



Focusing on the Future of Chemistry

NERM 2022

October 2-5, 2022

Rochester Riverside Convention Center and the Hyatt Regency, Rochester NY

The overall NERM schedule will be:

Sunday, October 2:

9 am - 5 pm: Short course in polymer cross linking from John Texter. Hyatt Regency.

12-2 pm: NERACS Board Lunch, Hyatt Regency.

12-5 pm: High-School Teacher professional development. Highland Rooms. Convention Center Highland rooms.

12-1:30 pm: Undergraduate panel discussion about applying to grad school. Highland Rooms at Convention Center.

1:30-5:00 pm: 4 professional development workshops about succeeding in grad school, networking, finding the best career, etc. Highland Rooms at Convention Center.

5:00-8:00 pm: Expo hall opening reception. Expo Hall at Convention Center.

6:00-8:00 pm: Undergraduate Poster Session. Expo Hall at Convention Center.

7-9:00 pm: YCC/SCC Networking and Mentoring Dinner, off site at the Rochester Museum and Science Center (RMSC). (For grad students and SCC mentors)

Monday, October 3:

8 am-4:30 pm: Oral Technical Sessions

9 am- 4:00 pm: Expo Hall Open

Times TBA: One on One ACS Career Consulting (Resume review, mock interviews, etc.), Hyatt Regency.

4:00 -6:00 pm: Poster session in the Expo Hall at Convention Center.

4:30 -6:00 pm: Ceremony commemorating Kodak Research Park as a National Historic Chemical Landmark. (off site at Kodak Research Park. Buses running from Convention Center).

6:00- 9:00 pm: Regional Awards Ceremony and Banquet at Kodak.

Tuesday, October 4:

8 am-4:30 pm: Oral Technical Sessions

8 am – 3:00 pm: Expo Hall Open

12-1:30 pm: WCC Luncheon, Riverside Court.

4:30-5:30 pm: YCC/SCC Mixer, Lilac Ballroom, all invited.

5:30-6:30 pm: Harrison Howe Award Plenary Lecture by Wilfred van der Donk, Lilac Ballroom, all invited.

6:30-8:30 pm: Poster session and Networking Mixer, Galleria and Riverside Court

Wednesday, October 5:

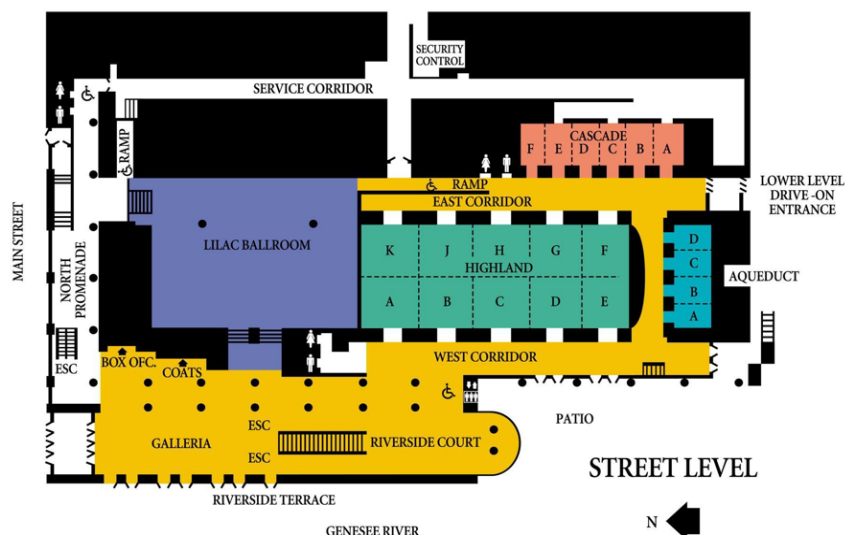
8:30 am -12:00 pm: Oral Technical Sessions

7:30-9:00 am: ACS Governance Social, Riverside Court

12:15- 3:00 pm: Small Chemical Business Round Table for Entrepreneurs, by invitation. Hyatt Regency.

Technical Sessions

Convention Center breakout rooms:



*Technical *asterisks indicate a change in schedule relative to the original schedule from MAPS. All speakers have been informed of these changes.*

SUNDAY AFTERNOON

Rochester Riverside Convention Center
Expo Hall

A. Charlebois, *Presiding*

5-8:00 pm Exhibition Hall Grand Opening

6-8:00 pm Undergraduate Poster Session

MONDAY MORNING

Rochester Riverside Convention Center
Aqueduct CD

Analytical Chemistry

R. S. Soman, *Presiding*

8:30 Introduction.

8:35 50. Multi-photon nonlinear laser wave-mixing spectroscopy for detection of SARS-COV2 nucleocapsid and spike proteins. **N. Shatirishvili**

9:05 51. Real time in vivo superoxide measurements using an electrochemical biosensor based on Cytochrome C. **A.S. DESHPANDE**, W.T. Muraoka, J. Wait, A. Colak, E. Andreescu

9:35 52. Getting to the “root” of the problem: Species identification of endangered wood by DART-HRMS and multivariate statistical analysis. **M. Ventura**, S. Beyramysoltan, B. Garosi, M. Appley, E. Espinoza, R.A. Musah

10:05 Intermission.

10:35 53. Utilizing quality structure retention relationships to predict retention times for per-/Poly-Fluoroalkyl substances (PFAS). **S. Simpson**, J. Antle, L. Halwatura, D.S. Aga

11:05 54. HPLC-UV method development and validation for quantification of human insulin from its degradation product. **I. Kimaru**, T. Smith

11:35 Concluding Remarks.

Rochester Riverside Convention Center
Aqueduct AB

Chemistry in Ceramics, Glass and Inorganic Materials

P. Tandon, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 131. Structural descriptors controlling sulfur solubility in borosilicate glasses. **A. Goel**, R. Saini, X. Xu, R. Youngman, H. Eckert, D. Neuville, J. McCloy

9:10 132. Photophysics and charge transfer properties of exciton polaritons. L. Qiu, A. Mandal, O. Morshed, M. Meidenbauer, W. Girten, P. Huo, A. Vamivakas, **T.D. Krauss**

9:45 Coffee Break in the Expo Hall.

10:15 133. Monolayer p-type doping in silicon using gallium and boron coordinate complexes. **S. Kurinec**, S. Williams, A. Taylor, C. Spaulding, G. Packard, G. Curvacho

10:45 134. Copper-containing glass-ceramic with high antimicrobial efficacy. **T. Gross**

11:20 135. Glass and Water. **M. Tomozawa**

Rochester Riverside Convention Center
Highland F

Environmental Chemistry

E. Stennett, *Organizer*

T. S. Dibble, N. Pflug, *Presiding*

8:30 Introduction.

8:35 257. Past and present variability in the oxidative capacity of the atmosphere. **L.T. Murray**, A.M. Fiore, D.T. Shindell, L.W. Horowitz, V. Naik, L. Yeung, A. Banerjee, H. Hu, Y. Yan, P. Martinerie, E. Witrant, J. Chappellaz, A. Orsi

9:15 258. Evaluation of the stable Isotopologue Budget of Methane with GEOS-Chem. **M. Shi**, L. Murray, J.D. Kessler, T. Weber

9:35 259. Characterizing sources of anthropogenic methane using co-emitted trace gases within the New York City metro area. **R. Commane**, L. Schiferl, A. Hallward-Driemeier, L. Murray, R. Toledo-Crow

9:55 Break.

10:15 260. Urban nitrous oxide emissions from New York City wastewater treatment. **A. Hallward-Driemeier**, R. Commane, L. Schiferl, R. Toledo-Crow, L. Murray

10:35 261. Integrating an N₂O mobile measurement system and atmospheric inversion technique. **C. Lonsdale**, K. Sun

10:55 262. Effects of an Interstate highway on atmospheric fine particles and adsorbed polycyclic aromatic hydrocarbons in Syracuse, New York. G. Townsend, **J.P. Hassett**

11:15 263. Wavelength dependent refractive index retrievals for vanillic acid: The influence of particle generation method. **V. Hosseinpour Hashemi**, M.E. Greenslade

11:35 264. Heterogeneous nucleation of a non-wetting vapor on NaCl aerosol nanoparticles and its implications on cloud forming and optical properties. **E. Demidov**, A. Khalizov

Rochester Riverside Convention Center
Highland H

Heterogeneous Catalysis

A. Ignatchenko, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 284. Reconciliation of published experimental data for structure-sensitive catalytic reactions. **X. Zong**, D.G. Vlachos

8:55 285. On-surface interactions and reactivity of metal-ligand single-atom heterogeneous catalysts. **S.L. Tait**

9:15 286. CO₂ hydrogenation on model Cu/ZrO₂/ZnO catalysts. L. Shi, J. Wang, **M.G. White**

9:35 287. Highly efficient and recyclable nickel-palladium bimetallic nanoparticles supported on multi-walled carbon nanotubes for copper-free Sonogashira cross-coupling reactions. **A.R. Siamaki**, K. Coker, L. Picinich

9:55 Break in the Expo Hall.

10:25 288. Active site requirements for chemoselective hydrogenation with binary and ternary intermetallics. **R.M. Rioux**, A. Dasgupta, H. He, G. Canning, A. Nyugen, M.J. Janik

10:45 289. Generalizing the mechanistic origins of reactivity and selectivity during ketone oxidative scission. **J. Bond**, R. Zhu, B. Liu, S. Wang

11:05 290. Competing dehydration reactions of branched alcohols on solid acid catalysts. **M. Todd**, T.J. Schwartz

11:25 291. Application and characterization of a novel Immobilized Cu(I) catalyst for heterogenous Copper-Catalyzed Azide-Alkyne cycloaddition of small molecules and bio-molecules in aqueous solutions. **R. Kandler**, S. Das, A. nag

Rochester Riverside Convention Center
Highland D

Nanoscale interaction and biosensing

X. Yong, *Organizer*

K. Du, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 381. Adhesive-free, stretchable, and permeable multiplexed biosensors for wound management. **A. Koh**, M. Brown

9:05 382. Novel single-molecule electrical detection method with applications in Cancer and Covid19 detection. **K.G. Pattiya Arachchillage**, S. Chandra, S. Rangan, J.M. Artes Vivancos

9:35 383. Role of metal-organic frameworks in the fabrication of sensors & biosensors. **A. Ensafi**

9:55 Coffee Break in the Expo Hall.

