2026 Midwest Regional Meeting

October 25-27, 2026

Manhattan, KS

General Chair

Daniel Higgins

Program Chair

Christine Aikens

Sunday, October 25, 2026

Registration

Time: 1:00 PM - 9:00 PM
Session type: Registration
Location: Second Floor Lobby

Badge pick-up and onsite registration.

Public Lecture: "Chemistry is Everywhere"

Time: 2:00 PM - 3:00 PM
Session type: Plenary
Location: Forum Hall, Ground Floor

Public lecture by Prof. Thomas Kuntzleman (Wayne State University)

Science Writing Workshop: From Data to Story: Making Your Writing Clear, Compelling, and Memorable

Time: 3:00 PM - 5:00 PM
Session type: Workshop
Location: Bluemont Room, Second Floor

Great science advances when scientists communicate it effectively, and this interactive workshop helps participants uncover and communicate the story behind their research so that others can understand, use, and cite it. Participants will learn how to move beyond presenting results to crafting clear, compelling narratives in their writing and, through hands-on exercises, will distill their work into core story elements and revise for clarity and impact. Pre-registration is required, $5.

Chemistry in Action

Time: 3:15 PM - 4:45 PM
Session type: Outreach
Location: Bosco Plaza

Demonstrations and interactive activities by Alpha Chi Sigma in honor of National Chemistry Week.

Plenary Lecture: "Curiosity, Science, and the Wisdom of Dr. Seuss"

Time: 5:00 PM - 6:00 PM
Session type: Plenary
Location: Forum Hall, Ground Floor
Sponsor(s): Kansas State University Office of the Provost and Office of the Vice President for Research

Plenary Lecture by Prof. Geri Richmond (University of Oregon)

Meet the Speaker Reception

Time: 6:00 PM - 7:00 PM
Session type: Social Event
Location: Forum Hall, Ground Floor

Sci-Mix

Time: 7:00 PM - 9:00 PM
Session type: Sci-Mix
Location: Grand Ballroom, Second Floor
Organizer(s): Christine M Aikens, Daniel A Higgins
Sponsor(s): Wakarusa Valley Local ACS Section, Kansas State University Local ACS Section, Cambrex, Shimadzu, Cintas, Taylor Chair of Chemistry at Kansas State University

Presentations:

7:00 PM [MW350] Label-free detection and identification of epitranscriptomic modifications using XToF nanofluidic device. **Presented by: Minaza Yahiya**

7:00 PM [MW355] Cu(II) adsorption behavior of an organic nanotube having inner amine groups. **Presented by: Mikynzie Tatro**

7:00 PM [MW422] Analyzing the role of microplastic size, surface area and chemical composition on PFAS sorption in sanitary water samples: A case study of the Galesburg area. **Presented by: Lumala Nelum Naullage**

7:00 PM [MW423] Correlation of high molecular weight-glutenin subunit allele Glu-B1-al with seed, milling, dough, and baking characteristics in hard winter wheat. **Presented by: Bruna Mattioni**

7:00 PM [MW434] Fourier transform infrared spectrometric quantification of volatile organic compounds emitted by common commercial 3D printers. **Presented by: Daphne Hedrick**

7:00 PM [MW06] Toward high-throughput quantitative measurements of RNA-protein binding. **Presented by: Prathapa Deepadul Perera**

7:00 PM [MW07] Machine learning guided discovery of isoform selective HDAC8 inhibitors through virtual screening and generative design. **Presented by: Bennett Garfinkel**

7:00 PM [MW101] Liquid chromatography-mass spectrometry lipidomic characterization for pulmonary arterial hypertension (PAH). **Presented by: Ella Jade Simmons**

7:00 PM [MW22] Gene expression & structural analysis of OAZ RNA in Neurospora crassa. **Presented by: Billy Bettis**

7:00 PM [MW28] De novo mini-protein binders for TREM2 associated with Alzheimer's disease. **Presented by: Doniesha Perera**

7:00 PM [MW218] Utilization of eye tracking to add to the validity of data obtained using the resonance concept inventory. **Presented by: Mary Simon**

7:00 PM [MW219] Utilization of chemical demonstrations as an experiential and collaborative learning strategy for general chemistry students. **Presented by: George P Nora**

7:00 PM [MW144] Design and development of Ln-MOF fluorophores for cellular multiplexing imaging applications. **Presented by: Brayden Schut**

7:00 PM [MW229] Interpretation of the electronic structure from experimental X-ray absorption spectra (XAS) using computational methods. **Presented by: Rhoda Cherotich Komen**

7:00 PM [MW233] Comparing the thermodynamic properties and reactivity of FeIII- and MnIII-hydroxo complexes. **Presented by: Anagha Puthiyadath**

7:00 PM [MW241] Functionalizing nanoporous metal-organic supercontainers for environmental remediation of illicit substances. **Presented by: MaKenna King**

7:00 PM [MW114] Selective formation of 1- and 1,8-substituted fluorenones and synthesis of fluorenylspirocyclopropene compounds. **Presented by: John N. Brunn**

7:00 PM [MW120] Tröger's base as a multifunctional platform for metallodrug and supramolecular design. **Presented by: Asanga Kasun Mannapperuma**

7:00 PM [MW124] One-step versus stepwise 2-electron electrochemical reduction of 6,6'-biazulenes. **Presented by: Ryan N Pierce**

