. Fuentes-Rivera, J.R. Long, J.J. Wilson, **P.J. Milner**

FRIDAY AFTERNOON

Virtual Room

Plenary: LaShanda Korley

Financially supported by University of Delaware
M. P. Watson, *Organizer*

L. Kayser, *Presiding*

1:00 Introductory Remarks.

1:05 285. Manipulating hierarchy, mechanics, and function in polyurea-peptide hybrids. **L. Korley**

1:50 Discussion.

Virtual Room

Dimensionality in Nanoscale Materials

Financially supported by Solenis

E. A. Hernandez-Pagan, *Organizer*

E. Hernandez-Pagan, *Presiding*

2:00 Introductory Remarks.

2:05 286. Insights into reaction intermediates to predict synthetic pathways for shape-controlled copper nanocrystals. **R. Buonsanti**

2:35 287. Chemically reversible isomerization in magic-sized clusters. **R.D. Robinson**

3:05 288. Laser-made nanocatalysts with controlled properties. **A.M. Müller**

3:35 Intermission.

3:45 289. Chelating agents in tandem with minimal concentrations of HF as an alternative method to produce highly crystalline MXene $\text{Ti}_3\text{C}_2\text{T}_x$ nanostructures. **L.R. De Jesus**, T.E. Mallouk

4:15 290. Design and synthesis of colloidal quantum dot nanostructures for photon upconversion. **T. Welsch**, J. Cleveland, M. Doty

4:45 291. Energy-based applications of multi-functional nanoscale systems. **S.S. Wong**

Virtual Room

Diversity in Polymer Chemistry and Engineering

Cosponsored by PMSE

Financially supported by Covestro

C. Fromen, L. Kayser, *Organizers, Presiding*

2:00 Introductory Remarks.

2:05 292. Merging organic synthetic and polymer chemistry: Toward accelerated catalysis and architecturally-diverse Sp^3 -enriched polymers. **E. Elacqua**

2:35 293. Two-dimensional perovskites with bifunctional ligands yield efficient and stable solar cells. **M. Ball**, X. Zhao, A. Kakekhani, T. Liu, A.M. Rappe, Y. Loo

3:05 294. Polymeric nanofiber scaffolds as an ex-vivo method for CD34+ Hematopoietic Progenitor Stem Cell (HPSC) growth and expansion. **C. Winstead Casson**, L. Lott

3:35 Intermission.

3:45 295. Responsive polymer nanocomposites. **S. Yang**

4:15 296. Precision polyolefins and the circular economy. **K. Beers**

4:45 297. New family of guanidine based n-type dopants and the structural effects on doping efficiency. **J.A. Schneider**, H. Nakayama, H. Wang, J. Read de Alaniz, M.L. Chabiny

Virtual Room

Excellence in Organic Chemistry and Chemical Biology Research with Undergraduates

Cosponsored by ORGN

S. A. Habay, *Organizer*

J. Fox, *Organizer, Presiding*

2:00 Introductory Remarks.

2:05 298. Observing and reversing the cysteine-perfluoroarene S_NAr reaction: towards a traceless tag for isolating expressed peptides. **J. Gavenonis**

2:35 299. Good things come in small packages: Cyclic peptide inhibitors to a protein-protein interaction initiating thrombosis and novel short peptide helices and turns. **D. Guarracino**

3:05 300. Designing 'intelligent' MRI contrast agents. **A.J. Rojas**

3:35 Intermission.

3:45 301. Untangling the mechanisms of chlorocarbene additions to strained bonds. **D.C. Merrer**

4:15 302. Bacterial capsule polymerases as tools for carbohydrate synthesis. **P.C. McCarthy**

4:45 303. From heterocycles to carbacycles: How to exploit nitrogen in small rings. **G. Moura-Letts**

Virtual Room

Nanoparticles: Characterization & Applications

S. L. Neal, *Organizer*

L. Gundlach, *Organizer, Presiding*

2:00 304. Manipulation of dimensionality, edge state, and strain in transition metal dichalcogenide nanocrystals. **T.J. Kempa**

2:40 305. Photo-induced charge transfer dynamics and mechanisms in thin-films of Sb_2S_3 . **E.R. Young**

3:10 306. Bidirectional excited-state charge-transfer and extended charge separation within covalently-tethered type-II CdSe/CdTe quantum dot heterostructures: Colloidal and multilayered systems. **C. McGranahan, G. Wolfe II, D. Watson**

3:40 Intermission.

3:55 307. Fibrous phosphorus quantum dots for cell imaging. P. Amaral, D.C. Hall, J. Krol, G. Ehrlich, **H. Ji**

4:25 308. Lipoic acid decorated gold nanoparticles and their application in the detection of lead ions. **W. GHANN**, T. Harris, J. Uddin

4:55 309. Long chain hydrosilanes as phase transfer agents. B.P. Chauhan, **E. Cook**, Q.R. Johnson