10:25 384. Implantable biosensors for real-time detection of dopamine in diagnostics. **E. DeVoe**

10:45 385. Precision synthesis of functional biointerfaces to direct microbial behaviors. **R. Yang**

11:15 386. Predicating the preclinical efficacy of anti-fibrosis agents using a force-sensing fibrosis on chip system. I. Hsia, M. Asmani, **R. Zhao**

Rochester Riverside Convention Center
Cascade CD

Organic Chemistry

B. E. Partridge, *Organizer, Presiding*
K. Houghtling, *Presiding*

8:15 427. Antimicrobial and structural characterization of streptothricin F, and the convergent synthesis of streptothricin analogs. **B. Miller**, M. Dowgiallo, M. Kassu, K. Smith, C. Morgan, A. Fetigan, Y. Marusyk, H. Warinner, J. Guo, E. Yu, J. Kirby, R. Manetsch

8:40 428. Enantioselective C–H bond functionalization of cyclic amines via biocatalytic carbene transfer. **X. Ren**, N. Liu, **B. Couture**, R. Fasan

9:05 429. Antimalarial activity of enantiopure tetrahydro- β -carboline benzofuran carboxamides. **H. Almolhim**, P.R. Carlier, M. Cassera, M. Totrov, Z. Rizopoulos

9:30 430. Modular synthesis of high-relaxivity prostate-cancer-targeted MRI contrast agents. **A.M. O'Brien**, D.M. Soika, H.F. Schmitthenner

9:55 Coffee Break.

10:25 431. Ligand-controlled carbopalladation regioselectivity in heteroannulation of 1,3-dienes: Regiodivergent synthesis of indolines. **J. Vaith**, D. Rodina, S.M. Paradine

10:50 432. Process chemistry development for end-to-end integrated continuous manufacturing of steroid API. **A. Neshchadin**, G. Zhu, Y. Li, Z. Fejedelem, J. Gamekkanda, A. Aloglu, S. Born, C. Hu

11:15 433. Haloalkane behavior in hydrophobic environments: Implications for drug design. **M.R. Ams**

Rochester Riverside Convention Center
Cascade AB

Innovations in Chemistry Education

S. Tysoe, *Organizer*

T. Goudreau Collison, C. L. Stanford, *Presiding*

8:30 Introduction.

8:35 306. Sign Language Incorporation in Chemistry Education (SLICE): How efforts made to include a few have rippling effects for many. **T. Goudreau Collison**

9:00 307. Exploring student's spatial understanding of molecules. **J. Bailey**

9:25 308. Power of analogies. **D.L. Newman**, C. Kapetenakis, S. Abdo, K. Wright

9:50 Coffee Break in the Expo Hall.

10:20 309. Protein landscape: A tool for exploring visual literacy in biochemistry. **K. Wright**, C. Dwyer, D.L. Newman

10:45 310. Establishing a sustainable infrastructure of peer mentors in first semester general chemistry to as in both academic and college culture acclimation. **S. Tysoe**, A. Ma, G. Korenowski, W. Colon, W. Woodward, J. Fayette

11:10 311. POGIL and The POGIL Project: Two decades of learner-centered pedagogy and professional development. **R.S. Moog**

11:55 Lunch.

1:10 312. Study habits in general chemistry with the COVID cohort. **A.S. McNeill**

1:35 313. Using smartphones to facilitate democracy in a large classroom. **B. Schabes**

2:00 314. Ensuring all students succeed: Methods implemented to support students with dyscalculia in General Chemistry. **J. French**

2:25 Coffee Break in the Expo Hall.

2:55 315. “Bio” chemistry for everyone as a DEI tool. **M. Colbert**

3:20 316. An asset-based approach to closing asymmetries in student success in general chemistry. **H. Sevian, K. Caushi**

Rochester Riverside Convention Center
Highland A

Advanced Materials and Technologies at Kodak

C. J. Coltrain, K. V. Heifferon, *Presiding*

8:30 Introductory Remarks.

8:50 9. Printed electronics – manufacturing using high-resolution flexography. **C. Ellinger**

9:15 10. Coordination complexes: Preparations and roles in imaging applications. **B.P. Cleary**

9:40 11. Engineering of self-supporting transparent membranes of fluorinated copolymers for 3D-printer technologies. **C.J. Coltrain, C.L. Bauer, L. Franklin, T. Jones**

10:05 Intermission in the Expo Hall.

10:20 12. Visual image formation in on-press developable lithographic printing plate precursors. **J. Huang**

10:45 13. Materials technology in the electrophotographic Kodak ASCEND Digital Press. P. Alexandrovich, M. Zaretsky, C. Kuo, K. Lofftus, **J. Honan**

11:10 14. Latex foam containing porous polymer microparticles in light blocking textile finishes: Tapping into the power of less. **M. Nair, J.S. Sedita, L.A. Lobo**

11:35 15. Kodak technology powering digital textile printing.. **G.L. French, K. Goodell**

Rochester Riverside Convention Center
Highland B

Advanced Polymer Materials 1 - Interfaces, Assemblies, and Composites

J. Texter, *Organizer, Presiding*

8:30 16. Keynote - Directed assembly of nanoparticles at oil/water interfaces. **E.P. Giannelis**

9:20 17. Unusual ionic conductivity of π -conjugated polymer, ionic liquid, and graphene nanocomposite films. **S. Krishnan**, A.P. Pitchiya, B.E. Slenker, T. Orimolade, A. Sreeram

9:55 Discussion.

10:30 18. Mesoscale modeling of reaction and assembly at colloid-polymer interface. **X. Yong**

11:05 19. Aliphatic polyesters based on 1,4-butanediol and C4 to C20 even numbered dicarboxylic acids. **J.R. Samonte**, M.J. Miri

11:25 20. Association of functional polymers with PFAS surfactants. **M. Tsianou**

Rochester Riverside Convention Center
Highland G

Chemistry of Emerging Technologies 1

H. Gysling, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 136. Nanozymes: Design, synthesis, and applications in bioassays. **X. Xia**

8:50 137. SunburstTM pretreatment: Enabling a true biorefinery. **S. Tudman**

9:35 138. Novel fluorescence-based binding characterization of small molecule ligands targeting CUG RNA repeats. **Z. Chang**, J. Sheng

10:05 Break in the Expo Hall.

10:35 139. Programmable RNA-targeting by CRISPR-CAS enzymes. **M. O'Connell**

11:20 140. OLEDWorks – growing OLED technology in Rochester. **J. Hamer**

Rochester Riverside Convention Center
Cascade EF

CO₂ Conversion and Utilization I

J. He, *Organizer*

A. M. Angeles Boza, *Organizer, Presiding*

8:30 150. Probing the distribution of alkali metal cations at the aqueous electrolyte/Au electrode interface under CO₂ reduction. **M. Waegele**

8:55 151. Controlling the product selectivity of electrocatalytic CO₂ reduction at [Mn(diimine)(CO)₃]⁻ catalysts. **J.J. Rochford**

9:20 152. Nanoparticle-catalyzed reduction of CO₂ via alkylcarbonate. **S. Sun**

9:45 Coffee Break.

10:10 153. Assemblies of gold nanoparticles on hydrophilic carbon fiber paper for aqueous CO₂ reduction. **C.P. Cox**, M. Wilsey, R. Forsythe, A.M. Müller

10:30 154. Deciphering the correlation between thermodynamic and kinetic hydricities of transition metal hydrides. **M.Z. Ertem**, M.R. Espinosa, A. Smith, N. Hazari, A.J. Miller

10:55 155. Solar CO₂ reduction using single atom catalysts on carbon nitride. E. Shaaban, E. Ahmad, T. Jin, A. St. John, **G. Li**

11:20 156. Monolayer molecular functionalization enabled by acid-base interaction for high-performance photochemical CO₂ reduction. **H. Wang**

11:45 157. Antimony Selenide as a promising photocatalyst for photoelectrochemical CO₂ reduction. **I. Sifat**, B. Li, A.G. Agrios

Rochester Riverside Convention Center
Highland K

Functional Materials I, Morning session

O. V. Zenkina, *Organizer*

S. Martic, O. Voznyy, *Presiding*

8:30 Introductory remarks.

8:35 271. Properties and surface chemistry of nanostructured electroactive materials. **S. Morin**

9:05 272. Optical and electrochemical sensors for biomedical applications. **S. Martic**

9:35 273. Investigating electrospun nanofibre materials and components for dye-sensitized solar cell applications. **B. Koivisto**, R. Mahmood

10:05 Coffee break.

10:30 274. From n-Heterocyclic Carbene-based metallopolymers to their corresponding metal nanoparticles. **A. Nazemi**

11:00 275. Of MOFs and MEF: Hybrid strategies for enhanced luminescent materials. **S. Impellizzeri**

11:30 276. Supramolecular materials based on Vibration Induced Emissive (VIE) fluorophores. **N.M. Ofodum**, Q. Qi, M. Tabor, X. Lu

Rochester Riverside Convention Center
Highland E

Optical Methods for Chemical and Biological Sensing

B. L. Miller, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 406. Synthesis of polymer sorbents for enhancing photonic sensor performance. **M. Yates**, E. Luta, J. Beard, B.L. Miller

9:15 407. Disposable Point-of-Care photonic diagnostics: COVID-19 immune surveillance. **D. Steiner**, M.R. Bryan, B.L. Miller

9:35 408. Activated platelet detection using a glycoprotein IIb/IIIa targeted near infrared fluorescence imaging probe. **K. Ha**

9:55 409. StaphAIR microarray detection of antibody responses to *Staphylococcus aureus* virulence factors in human serum. **A. Klose**, J. Daiss, L. Ho, C. Striemer, C. Beck, G. Muthukrishnan, B.L. Miller, L. Beck

10:15 Coffee Break in the Expo.

10:45 410. Plasmonic-enhanced fluorescence for rapid, multiplexed diagnostics. **N. Cady**

11:25 411. Development of a disposable photonics platform for clinical diagnostics and its application to SARS-CoV-2. **J.N. Butt**, M.R. Bryan, B.L. Miller

11:45 412. Combining DNA and protein engineering to construct a luminescent biosensor. **H. Sekhon**, S.N. Loh

Rochester Riverside Convention Center
Highland C

Polymer, Supramolecular and Nanoscale Materials I

X. Lu, *Organizer, Presiding*

8:00 Symposium Opening Remarks.

8:05 524. Programmable nanoscale materials. **O. Gang**

8:50 525. Nanostructured block polymer muscles exhibiting reversible actuation. **R. Hickey**

9:15 526. Recyclable network polymers via disulfide exchange derived from thiolactone-containing monomers. Y. Wu, A. Rolsma, **D.A. Shipp**

9:40 Coffee Break.

10:00 527. Biodegradable polymer-drug conjugates for pH-responsive release of anticancer drugs. **C. Cheng**

10:25 528. Regulating reactivities using mechanical force. **X. Hu**

10:50 529. Multiscale mechanically responsive polymeric systems: Design, applications, and beyond. **X. Lu**

11:15 530. Squitex: Biomanufacturing of Protein based fibers for creating Sustainable Materials. **M.C. Demirel**

11:55 Session Closing Remarks.

Rochester Riverside Convention Center
Highland J

Quantum Dynamics and Light-Matter Interactions

P. Huo, *Presiding*

8:00 538. First-Principles Study of Peridinin Chlorophyll- $\{it a\}$ Protein: Influence of initial excitation on energy transfer relaxation timescale. **D. Coker**

8:35 539. Simulating photo-induced electronic dynamics via quantum master equations. **E. Geva**

9:10 540. A uniform semiclassical framework for mixed quantum-classical nonadiabatic dynamics. **N. Ananth**

9:45 Intermission (coffee break).

10:15 541. Non-adiabatic quantum dynamics via ring polymer surface hopping. **F.A. Shakib**

10:50 542. Quantum dynamics via the exact factorization approach. **N. Maitra**

11:25 543. An exact formulation of quantum time correlation functions in terms of an open-chain path integral distribution. **M.E. Tuckerman**

MONDAY AFTERNOON

Hyatt Regency Rochester
Hyatt Susan B Anthony Room

Making Bonds and Breaking Boundaries: Modern Developments in Catalysis I

C. Kennedy, *Organizer*
S. M. Paradine, *Organizer, Presiding*

1:00 . New strategies in copper-catalyzed oxidative decarboxylation reactions. **J.M. Hoover**

1:30 122. Development of alkylaluminum scavengers to eliminate oligomer formation in polyethylene catalysis. **A. Young**, H. Do, P. Fontaine, D.M. Pearson

2:00 .* Radical tools to transform biomass sugars. **H.M. Carder**, A.E. Wendlandt

2:30 Break.

2:50 125.* Handling gases as solids: Fluorinated gas reagent delivery using metal-organic frameworks. **P.J. Milner**

3:20 . Photoenzymatic catalysis – using light to reveal new enzyme functions. **T. Hyster**

Rochester Riverside Convention Center
Aqueduct AB

3D Printing

B. J. LeSuer, *Organizer, Presiding*

1:00 1. On-demand modulation of 3D-printed elastomers using programmable droplet inclusions. **T. Mea**, J. Wan

1:25 2. Covalently functionalized cellulose nanocrystal-reinforced thermosetting polyurethane for 3D printing application via stereolithography. **N. Palaganas, J.O. Palaganas**, J.C. Millare

1:50 3. Sidekick: An inexpensive open-source 3D printed liquid dispenser. **B.J. LeSuer**

2:15 Break in the Expo Hall.

Rochester Riverside Convention Center
Highland A

A Century of Kodak Research: Historical Reflections

C. J. Coltrain, *Organizer*

J. H. Reynolds, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 4. Two hundred years of photographic history: A retrospective. **T. Gustavson**

1:45 5. Historical reflections of latent image formation studies in silver halide. **R.C. Baetzold**

2:10 6. Making Kodak film: State-of-the-art film manufacturing. **R.L. Shanebrook**

2:35 Coffee Break.

2:55 7. Expanding the heart of imaging – Reflections on the history of the Kodak Research Labs. **N.S. Ferris**

3:20 8. Disruptive innovation: The story of the first digital camera. **S. Sasson**

Rochester Riverside Convention Center
Highland B

Advanced Polymer Materials 2 - Colloids, Coatings, and Amphiphilic Copolymers

J. Texter, *Organizer*

T. Long, *Presiding*

1:30 21. Microcapsule-based smart polymer composites. **X. Lu**

2:05 22. Xanthan gum polysaccharide aqueous solution viscosity: salt and temperature effects. **E.M. Nsengiyumva**, M.P. Heitz, P. Alexandridis

2:25 Coffee Break in the Expo Hall.

2:55 23. Nanostructured materials from bottlebrush copolymers. **J. Rzayev**

3:30 24. A novel triblock copolymer: Synthesis and self-assembly. **P. Chuquimarca**, A. Sarkar

Rochester Riverside Convention Center
Highland F

Environmental Chemistry

T. S. Dibble, N. Pflug, *Presiding*

1:00 224. Environmental effects in the photosensitized conversion of NO₂ into HONO on humic acid films. H.M. Ricker, A.L. Leonardi, **J.G. Navea**

1:20 225. Atmospheric fate of H₂O₂: The Hg(II) product of OH-initiated oxidation of Hg(0). **D. Hewa Edirappulige**, C.K. Beckett, I.J. Kirby, T.S. Dibble

1:40 226. Exploring the uncanonical chemistry of carbonyl-substituted peroxy radicals in atmospheric oxidation chemistry. **V. Barber**, Y. Li, F. Keutsch, W.H. Green, J.H. Kroll

2:00 Break in Expo Hall.

2:30 227. Development of analytical tools for rapid low-cost detection of emerging contaminants and perfluoroalkyl substances. **E. Andreescu**

3:10 228.* Up against the wall: Comparative examination of the ease of antibiotic and fungicide oxidation by Fe-TAML/H₂O₂. **H. Frame**

3:30 229. Phytoremediation of PFAS compounds by *Pistia stratiotes* and *Eichhornia crassipes*. A. Kenyon, **L. Newman**

Rochester Riverside Convention Center
Highland D

Nanoscale interaction and biosensing

K. Du, *Organizer*

X. Yong, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 387. CRISPR-powered biosensing for molecular diagnostics of infectious diseases. **C. Liu**

1:35 388. Enhancing plasmonic biosensing via integrated physical and chemical approaches. **Q. Yu**

2:05 Coffee Break in the Expo Hall.

2:35 389. RNA electrical conductivity, biomolecular interactions, and single-molecule electrical biosensing. K.G. Pattiya Arachchilage, S. Chandra, A. Castillo, S. Rangan, **J.M. Artes Vivancos**

2:55 390. Computational modeling of interactions between arbitrary shaped nanoplastics and cell membranes. **D. Redwan**, K. Du, X. Yong

3:15 391. Polyvinylpyrrolidone-induced photocatalysis of gold nanorod growth with interband excitation. **B. Roche**, V. Singla, T. Vo, W. Chang

Rochester Riverside Convention Center
Aqueduct CD

Plastics Recycling Chemistry for a Sustainable Future

P. Alexandridis, *Organizer*
L. A. Velarde, *Presiding*

1:00 Introductory Remarks.

1:05 518. Mechanochemistry based recycling of polyethylene into smaller hydrocarbons. **Y. Ghosh**, D. Theberge, L. Wilcox

1:35 519. Molecular-level automation for mechanical sorting of plastic waste: High-throughput multi-modal sensing and computer vision for sustainable recycling industries. **N. Stavinski**, V. Maheshkar, Y. Zhao, T. Thundat, K. Dantu, L.A. Velarde

2:05 520. Dissolution/precipitation process for the chemical recycling of plastic waste. **C. Ferger**, N. Cejic, J. Mazer, P. Alexandridis, M. Tsianou

2:25 Coffee Break in the Expo Hall.

2:55 521. Dissolution of semicrystalline polyethylene in the chemical recycling of polyolefins. **A. Ghasemi**, C. Ferger, P. Alexandridis, M. Tsianou

3:15 522. Polyethylene upcycling through controlled breakdown and functionalization. **G. Kerr**, J. Rzyayev

3:35 523. New methods for polymer chemical recycling to monomer. **L.H. Kugelmass**, E. Stache

Rochester Riverside Convention Center
Highland E

Advancements in Protein Chemistry and Applications

R. Fuanta, *Organizer, Presiding*

1:00 Introductory remarks.

1:05 41. Structural effects of Ser165 phosphorylation in α -tubulin. V. Maddula, N.S. Holtzman, M.C. Nagan, **S.A. Rotenberg**

1:25 42. Insights into the structure and topography of caveolin. **K.J. Glover**

1:45 43. Triggering toxicity: Detecting outer membrane vesicles released from Escherichia coli in the presence of antibiotics. **L. Vacca Michel**, N. Singh, M. Videva, T. Gaborski

2:05 44. Autophosphorylation of tyrosine kinases regulate biofilm formation in the bacteria Bacillus subtilis. **S. Wacker**, M. Duncan, M. Elsaid

2:25 Break.

2:55 45. Investigation of protein corona by amyloidogenic peptides and nano-size dependent aggregates formation. **K. Yokoyama**

3:15 46. Peptide and protein aggregation and inhibition: From small molecules to large antibodies. **S. Martic**

3:35 47. Design, synthesis, and evaluation of anti-inflammatory antibody-drug-conjugates (ADCs) that target monocytes and macrophages. J.M. Howe, S. Fang, B. Brems, K.A. Watts, F. Xu, J.T. Miller, **L.N. Tumey**

3:55 48. Predicting de novo peptides binding to TRAP protein for drug delivery design. **Q.L. Campbell**, Z. Yang, A.D. White

4:15 49. Droplets, tails and loops: the role of intrinsic disorder in R-loop biology. **L. Dettori**, D. Torrejon, A. Chakraborty, A. Dutta, M. Mohamed, C. Papp, V. Kuznetsov, P. Sung, W. Feng, A. Bah

Rochester Riverside Convention Center
Highland G

Chemistry of Emerging Technologies 2

H. Gysling, *Organizer, Presiding*

1:00 141. Metal-Organic frameworks at the Interface of organic chemistry and materials science: From catalysis to chemical separations. **P.J. Milner**

1:50 142. Chemistry and materials science in additive manufacturing. **B. Kahn**

2:30 Break in the Expo.

3:00 143. Transition metal nanoparticle inks for printed electronics and additive manufacture. **K. Reed**, J. Fagnoli, D. Cormier, T. Hull

3:45 144. Artificial Intelligence-powered chemistry. **X. Zhang**

Rochester Riverside Convention Center
Cascade EF

CO2 Conversion and Utilization II

A. M. Angeles Boza, *Organizer*

J. He, *Organizer, Presiding*

1:00 158. Well-defined catalyst for CO₂ conversion. **S. Zhang**

1:25 159. Computational study on the reactivity of imidazolium-functionalized manganese bipyridyl tricarbonyl electrocatalysts [mn[bpyme(im-r)](co)₃br]⁺ (R = ME, ME₂ and ME₄) for CO₂-to-CO conversion over H₂ formation. **J. Panetier**

1:50 160. In-situ investigations of dynamic structural evolution of Cu-based bimetallic catalysts during the electrochemical CO₂ reduction. **H. Zhu**

2:15 161. Carbon dioxide reduction with a synthetic biocatalyst. **A. Salamatian**, J.L. Alvarez-Hernandez, K. Bren

2:35 Coffee Break.

3:05 162. Nanoarray engineered catalysts for CO₂ conversion at high efficiency and low cost. **P. Gao**

3:30 163. Positively tuning the microenvironment of CO₂ reduction catalysts using local cations. **G. Manbeck**, L. Rotundo, M.Z. Ertem

3:55 164. Artificial leaf design with remarkable quantum conversion efficiency in bicarbonate to formate. **M.D. Heagy**

4:20 165. Control of clean syngas compositions from electrochemical CO₂ reduction using ionomer overlayers on carbon fiber paper electrode assemblies. **R. Forsythe**, C.P. Cox, M.K. Wilsey, A.M. Müller

Rochester Riverside Convention Center
Highland K

Functional Materials II, Afternoon session

O. V. Zenkina, *Organizer*
S. Impellizzeri, A. Nazemi, *Presiding*

1:00 265. Applying machine learning to search for new materials for clean energy. **O. Voznyy**

1:25 266. Correlation analysis to study disorder in solid-state electrocatalysts. **R.D. Smith**

1:50 267. Recent advances in doped metal oxide fuel cell catalyst supports. **E.B. Easton**, R.A. Esfahani, K. Black-Araujo, P.D. Melino, M.T. Sullivan

2:15 Coffee break.

2:45 268. Surface ligand-mediated synthesis of chemically tailored two-dimensional all-inorganic perovskite nanocrystals. **W. Zheng**

3:10 269. Facilitated electron transfer by MN dopants in 1-dimensional CDs nanorods for enhanced photocatalytic water splitting. **W. MacSwain**, H. Lin, S. Li, C. Chu, W. Zheng, G. Leem

3:35 270. Synthesis of all-inorganic perovskite/double perovskite core/shell NCs. **H. Lin**, W. Zheng

4:00 Concluding remarks.

Rochester Riverside Convention Center
Highland H

Metal Oxide Clusters and Materials I

K. E. Knowles, E. M. Matson, *Presiding*

1:00 365. Emergent phenomena in colloidal d0 metal oxide semiconductor nanocrystals. **K.R. Kittilstved**

1:25 366. Pulsed laser in liquids synthesis of nanocatalysts for sustainable electrocatalytic processes. **A.M. Mueller**

1:50 367. Catalytic oxidative alcohol dehydrogenation by perfluorinated v oxo-alkoxide systems. M.I. Kitt, E. Amir, E. Sloane, C.M. Sabanos, S.M. Moore, A.B. Beeler, J.K. Snyder, **L.H. Doerrer**

2:15 368. Hydrogen atom binding to nickel oxide electrodes and its catalytic implications. **H. Noh**, M. Houck, J.M. Mayer

2:40 Break in the Expo Hall.

3:10 369. MxMyV₂O₅-quantum dot heterostructures with programmable electronic structure for excited-state charge transfer and photocatalysis. **D. Watson**

3:35 370. Surface ligands influence the selectivity of cation uptake in polyoxovanadate-alkoxide clusters. **E. Schreiber**, R.E. Garwick, W.W. Brennessel, J.R. McKone, E.M. Matson

4:00 371. Examining proton and electron transfers in aqueous iridium oxide nanocrystals. **J.L. Lee**, J.M. Mayer

Rochester Riverside Convention Center
Cascade CD

Organic Chemistry

B. E. Partridge, *Organizer, Presiding*
J. Vaith, *Presiding*

1:00 413. Study on amide bond conformation of the heterocyclic backbone containing peptide. **S. Suwal**

1:25 414. Ultra-tight binding affinity, strong positive cooperativity, and supramolecular isomerism of a new class of aromatic oligoamide macrocycles with a cyclodirectional backbone. **T.A. Sobiech**, Y. Zhong, B. Gong

1:50 415. Aerobic copper-catalyzed aminooxygenation of β,γ -unsaturated carbamates: Synthesis of 4-benzoyl-oxazolidin-2-ones. **C. McNichol**, S.M. Paradine

2:15 416. Use of building blocks symmetry for the diversification of the carbon Schwarzites bottom-up synthetic design. **A. Ignatchenko**, J.P. Willower, S.M. French

2:40 Coffee Break in the Expo Hall.

3:10 417. Withdrawn

3:35 418. Urea ligands and palladium catalyze the heteroannulation of diverse multicyclic heterocycles. **K. Houghtling**, O. Monteferrante, S.M. Paradine, A. Kropiwnicki

4:00 419. Biosynthesis of multifunctional polycyclic peptides via pCmF-mediated cyclization. **A. Saseendran**, E. Yeung, R. Fasan

Rochester Riverside Convention Center
Highland J

Quantum Dynamics and Light-Matter Interactions

P. Huo, *Organizer*

N. Maitra, F. A. Shakib, *Presiding*

1:00 563. Diffusive to ballistic transport of exciton polaritons. **A. Mandal**, D.R. Reichman

1:30 564. Semiclassical simulations of polariton chemistry. **T. Li**, S. Hammes-Schiffer

2:00 565. Incorporating Lindblad decay dynamics into mixed quantum-classical simulations. **E. Koessler**, A. Mandal, T.D. Krauss, P. Huo

2:30 intermissions (Coffee Break).

3:00 566. Resolution of gauge ambiguities in molecular cavity quantum electrodynamics. **M. Taylor**, A. Mandal, P. Huo

3:30 567. Modeling polaritonic chemistry via exact factorization-based trajectory methods. **S. Roy**, N. Maitra

4:00 568. Resonant cavity modification of ground state chemical kinetics. **L. Lindoy**, A. Mandal, D.R. Reichman

Rochester Riverside Convention Center
Highland C

Polymer, Supramolecular and Nanoscale Materials II

X. Lu, *Organizer, Presiding*
D. A. Shipp, *Presiding*

1:00 Session Opening Remarks.

1:05 531. Active matter swarms for cargo capture, transport, and delivery. **A. Sen**

1:50 532. Tuning emergent crystalline order in self-assembly simulations. **J. Dshemuchadse**

2:15 533. Interconverting electrical and mechanical energy with organic self-assembled piezoelectric films. **G. Hutchison**

2:40 Coffee Break.

3:00 534. Degradation of organic molecules by Tribovoltaic mechano-electrochemistry. **J. Liu**

3:25 535. Smart materials with tunable properties based on low melting point alloys. **W. Shan**

3:50 536. Design and synthesis of soft actuators for photo-control of multiscale movement. J. Gomez, S. Talebi, S. Kim, E. Doukmak, **R. Steinhardt**

4:15 537. Soft intelligent materials with liquid metal and liquid crystal elastomer. **C. Majidi**

4:55 Session Closing Remarks.

Rochester Riverside Convention Center
Aqueduct AB

Multiscale assembly of living and physical materials

J. A. Diaz, *Organizer, Presiding*

3:00 Introductory Remarks.

3:05 378. Programming the hierarchical assembly of biological and bioinspired molecules. **B.E. Partridge**

3:45 379. Detailed control of droplet size for self-assembly. **T. Niper**, J.A. Diaz

4:15 380. Porous mesoscale colloids with adjustable shape. **L. Galeano Tirado**, J.A. Diaz

4:45 Concluding Remarks.

Rochester Riverside Convention Center
Expo Hall

4-6:00 pm Poster Session for Environmental Chemistry, Physical Chemistry, Analytical Chemistry, Organic Chemistry, Inorganic Chemistry and Chemical Education.

TUESDAY MORNING

Rochester Riverside Convention Center
Aqueduct CD

Oxidations and Electrochemistry in Organic Synthesis: The James Bobbitt Memorial Symposium

N. E. Leadbeater, J. Rusling, *Presiding*

8:30 Introductory Remarks.

8:35 467. Highlighting James Bobbitt's legacy in undergraduate education: Recent applications of oxoammonium salts in the undergraduate teaching and research laboratories. **J. Milligan**, K.M. Lambert, C. Kelly, L.J. Tilley

8:55 468. Ligand effect in electroreduction of CO₂: N-heterocyclic carbene-capped polymers to promote catalytic efficiency. **J. He**

9:15 469. Monovalent nickel-mediated radical formation: A concerted halogen-atom dissociation pathway determined by electroanalytical studies. **T. Diao**

9:35 470. Electrochemical recycling of adenosine triphosphate in biocatalytic Cascades. **S. Ruccolo**, G. Brito, M. Christensen, T. Itoh, K. Mattern, K. Stone, N. Strotman, A. Sun

9:55 471. Enhancing oxidant strength via induction: Novel α -perfluoroalkyl Bobbitt salt variants.. **L.J. Tilley**, D. Del Sesto, J. Freeman, A. Hoang

10:15 Break in the Expo Hall.

Rochester Riverside Convention Center
Highland B

Advanced Polymer Materials 3 - Nanofluids, Energy, and Interpenetrating Networks

J. Texter, *Organizer*
C. J. Coltrain, *Presiding*

8:30 25. Solvent-free nanofluids for advanced materials. **J. Texter**

9:05 26. Silicon polymer interactions and their relevance in energy storage. **S. Moganty**

9:40 27. Auto-dispersing polyester nanofluids. **Y. Bian**, J. Texter

10:00 Coffee Break in Expo Hall.

10:30 28. Keynote - Mechanics and percolation in extracellular matrices of soft tissues. **M. Das**

11:20 29. Reactive CeO₂ nanofluids for UV protective coated films. **K. Reed**, R. Maniglia, J. Texter

Rochester Riverside Convention Center
Highland G

Battery and Energy Storage

M. Ganter, C. J. Patridge, P. Taboada-Serrano, *Organizers*
H. Liu, *Organizer, Presiding*

8:30 82. Interaction and transformation of defects in energy materials. **A. Singer**

8:55 83. Using nuclear magnetic resonance to connect interphase composition and performance in K-ion batteries. **D. Ells**, R. May, L. Marbella

9:20 Break.

9:45 84. Towards the applicability of density functional tight binding to charge transport in quinones in solution and in the solid state. **P. Goyal**, M.M. Kithika, M. Redington, J. Zhang, Y. Yao, J. Andrews

10:10 85. Battery simulations with ab initio molecular dynamics. **M. Smeu**

10:35 86. Process design for calcination of nickel-based cathode materials by in situ characterization. **F. Wang**

11:00 87. Using in situ Raman spectroscopy to track electrochemical reactions. P. Xu, B. Bruno, **J. Suntivich**

Hyatt Regency Rochester
Hyatt Susan B Anthony Room

Chemistry and Patent Law

J. Barrera, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 127. Contact lens wars: CibaVision v. Bausch and Lomb. **J. Barrera**

9:10 128. Chemists & chemical engineers as patent practitioners: Careers in intellectual property. **D.J. Jakiela**

9:45 Break.

10:05 129. Chemical patents: Completion and possession of invention. **J. Barrera**

10:40 130. Panel discussion: Transition from scientist to patent attorney/agent. **J. Barrera**

Rochester Riverside Convention Center
Highland E

Emerging Strategies for Chemical Probing and Control of Biological Processes

R. Fasan, *Organizer, Presiding*

8:30 210. Modular synthesis of peptide-based targeted molecular imaging and therapy agents for cancer. **H.F. Schmitthener**, E.C. Stafford, M.V. Law, M.P. Henry, J.C. Crandall, C.R. Kelly, J. Lapham, S.N. Shaut, C.W. DeNyse, **A.M. O'Brien**, M.C. Ferran

9:00 211. Photoresponsive probes for dopamine and serotonin receptors: chemoproteomics and bioorthogonal control. **R. Steinhardt**, S. Kim, E. Doukmak, M. Shanguhya

9:30 212. Chemical control of human Hedgehog ligand biosynthesis with conditional protein autoprocessing: A test system for synthetic vitality. **B.P. Callahan**

10:00 Coffee Break in Expo Hall.

10:30 213. Functional delivery of siRNA by cyclic amphipathic peptides. **B.L. Nilsson**

11:00 214. Light-responsive probes: Guiding clinician decision-making and destroying cancer. **A. Beharry**

11:30 215. Chemoenzymatic synthesis of a diverse collection of natural product-like compounds with anti-cancer activity. **J.M. Bennett**, A.R. Bortz, R. Fasan

Rochester Riverside Convention Center
Highland F

Environmental Chemistry

N. Pflug, E. Stennett, *Presiding*

8:30 Introduction.

8:35 249. “Free drugs”, “superbugs”, and “forever chemicals” in the environment: Occurrence and implications. **D.S. Aga**

9:15 250. Selective organophosphate removal by adsorption on metal hydroxides/oxides nanowires. **G. Pathiraja**, H.P. Rathnayake, S.O. Obare

9:35 251. Elucidating photoelectrocatalytic degradation of carbamazepine in a dye-sensitized photoelectrochemical cell. **M. Frame**, U.K. Wijethunga, L. Powers, N. McMillan, B. Sherman, S. Fernando, C. Bunker, G. Leem

9:55 252. Drivers affecting the aging of plastics in freshwater ecosystems. **N.C. Eddingsaas**, M. Cureaux, C. Tyler

10:15 Break.

10:35 253. Association of ambient fine particulate air pollution (PM_{2.5}) with cardiovascular morbidity in a Megacity Karachi, Pakistan. **H. Khwaja**

10:55 254. Assessment of personal exposure of size-segregated particulate matter and black carbon. **A. Jamal**

11:15 255. Bioaccessability of metal(loid)s in high-latitude mineral dust aerosol by inhalation-ingestion assay. **A. Downey**, A. Dourlent, J. King, P. Hayes

11:35 256. In utero exposure to lead, cadmium, mercury, and arsenic: assessing umbilical cord tissue for trace element analysis in human biomonitoring studies. **D.R. Luneau**, A.L. Galusha, A.C. Farnsworth, T.M. O'Shea, R.C. Fry, P.C. Kruger, P. Parsons

Rochester Riverside Convention Center
Highland H

Heterogeneous Catalysis II

A. Ignatchenko, *Organizer*

8:30 Break in the Expo Hall.

8:35 292. Simulation of pore filling in meso- and micro-porous catalyst supports. **B.M. Walden**, S.W. Bonnevie, R.A. Pollock, B.G. Frederick, F.G. Amar

8:55 293. Nano catalysts in heterogeneous catalytic and electrocatalytic reactions. **C. Zhong**

9:15 294. Kinetic model of tungsten oxide catalyzed conversion of glucose to lactic acid and hydroxymethylfurfural. **C.K. Boucher**, A. Mahdavi-Shakib, T.J. Schwartz, B.G. Frederick

9:35 295. Water oxidation reaction: From high-valent metal oxo species to photoactive assemblies. **R. Ezhov**, Y. Pushkar

9:55 Introductory Remarks.

10:25 296. Morphology controlled WO₃ for the photocatalytic partial oxidation of CH₄ to CH₃OH. **D. Premachandra**, M.D. Heagy

10:45 297. Measuring speciation of dilute low-Z dopants in photocatalysts with fluorescence XAFS. **C. Geci**, B.G. Frederick, R.W. Meulenberg

11:05 298. Identifying descriptors for electrochemical anion adsorption. **I. McCrum**

11:25 299. Unraveling the complexities of selective electrochemical oxidations of hydrocarbons. **M. Wilsey**, M.R. Forney, A.M. Mueller

Rochester Riverside Convention Center
Cascade AB

Innovations in Chemistry Education

T. Goudreau Collison, C. L. Stanford, *Organizers*
S. Tysoe, *Presiding*

8:30 Intro.

8:35 300. Reformed Experimental Activities (REActivities): Assessing student and instructor engagement in an undergraduate organic chemistry lab.. **T. Goudreau Collison**

9:00 301. Evaluating the development of transferable skills and content knowledge in an organic chemistry laboratory curriculum. **C.L. Stanford**, T. Goudreau Collison, J. Fernandes, I. Gaston, E. Ham, E. Schneider

9:25 302. Illustrating key concepts: Introducing small-molecule crystallography to chemistry undergraduates using a flexible laboratory module. **S. Zheng**

9:50 Break.

10:20 303. Development and implementation of a multi-year, CURE-based chemistry lab curriculum. **J.J. Peterson**, E. Helms, M. Webb

10:45 304. Developing guided-inquiry labs for general chemistry that incorporate inclusivity, continuity, and engaged student learning. **C.L. Stanford**, J.W. Ribblett, S. Beechboard, E. Danzeisen, B. Miller, T. Ratliff

11:10 305. Pathways into chemistry education research – A case study. **T.D. Kim**

Rochester Riverside Convention Center
Highland D

Nanoscale interaction and biosensing

X. Yong, *Organizer*

K. Du, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 392. Toward the development of nanopocket membranes for the purification and fractionation of extracellular vesicle subpopulations. **T. Gaborski**

8:55 393. Development of 3D-printable nanocomposite for colorimetric lactate sensing in sweat. **I.Y. Dong**, O.S. Popoola

9:15 394. Investigation of adsorption of SARS-CoV-2 spike protein onto gold nanocolloids. **K. Yokoyama**

9:35 395. Nanoparticle-blocked nanopores: Fundamentals and applications. **C. Duan**

9:55 Coffee Break in the Expo Hall.

10:25 396. Measuring charge transport properties in single and double-stranded RNA oligonucleotides at the Nanoscale. **S. Chandra**, K.G. Pattiya Arachchillage, J.M. Artes Vivancos

10:45 397. Label-free aptamer sensor for early detection of SARS-CoV-2 from enriched wastewater with all-portable in-line sampling and sensing. **P. Sen**, Z. Zhang, P. Li, T. Guo, B. Adhikari, J. Gu, A.R. Macintosh, Y. Li, L. Soleymani

11:05 398. Molecular challenges to treating Alzheimer's disease. **S. Nangia**

Rochester Riverside Convention Center
Aqueduct AB

Computational Tools for Materials Science I

P. Padmanabhan, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 166. Crystal growth and design with coarse-grained particle models. **J. Dshemuchadse**

9:15 167. Machine-learned features to solve crystal structure classification problems. **S. Lee**, A.O. Oliynyk

9:35 168. Colloidal coarse-grained simulations of SNIPS self-assembled block copolymers. **L.A. Nieves Rosado**, F. Escobedo

9:55 169. MELD-Bracket: Quickly screen for the most stable state. **E. Brini**, C. Liu, K. Dill

10:15 Break in Expo Hall.

10:40 170. Understanding the effect of solvent quality on the cooperativity of polymer adsorption on faceted nanoparticles via molecular simulations. **M.S. Alshammasi**, F. Escobedo

11:00 171. Molecular model agnostic counterfactual explanations (MMACE) in explainable AI. **G.P. Wellawatte**, A. Seshadri, A.D. White

11:20 172. Thermodynamics of chiral block copolymers. **M. Grant**, P. Padmanabhan

11:40 173. Computational study of nano-porous metal-organic frameworks for adsorptive desulfurization of Petroleum. **D. Limbu**, Y. Shi, M. Momeni, F.A. Shakib

Rochester Riverside Convention Center
Cascade EF

Defining and Encouraging DEIR

A. Charlebois, L. Daniele, R. E. Rogers, K. Sanchez Lievano, *Organizers*
T. E. Pagano, *Presiding*

8:30 Introductory Remarks.

8:35 182. A Chemist, a Biologist, and a Sociologist walk into a bar: Creating DEIR in higher education. **B. Chan**

8:55 183. Dow and NTID: Learnings from a decade of partnership. **S.T. Wills**

9:15 184. Improving inclusivity for students who are deaf and hard-of-hearing in chemistry classrooms and laboratories. **A.D. Ross**, T. Sarchet, T.E. Pagano

9:35 185. Equity for women faculty in STEM at primarily undergraduate institutions: Issues and solutions. **W. Pogozeleski**, S.A. Wasileski, K. West, C. Mills, J. Rodriguez, C. Margherio, D. Dembroski

9:55 Intermission.

10:20 186. Experimentalism to drive systemic change to create equity in chemistry courses. **B. Chan**

10:40 187. Techniques and a template for inclusivity and engagement in chemistry courses. **M. Colbert**

11:00 188. Best practices for the Advancement of diversity, equity, and inclusion in chemistry and chemical engineering education. **R.E. Rogers**, T.E. Pagano

11:20 189. Panel discussion: Moving forward with DEIR. **L. Daniele**

Rochester Riverside Convention Center
Highland K

Functional Materials III

O. V. Zenkina, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 277. Relating non-covalent interactions of conjugated materials to optical properties for applications in optoelectronics. **E. Guzman**, S.W. Thomas

9:05 278. Inserting an “atomic trap” for directional dopant migration in core/multi-shell quantum dots. **C. Chu**, E. Hofman, A. Khammang, J.T. Wright, J. Franck, R.W. Meulenberg, W. Zheng

9:35 279. Ionic Reverse Osmosis Membranes for Purifying Water: A New Generation of Resistance. **M. Mecham**, M. Armstrong, T. Schumacher, J. Riffle

10:05 Break in the Expo Hall.

10:30 280. Properties of materials used in clear face masks. **B.M. Strohm**, **P.J. Nikolai**, **A. Jahn**, S.M. Demyttenaere, M.J. Miri

11:00 281. High-performance 3D-printable wearable devices for UV-sensing applications. **R. Chandradat**, A. Finny, O. Popoola, Q. Qi, E. Andreescu, X. Lu

11:30 282. Plant-derived nanocarriers for aerosol drug delivery to treat bacterial pulmonary infections. D. Ali, L. Gravel-Tatta, A. Badia, **C. DeWolf**

Rochester Riverside Convention Center
Highland A

Inorganic Chemistry

E. S. Cueny, *Organizer, Presiding*

8:00 329. Synthesis of teatherable BIS-Iminopyridine ligands for heterogeneous catalysis. **J.R. Andreatta**

8:25 330. Breaking the C₃-symmetry of tris(amido)amine ligands: Synthesis, structure and metalation. **M. Naeem**, D.R. Manke

8:45 331. Copper(II) complexes of pyrazine-1,4-dioxide: Chains and layers. R. Rodríguez Pérez, C.P. Landee, L.N. Dawe, M. Deumal, D.A. Dickie, **M.M. Turnbull**

9:10 332. Introducing dopants into magic-size semiconductor nanocrystals. J. Denhardt, H. Kim, **K.R. Kittilstved**

9:35 333. Kinetic and mechanistic analysis of alkene polymerization via chromophore quench labeling. **E.S. Cueny**

10:00 Coffee Break in the Expo Hall.

10:30 334. Insight into reaction mechanism of amino-oxygenation of olefins with functionalized hydroxylamines. **A.G. Radovic**, N. Wolford, M.L. Neidig

10:55 335. O-atom vacancy formation in anionic POV-alkoxides with variable surface ligands. **C.Y. Peter**, A.A. Fertig, E. Schreiber, **E.M. Matson**

11:20 336. Node-based functionalization to enhance properties of zirconium-based metal-organic polyhedra. **M.G. Sullivan**, G.E. Sokolow, T.R. Cook

11:40 337. Copper(II) halide salt complexes of 5-bromo-2-aminopyridine and 3,5-dibromo-2-aminopyridine. **C.P. Bedford**, C.P. Landee, J.L. Wikaira, M.M. Turnbull

Rochester Riverside Convention Center
Highland C

Materials Design, Manufacturing and Devices

X. Lu, *Organizer, Presiding*

8:00 Session Opening Remarks.

8:05 358. Future smart materials systems from ultrasmall silica nanoparticles. **U.B. Wiesner**

8:50 359. Shape-memory polymer programming via printing. **J. Henderson**

9:15 360. Direct laser writing of shape-memory networks. **M.L. Anthamatten**, M.P. Jeske, D.R. Harding

9:40 Coffee Break.

10:00 361. Upcycling compact disks for advanced soft bioelectronics. **A. Koh**, M. Brown

10:25 362. Hybrid laser platform (HLP) for printing 3D multiscale multi-material hydrogel structures. **P. Soman**

10:50 363. Multi-color 3D Printing via single-vat grayscale digital light processing. X. Peng, L. Yue, **C. Cheng**, H. Qi, R. Zhao

11:15 364. Rubbery electronics and circuits. **C. Yu**

11:55 Session Closing Remarks.

Rochester Riverside Convention Center
Cascade CD

Organic Chemistry

B. E. Partridge, *Organizer, Presiding*
E. DeCicco, *Presiding*

8:30 Introductory Remarks.

8:35 420. Multi-turn helical aromatic oligoamide foldamers: Synthesis, structural analysis and host-guest binding study. **Y. Zhong**, T.A. Sobiech, B. Gong

9:00 421. Aerobic copper-catalyzed aminooxygenation of β,γ -unsaturated carbamates: Synthesis of 4-benzoyl-Oxazolidin-2-ones. **E. DeCicco**, C. McNichol, A. Canfield, D. Carstairs, S.M. Paradine

9:25 422. Synthesis of novel “Steramers” as tethers for intracellular protein-nucleic acid conjugates. **J. Pezzullo**, J.P. Giner

9:50 423. Copolymerization of C1 monomers with acrylates to access novel and photodegradable polymeric structures. **L. Camdzic**, E. Stache

10:15 Coffee Break in the Expo Hall.

10:45 424. Lewis acid-enabled aminoboration of olefins via Pd-catalysis. **B. Gay**, Y. Wang, S. Bhatt, A. Tarasewicz, D. Cooke, K. Hull

11:10 425. Convergent synthesis of dihydrobenzofurans via urea ligand-enabled heteroannulation of 2-bromophenols with 1,3-dienes. K. Houghtling, **A. Canfield**, S.M. Paradine

11:35 426. Experimental and computational insights into the cycloadditions of bis-borylated dienes. **J.M. Bray**, S.M. Stephens, S.M. Weierbach, **G. Adornato**, J. Schrider, K.M. Lambert

Rochester Riverside Convention Center
Highland J

Quantum Dynamics and Light-Matter Interactions

P. Huo, *Organizer*

A. V. Akimov, S. A. Lopez, *Presiding*

8:00 550. Computational study of charge carrier dynamics in photo-electrocatalysis.
M. Dupuis

8:35 551. Photodynamics simulations explain photochemical reactivity and selectivities towards strained molecules. **S.A. Lopez**

9:10 552. Characterization of the excited state properties of isomers of Dodecylthio perylene Diimides via Stark spectroscopy. **P.H. Dinolfo**, A.J. Riives, J. Brinker, W.D. Arthur

9:45 Intermission (Coffee Break).

10:15 553. Extending timescale and system size in nonadiabatic dynamics simulations. **A.V. Akimov**

10:50 554. The role of interfaces and heterostructures in charge transfer processes in nanocomposites. **S. Kilina**

11:25 555. Photoinduced molecular dynamics of chemical reactions. **D. Kilin**

TUESDAY AFTERNOON

Rochester Riverside Convention Center
Aqueduct CD

Oxidations and Electrochemistry in Organic Synthesis: The James Bobbitt Memorial Symposium

J. He, J. Rusling, *Presiding*

1:00 Introductory Remarks.

1:05 462. Biocatalysis and bioelectrocatalysis in microemulsions. **J. Rusling**, R. Kankanamage, J. Hena, J. He

1:25 463. Methods development in academic and industrial settings: A career shaped by an oxoammonium salt. **C.B. Kelly**

1:45 464. Chemoselective oxidation of thiols with Bobbitt's salt. **K.M. Lambert**, S.M. Weierbach, R.P. Reynolds, S.M. Stephens, K.V. Vlasakakis, R.T. Ritter, O.M. White, N.H. Patel, E.C. Hayes, S. Dunmire

2:05 465. Development of electrocatalytic reactions for the fluorination of arenes. **C.A. Malapit**

2:25 466. Adventures in oxoammonium cation chemistry: development of new routes for oxidative functionalization reactions. **N.E. Leadbeater**

2:45 Coffee Break in the Expo Hall.

Rochester Riverside Convention Center
Highland B

Advanced Polymer Materials 4 - Elastomers, Devices, and Signaling

J. Texter, *Organizer*
H. Gysling, *Presiding*

1:00 30. Dynamic covalent exchange in polyanhydride materials provides self-healing and recycling possibilities. A.L. Santefort, P. Sivablana, **D.A. Shipp**

1:35 31. Highly stretchable elastomers based on ionically-bonded network. **H. Cai**, Z. Wang, N. Utomo, Y. Vidavsky, M.N. Silberstein

1:55 32. Charge-balanced, ambipolar, and high-entropy molecular glass mixture hosts for high-efficiency and long-life white OLED devices, having low efficiency roll-off. **M.F. Molaire**, D.S. Weiss, M. Juba

2:30 Break in the Expo Hall.

3:00 33. New cues for new mechanobiology? Development of soft actuators to signal to cells. J. Gomez, S. Talebi, **R. Steinhardt**

3:35 34. Stereocomplexation of stereoregular aliphatic polyesters: Change from amorphous to semicrystalline polymers with single stereocenter inversion. **Y. Lu**, Y. Popowski, G.W. Coates, W.B. Tolman

3:55 35. Thermodynamic effects of chirality on the lamellar phase using particle-based simulations. **N. Buchanan**, P. Padmanabhan

Rochester Riverside Convention Center
Highland G

Battery and Energy Storage

M. Ganter, P. Taboada-Serrano, *Organizers*
H. Liu, C. J. Patridge, *Organizers, Presiding*

1:00 75. Understand the potentiodynamics of the charge transfer and transport process in aqueous zinc-ion batteries using Operando tools. **X. Teng**

1:35 76. Towards rechargeable aluminum-graphite batteries for low-temperature space & electromobility applications. **R.J. Messinger**, T. Schoetz, J. Wang, J.H. Xu, S.S. Kt, C. Ilkow

2:00 77. Electrochemical sodiation mechanism in magnetite nanoparticle-based anodes: understanding of nanoionics-based sodium ion storage behavior of Fe₃O₄. **M. Islam**, J. Bouldin, S. Han, J. Yang

2:25 Break.

2:55 78. Interface Engineering and Understanding for the Next-generation Batteries. **Y. Zhao**

3:20 79. Polymer electrolytes for next generation calcium batteries. **I.D. Hosein**

3:45 80. Investigation of Ca intercalation into eVOPO₄ for high-capacity Ca-ion battery cathodes. **J. Wang**, H. Liu

4:10 81. Investigating in-situ formation and evolution of solid electrolyte interphase at interface of beyond lithium-ion battery materials. **S. Cora**, N. Sa

Rochester Riverside Convention Center
Highland F

Biomedical Engineering - Session I

D. J. Jakiela, *Organizer, Presiding*

1:00 102. Engineered salivary gland tissue chips for radioprotective drug screening. **J. Mereness**, D. Benoit

1:40 103. Colloidal gel matrix provides spatial guidance for cell morphogenesis. **D. Sarkar**, M. Lin

2:00 104. Modeling macrophage-regulated pulmonary fibrosis with engineered membranous lung microtissues. X. Ying, **R. Zhao**

2:20 . Attempt for formation and detection of gold colloid aggregates at the hippocampus of the Alzheimer's disease rat. **K. Yokoyama**

2:40 Break in the Expo Hall.

3:10 106. The discontinuous surface of porous membranes can be engineered to reduce cell-substrate interactions similarly to soft materials. **T. Gaborski**

3:30 107. 3D printing of engineered bacteria for the production of biofilms-on-a-chip. **A. Meyer**

3:50 108. Tuning cysteine reactivity in peptides for efficient and reproducible thiol-ene reactions within poly(ethylene glycol) hydrogels for use in regenerative medicine. **B.L. Abraham**, A. March, S. Basu, A.R. Srivatsava, T. Nguyen, D.S. Benoit

4:10 109. Tumor targeted delivery of TLR7 agonists for anti-cancer therapy. **S. Fang**, B. Brems, E. DeYoung, E. Olawode, T. Brooks, L.N. Tumey

Rochester Riverside Convention Center
Aqueduct AB

Computational Tools for Materials Science II

P. Padmanabhan, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 174. Atomistic elucidation of electron transfer pathways in transition metal complexes. **N. Ananth**

1:45 175. Effect of graphene oxide on the photocatalytic properties of ZnO nanoclusters: A theoretical study. **D.C. Perera**, J.C. Rasaiah

2:05 176. A new experimentally guided computational database for 2D metal-organic frameworks. **Z. Zhang**, D. Valente, Y. Shi, D. Limbu, M. Momeni, F.A. Shakib

2:25 177. Computational approach for predicting ionic salt association in extreme ultraviolet photoresists. **P. Bangalore Prakash**, F. Escobedo

2:45 Break in the Expo Hall.

3:15 178. Defects in oxide heterostructures. **P.P. Dholabhai**, C. Marzano, W. Ebmeyer

3:35 179. Polaronic optical transitions in metal oxides revealed by first-principles electron-phonon coupling. **J.L. Shelton**, K.E. Knowles

3:55 180. Influence of size, composition, and morphology on the transformation mechanics of gold-silver bimetallic nanoparticles. **O. Uche**

4:15 181. Atomistic molecular dynamics simulation view of water local structure and dynamics on the surface of zeolitic-imidazolate framework nanoparticles. **Y. Shi**, D. Limbu, M. Momeni, F.A. Shakib, S. Abdelhamid

Rochester Riverside Convention Center
Highland D

Electron Transfer Across Semiconductor Surfaces I

D. McCamant, *Organizer*
L. A. Velarde, *Presiding*

1:00 . Spectroscopic probes of two-step (electro)photocatalysts. A. Vonder Haar, D. Bain, A. Lara, J. Kim, **A. Musser**

1:30 191. Heterostructured photocatalysts of Ni²⁺ doped CDs quantum dots and β -pb_{0.33}v₂o₅ nanowires: Towards selective CO₂ reduction. **K.E. Garcia-Pedraza**, D. Watson

1:50 192. Electrochemical oxidative desulfurization at iron oxide surfaces. **J. Swierk**

2:20 193. Quantitative assessment of dye-sensitized Pt/TiO₂ photocatalysis system with chemical actinometry. **L. Cai**, D. McCamant

2:40 Coffee Break in the Expo Hall.

3:10 194. Chalcogenoxanthylum dye-sensitized CuAlO₂ for solar hydrogen production. **M. Clark**, D. Watson

3:30 195. Selenoxanthylum based dye at organic/inorganic interfaces for application in dye sensitized technologies. **B. Breeman**, L.A. Velarde

3:50 196. Potential of zero charge measurement by second harmonic generation. **J. Suntivich**

Rochester Riverside Convention Center
Highland E

Emerging Strategies for Chemical Probing and Control of Biological Processes

R. Fasan, *Organizer, Presiding*

1:30 204. Bioorthogonal chemistry approach to study class B GPCR dynamics. **Q. Lin**

2:00 205. Isomerization of bioactive acylhydrazones triggered by light. **A. Woolley**

2:30 206. Developing ‘cyclopeptibodies’ as a new class of protein-targeting agents. **Y. Gu, M. Hendricks, R. Fasan**

2:50 break.

3:10 207. Combinatorial assembly of primary metabolites in animal model systems. **F.C. Schroeder**

3:40 208. Non-canonical roles of lipids in cell fates. **G. Atilla-Gokcumen**

4:10 209. Identifying descriptors for electrochemical anion adsorption. **C. DeNyse, S. Shaut, M. Law, H.F. Schmitthenner**

Rochester Riverside Convention Center
Cascade EF

Enabling New Methodologies in the Field of Organic Chemistry

P. Z. Musacchio, *Organizer, Presiding*

1:00 216. Synthesis or substitution? Preparation of N-(hetero)aryl piperidines. **A.C. Sather**

1:35 217. Deaminative Cross-Couplings. **M.P. Watson**

2:00 218. Enabling challenging chemo- and biocatalyzed transformations for medicinal chemistry programs – a series of vignettes from the applied synthesis technologies group. **H. Yayla**

2:25 219. Enantioselective synthesis of alcohol and amine derivatives via copper-catalyzed alkene difunctionalization. **S.R. Chemler**

2:50 Break.

3:05 220. Anaerobic heteroatom transfer reactions using photoexcited nitroarenes. **M. Parasram**

3:30 221. Solvated nickel complexes as stoichiometric and catalytic trifluoromethylation agents. **D.A. Vicic, S. Shreiber**

3:55 222. Room temperature decarboxylative amination of benzoic acids. **R. Basnet, J.M. Hoover**

4:20 223. Molecular editing of carbohydrates. **M. Ngai**

Rochester Riverside Convention Center
Highland A

Inorganic Catalysis I

M. L. Neidig, *Organizer*

W. D. Jones, *Organizer, Presiding*

1:00 317. Forged in iron: Sustainable catalysis for the 21st century. **M.L. Neidig**

1:25 318. Chelation equilibria and π -electron delocalization and in organosilicon complexes of 1-hydroxy-2-Pyridinone and 2-pyridithione. **B.M. Kraft**

1:50 319. Organometallic bidentate PN-Zn(II) hydrogenation catalysts. **S. Paul**, P. Morgante, S.N. MacMillan, J. Autschbach, D.C. Lacy

2:15 Coffee Break.

2:45 320. How does Milstein's catalyst really work? Identifying the active species in ruthenium-catalyzed hydrogenations. **A.R. Chianese**

3:10 321. Computational study for CO₂-to-CO conversion over proton reduction using [re[bpyme(im-r)](co)₃cl]⁺ (R = ME, ME₂, and ME₄) electrocatalysts and comparison with the manganese analogs. **J. Panetier**

3:35 322. Exterior decorating: Boron-based secondary coordination spheres for cross-coupling reactivity. **M.W. Drover**, J. Zurakowski, B. Austen

Rochester Riverside Convention Center
Cascade CD

Making Bonds and Breaking Boundaries: Modern Developments in Catalysis II

S. M. Paradine, *Organizer*

C. Kennedy, *Organizer, Presiding*

1:00 . Harnessing radicals to enable unconventional reactivity. **D. Nagib**

1:40 120. Exploration in deaminative cross-couplings of pyridinium salts for peptides diversification. **A. Dion**, M.P. Watson, D. Kalyani, D.M. Schultz, C. Twitty, Y. Hong, B. Garcia

2:10 . Catalytic reduction of C-O π bonds using sulfonamide-based complexes. **A.R. O'Connor**

2:40 Break.

3:10 117.* New synthetic strategies for controlled radical polymerizations. **E. Stache**, S. Dadashi Silab, L. Camdzic

3:40 . Radical pathways mediated by nickel catalysts and applications to peptide modification. **T. Diao**

Rochester Riverside Convention Center
Highland H

Metal Oxide Clusters and Materials II

K. E. Knowles, *Organizer*
E. M. Matson, *Presiding*

1:00 Introductory Remarks.

1:05 372. Chemical transformation reactions of oxide-based nanomaterials. **R.E. Schaak**

1:50 373. Accurate Nanotitania surface models. G. Repa, A.S. Malik, **L.A. Fredin**

2:15 374. Understanding the effects of cation inversion on the electronic structure and photophysics of spinel zinc ferrite nanocrystals. **J. Stair**, K.E. Knowles

2:40 Coffee Break in the Expo Hall.

3:10 375. STM reveals the atomic-scale chemistry of TiO₂ in aqueous and ambient environments. **M.A. Hines**

3:35 376. Photochemical conversion of organotin clusters into SnO₂ and their use as precursors for thin-film photoresists. **D. Marsh**

4:00 377. Probing the influence of metal oxide nanoparticle surfaces in catalysis. **R.N. Austin**, J.D. Sempel, A. Mahdavi-Shakib, M. Hoffman, A. Oza, E. Bennett, J.S. Owen, A.R. Chokanlu, T.J. Schwartz, B.G. Frederick

Rochester Riverside Convention Center
Cascade AB

Physical Chemistry I

D. McCamant, *Organizer*
E. J. Robertson, *Presiding*

1:00 Opening Remarks.

1:05 488. Optoelectronic behavior of spinel oxides: insights into the contributions of 3D bands to photophysical properties. **E.P. Craddock**, K.E. Knowles

1:30 489. Photophysical characterization of acridinium photoredox catalysts by stark spectroscopy. **R. Ryan**, P.H. Dinolfo

1:55 490. Bell-shaped temperature dependence of electrical conductivity in a multi-heme microbial nanowire: structural transitions or something else?. **M.J. Guberman-Pfeffer**

2:20 491. Investigation of adsorption orientation and surface coverage of amyloidogenic peptides over nano-gold colloid surface. **K. Yokoyama**

2:45 Intermission.

3:15 492. Peptoid nanosheet synthesis at the oil-water interface: A generalizable route for producing freely-floating metal nanoparticle arrays. **E.J. Robertson**

3:40 493. Fluorescence quenching by gold nanoparticles in a model bio-sensing system. **J.J. Peterson**

Rochester Riverside Convention Center
Highland J

Quantum Dynamics and Light-Matter Interactions

P. Huo, *Organizer*
D. Kilin, S. Kilina, *Presiding*

1:00 544. Path integral molecular dynamics simulations of the nanoconfined water at interface. **M. Momenitaheri**, D. Limbu, F.A. Shakib

1:30 545. Non-Adiabatic Mapping Dynamics in the phase space of SU(N) Lie group. **D.L. Bossion**, W. Ying, P. Huo

2:00 546. Floquet engineering optical absorption properties of matter. **V. Tiwari**, I. Franco

2:30 Intermission (Coffee Break).

3:00 547. Properties of molecular exciton-polaritons: coupling ab initio calculations with quantum optics. **B. Weight**, P. Huo

3:30 548. Exact factorization-based coupling terms for mixed quantum- classical dynamics. **E. Villaseco Arribas**, N. Maitra

4:00 549. Singlet and triplet lowest excitons in covalently functionalized (11,0) carbon nanotube. **S. Kilina**, D. Thapa, H. Woods

Rochester Riverside Convention Center
Highland C

Bioinspired Materials and Biomedical Applications

X. Lu, *Organizer, Presiding*

1:00 Session Opening Remarks.

1:05 95. Stimuli-responsive and self-regulating liquid crystals. **N.L. Abbott**

1:50 96. Activated macrophage targeting nanoparticles-in-microparticles for treatment of post-traumatic osteoarthritis. P.N. Sago, Y. Espiritusanto, **E. Jain**

2:15 97. Greasing proteins wheel: Harnessing post-translational lipidation for the biosynthesis of smart Nanobiomaterials. **D. Mozhdehi**

2:40 Coffee Break.

3:00 98. One-pot chemical-free surface functionalization via silk fibroin self-assembly. T. Fink, C. Wigham, A. Ziemba, R. Gilbert, **R.H. Zha**

3:25 99. Innovating and characterizing bioinspired soft materials with multiscale models and machine-learned metamodels. **J. Yeo**

3:50 100. Developing virucidal N95 respirator materials. **E. Palermo**, R.H. Zha, C. Heldt, M. Sorci, T. Fink, V. Sharma, S. Singh, R. Chen, B. Arduini, K. Dovidenko

4:15 101. Bioresorbable metals as smart medical implants. **D. Zhu**

4:55 Symposium Closing Remarks.

Rochester Riverside Convention Center
Lilac Ballroom

Harrison Howe Plenary Lecture

D. McCamant, *Organizer, Presiding*

4:30 SCC/YCC Mixer, All Invited.

5:30 Introductory Remarks.

5:40 283. Biosynthesis and Engineering of Macrocyclic Peptides.
W.A. Van Der Donk, 2020 Harrison Howe Award Winner

Poster Session:

6:30- 8:30 pm. Poster Session in the Galleria (Convention Center, outside Lilac Ballroom) for Physical Chemistry, Analytical Chemistry, Organic Chemistry, Inorganic Chemistry and Chemical Education.

WEDNESDAY MORNING

Rochester Riverside Convention Center
Highland B

Advanced Polymer Materials 5 - Manufacturing, Coatings, and Catalysis
J. Texter, *Organizer, Presiding*

8:30 36. Keynote - Designing advanced macromolecules for advanced manufacturing: Striving for sustainability. **T.E. Long**, C.B. Williams

9:20 37. Reactive polyurethanes for UV-cure printing. **H. Gupta**

9:55 Coffee Break in Galleria.

10:30 38. Polymer-stabilized enzymes on nanoparticles for high temperature biocatalysis. **J. Rusling**, R. Kankanamage, J. Hena, J. He

11:05 39. Molecular mechanisms relevant during high-throughput processing of extreme-strength two-dimensional polymers. A. Maxwell, E. Rankin, E. Borza, E. Sandoz-Rosado, O. Uche, **P. Padmanabhan**

11:30 40. Equilibrium glass transitions in polymer systems. **J. Texter**, N. Dixit, K. Bian, H. Gupta

Rochester Riverside Convention Center
Highland F

Biomedical Engineering - Session II

D. J. Jakiela, *Organizer, Presiding*

8:30 110. mRNA delivery from fibrous scaffolds for nervous system regeneration. D. Puhl, J. Funnell, T. Fink, A. Swaminathan, M. Oudega, R.H. Zha, **R. Gilbert**

9:10 111. Liposome-display of antigens: A versatile approach for vaccine development. **J.F. Lovell**

9:30 112. Adaptive recombinant nanobiomaterials from genetically encodable amphiphiles. **D. Mozhdehi**

9:50 Break.

10:20 . Using imaging to understand and engineer DNA origami interactions with biological systems. **L. Chou**

10:40 114. Structural design of phosphate bioactive glasses for tissue engineering applications. **S. Lau**, Q. Qin, A. Goel

11:00 115. Engineering an adaptable biosensor scaffold with monobody alternate frame folds. **M.F. Presti**, J. Ha, S.N. Loh

11:20 116. Robust antimicrobial surface with ZnO nanowire patterned micro-armor. H. Yuqing, J. Silva, **K. Du**

Rochester Riverside Convention Center
Highland A

Inorganic Catalysis II

W. D. Jones, *Organizer*

M. L. Neidig, *Organizer, Presiding*

8:30 323. Surface-confined terpyridine coordination-cased monolayers for ultra-durable electrochromic materials. **O.V. Zenkina**, E.B. Easton, R. Ahmad, N. Laschuk

8:55 324. Intramolecular proton shuttle enhances hydrogen production by metalloprotein electrocatalysts in water. **J. Han**, J.L. Alvarez-Hernandez, K. Bren

9:20 325. Bioinspired transfer hydrogenation using diiridium catalysts at nano molar concentrations. **A. SRIMANI**, L.H. Do

9:45 Coffee break.

10:15 326. Sometimes two metals are better than one: Dinuclear Mn(I) catalysts in E-selective alkyne semihydrogenation. **D.C. Lacy**

10:40 327. Synthesis of nickel complexes of bidentate, pyridone-containing ligands and their applications. **A.A. Kadam**, M. Afandiyeva, R. Kennedy

11:05 328. Development of new first-row metal Fox complexes for alcohol dehydration. O. Nachtigall, A. VandeWeide, A. Panda, **W.D. Jones**

Rochester Riverside Convention Center
Cascade AB

Physical Chemistry II

D. McCamant, *Organizer*
E. J. Robertson, *Presiding*

8:00 Opening Remarks.

8:05 495. The search for molecular corks beyond carbon monoxide: A quantum mechanical study of N-Heterocyclic carbene adsorption on Pd/Cu(111) and Pt/Cu(111) single atom alloys. **S. Simpson**

8:30 496. From fast water on surfaces to nearly immobile nano-confined water: Exploring and expanding the dynamic range of Overhauser dynamic nuclear polarization. A. Beaton, A. Guinness, F.F. Syed, **J. Franck**

8:55 497. Insight into the internal water pools of reverse micelles *via* magnetic resonance relaxometry techniques. **A.A. Beaton**, A. Guinness, J. Franck

9:20 498. Hydrate-based technologies for gas storage/transportation and mixtures separation: methods for accelerating gas hydrate formation. **A. Stoporev**, A. Semenov, R. Pavelyev, A. Manakov, M. Varfolomeev

9:45 Intermission.

10:05 499. Assessing rotation and rotation dynamics in glyceline deep eutectic solvent and its solutions with methanol. **C. Green**, M.P. Heitz

10:30 500. Coumarin 153 solvation dynamics in methanol-water binary mixtures: Are there implications for ionic liquid solutions?. **M.P. Heitz**, S. Robillard, D.M. Heitz, D. McCamant

10:55 501. V-shaped temperature dependences and pressure dependence of elementary reactions of hydroxyl radicals with several organophosphorus compounds. **X. Zhang**

11:20 502. Ruthenium complexes and their applications towards Dye-Sensitized Solar Cells (DSSCs). **B. Brekke**, A. Hussain, K. Mariappan, A.G. Sykes

Rochester Riverside Convention Center
Highland G

Battery and Energy Storage

H. Liu, P. Taboada-Serrano, *Organizers*
M. Ganter, C. J. Patridge, *Organizers, Presiding*

8:30 88. Vanadium: A positive electrode material in lithium-ion batteries. **B.J. Schultz**

9:05 89. Thermal runaway in Li-ion batteries: an electrolyte perspective. **S. Moganty**

9:30 90. Thin film composite separators to enable Li metal anodes. **F. Hu, W. Tenhaeff**

9:55 Break.

10:25 91. Advanced lithium ion battery separators prepared by polymerization-induced phase separation. **W. Tenhaeff**

11:00 92. Fe(III)/Fe(II) redox flow batteries for brackish water desalination. **G. Mohandass, W. Chen, S. Krishnan, T. Kim**

11:25 93. The development of heterocyclic compounds as novel high potential anolytes in non-aqueous redox flow battery. **C.A. Malapit**

11:50 94. Effect of solid-electrolyte pellet density on failure of solid-state batteries. **Q.Q. Tu**

Rochester Riverside Convention Center
Highland H

Chemists as Entrepreneurs

H. Gysling, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 145. Scientists as existential Entrepreneurs. **K. Reed, J. Fagnoli**

9:15 146. Thin film electronic materials research - pathway for chemical entrepreneurship. **T. Royster**

9:55 Intermission.

10:10 147. Catalyzing innovation for high-tech companies looking to grow and maintain their technological edge. **J. Sinnott**

10:45 148. Nanopore filters for proteins. **T. Gaborski**

11:25 149. ACS Division of Small Chemical Businesses (SCHB) activity, member benefits, and opportunities. **J.E. Sabol, X. Simon**

Rochester Riverside Convention Center
Highland D

Electron Transfer Across Semiconductor Surfaces II

D. McCamant, L. A. Velarde, *Organizers*
K. E. Knowles, *Presiding*

8:30 Welcome remarks.

8:35 197. Semiconductor nanocrystal photocatalysis for the production of solar fuels. K. Bren, E.M. Matson, D.J. Weix, **T.D. Krauss**

9:05 198. Long-range exciton to ligand vibronic coupling in quantum dots probed by surface nonlinear optics. **M. Rajapakse**, L.A. Velarde

9:25 199. Electron-hole recombination and hot carrier cooling in 0D, 2D, and 3D materials: Theory meets (?) Experiment. **A.V. Akimov**

9:55 Coffee Break.

10:20 200. Influence of excited state surface chemistry on charge dynamics of lead sulfide quantum dots. **J.B. Asbury**

10:50 201. Heterostructures of cadmium chalcogenide quantum dots and MoS₂ nanoplatelets prepared by linker-assisted assembly: Influence of ligand properties on excited-state charge transfer and photocatalysis. **A. Rothfuss**, D. Watson

11:10 202. Interfacial charge transfer in rhodamine-based dye-sensitized TiO₂ quantum dots with ab initio non-adiabatic excited state dynamics simulations. **B. Weight**, P. Huo

11:30 . Mapping out the density of electrochemically accessible states in metal oxide semiconductor films using electrochemical impedance spectroscopy. M.D. Koch, L. Cai, D.A. Brewster, D. McCamant, **K.E. Knowles**

Rochester Riverside Convention Center
Cascade EF

Natural Product Synthesis and Discovery

J. Wu, *Organizer, Presiding*

8:30 399. Plant-derived products of *Caspella Bursa-Pastoris* and *Parthenium Hysterophorus* and their biological effects on *Escherichia coli* and Triple Negative Breast Cancer. **K.A. Salinas**

8:45 400. Catalytic Markovnikov hydrothiolation of dehydroamino acids. **C.P. Ting**

9:15 401. Photoacid catalyzed functionalization of carbonyls. **J.J. Badillo**

9:45 405. Game of tropones: Studies on the synthesis and function of cycloheptatrienones. **R.P. Murelli**

10:15 Intermission.

10:45 403. Development and investigation of micheliolide-based anticancer agents via late-stage chemoenzymatic C-H functionalization. **R. Potenzino**, H. Alwaseem, B. Frisch, R. Fasan

11:00 404. Mild strategies in the direct generation of carbocation intermediates from C(sp³)-H bonds. **P.Z. Musacchio**, Y. Zhang, N. Fitzpatrick, M. Das, L. Zamani, I. Bedre

11:30 402. Rapid access to pyrroloindolines by visible-light-induced radical cascade reactions. **T. Wang**

Rochester Riverside Convention Center
Highland J

Quantum Dynamics and Light-Matter Interactions

P. Huo, *Organizer*

D. L. Bossion, A. Mandal, *Presiding*

8:00 556. Chemistry of quantum decoherence. **I. Gustin**

8:30 557. A practical quantum dynamics method for condensed phase chemical systems by incorporating tensor network strategies into hierarchical equations of motion. **X. Chen**, I. Franco

9:00 558. Symmetric molecular dynamics. **S. Cox**, A.D. White

9:30 559. Nonadiabatic molecular dynamics in periodic solids and nanoscale materials. **M. Shakiba**, A.V. Akimov

10:00 Intermission (Coffee Break).

10:30 560. Significant luminescence from SiC quantum flakes with oxygen defects..
J. Granlie, D. Kilin

11:00 561. Light Induced spin crossover in 2D Hoffman-type metal organic frameworks. **D.S. Valente**, Z. Zhang, F.A. Shakib

11:30 562. Understanding the problem of unphysical divergence in quadratic response TDDFT. **D. Dar**, S. Roy, N. Maitra

Rochester Riverside Convention Center
Highland C

Sustainability and Green Chemistry

M. G. Coleman, *Organizer, Presiding*
R. Tandon, *Presiding*

8:30 Sustainability and Circular Economy – Talk 1: Dr. Susan E. Powers, Clarkson University.

8:50 Sustainability and Circular Economy – Talk 2: Dr. Alan Rae, University at Buffalo.

9:10 Discussion.

9:20 569. Recent development of sustainable polyesters. **M.J. Miri**

9:45 570. Photoelectrocatalytic chemical transformations in lignin under ambient conditions. **G. Leem**

10:10 Intermission.

10:25 571. Solvent-free high speed ball milling: Mechanochemical carbene transfer reactions. **M.G. Coleman**

10:45 572. Production of renewable diesel and jet fuel via selective ring opening of decalin. **M. Kline**, S.A. Karunaratne, T.J. Schwartz, M.C. Wheeler

11:05 573. Development of 3D-printable nanocomposite for smart antimicrobial food packaging. **O.S. Popoola**, A. Finny, E. Andreescu

11:20 574. Reinforcement of epoxy acrylate UV-curable oligomers using functional dewaxed cashew shell. **M.M. Adjoumane**

11:35 575. Resin-assisted ball milling of esterified maple wood nanomaterials for industrial applications. **J. DOE-MENSAH**, M. Driscoll, R. Meyer

11:50 576. Dehaloperoxidase catalyzed stereoselective synthesis of cyclopropanol esters. **M.G. Siriboe**, D.A. Vargas, R. Fasan

12:05 Closing Remarks.