7:00 PM [MW166] Total synthesis of the trikentrins and the trikentramides using one-pot tandem Bartoli syntheis/indole aryne Diels-Alder cycloaddition methodologies. **Presented by: An Nguyen**

7:00 PM [MW441] *Withdrawn*

7:00 PM [MW442] *Withdrawn*

7:00 PM [MW446] Uniformity from disorder in electrochemical reaction networks. **Presented by: Olivia Underwood**

7:00 PM [MW447] Ultrafast study of a pH-sensitive azobenzene photoswitch in basic conditions. **Presented by: Jaden Riddle**

7:00 PM [MW309] Ctrl-X, Ctrl-V, Ctrl-PET: Rapid, selective, and mild depolymerization of poly(ethylene terephthalate). **Presented by: Benjamin Heiderscheit**

7:00 PM [MW311] Polymer infiltration in UiO MOFs monitored by NMR: Exploring the role of polymer chain length. **Presented by: Colton Rhoads**

7:00 PM [MW331] Designing antimicrobial polymers to combat antibiotic-resistant bacteria. **Presented by: Marie Kerschen**

7:00 PM [MW332] Ground state destabilization as a means to access transformable poly(acrylamides). **Presented by: Alexis Redwine**

7:00 PM [MW335] Development of a free, open-source Python kinetic simulation package for modeling, fitting, and mechanism discovery. **Presented by: Taylor Paez**

7:00 PM [MW337] Comparing machine-learned interatomic potentials for diamond stability in liquid metals. **Presented by: Amin Ahmadisharaf**

7:00 PM [MW402] Multiscale modeling of the NarK nitrate/nitrite antiporter using adaptive-partitioning algorithms based on hierarchical truncated many-body expansion (PAP-HMBE). **Presented by: Julia Roma**

7:00 PM [MW415] Enhanced sampling approaches to Li-ion transport across the solid electrolyte interphase. **Presented by: Hiruni Wimalasiri**

Monday, October 26, 2026

Registration

Time: 7:00 AM - 9:00 PM
Session type: Registration
Location: Second Floor Lobby
Badge pick-up and onsite registration.

Biochemistry and Chemical Biology

Time: 8:00 AM - 9:40 AM
Session type: Poster
Location: Grand Ballroom, Second Floor
Organizer(s): Ping Li
General poster session featuring biochemistry and chemical biology research

Presentations:

8:00 AM [MW05] Stabilization of aryl diazonium groups for intracellular affinity-driven labeling of proteins. **Presented by: Kyler McConnell**

8:00 AM [MW06] Toward high-throughput quantitative measurements of RNA-protein binding. **Presented by: Prathapa Deepadul Perera**

8:00 AM [MW07] Machine learning guided discovery of isoform selective HDAC8 inhibitors through virtual screening and generative design. **Presented by: Bennett Garfinkel**

8:00 AM [MW08] Novel path to clean power: Increasing electrode performance of microbial fuel cells. **Presented by: Ayush Jalani**

8:00 AM [MW09] Discovery and optimization of thienopyrazine RNA-splicing modulators for the treatment of Huntington's disease. **Presented by: Chaofan Xu**

8:00 AM [MW10] Effects of propylene glycol on the stability of nanostructured lipid carriers. **Presented by: Mahsa Hosseini**

8:00 AM [MW11] Volatile organic compound enrichment from exhaled breath using cryogenic condensation for electrochemical sensing. **Presented by: Lida Khalafi**

8:00 AM [MW12] Screening of bioactive algal lipids as natural antimicrobial agents. **Presented by: Kritika Jaswal**

8:00 AM [MW13] Optimizing expression, purification, and crystallization conditions for FlrB 7–123 wild-type as a foundation for mutant structural studies. **Presented by: Avery Ferguson**

8:00 AM [MW14] HPLC-UV analysis of hemp-derived cannabinoids in honey bee tissues. **Presented by: P Alex Swider, Qiyang Zhang**

8:00 AM [MW15] CRISPR knock-in to identify tethering factor association of recombinant adeno-associated virus (rAAV) to the human genome. **Presented by: Josie Diffendaffer**

8:00 AM [MW16] Investigating evolutionary conservation of 7SK stem-loop 3 RNA structural dynamics. **Presented by: Shrimai Raghuvanshi**

8:00 AM [MW17] Investigating landfill and soil communities for potential rubber-degrading abilities. **Presented by: Drew C Harris**

8:00 AM [MW18] Identification of Citrus bergamia flavonoids responsible for HMG-CoA reductase inhibition. **Presented by: Alaina Worland**

8:00 AM [MW19] Pyruvate dehydrogenase complex inhibitors. **Presented by: Mason Bach**

8:00 AM [MW20] Development of novel fluorogenic dyes to explore the role of fluorine in fluorescence activation. **Presented by: Josephine Alesio**

8:00 AM [MW21] Reductive nitrogen metabolism by bryophyte non-symbiotic hemoglobins. **Presented by: Anastasia Jankowski**

8:00 AM [MW22] Liquid chromatography-mass spectrometry lipidomic characterization for pulmonary arterial hypertension (PAH). **Presented by: Ella Jade Simmons**

8:00 AM [MW23] Synthesis and characterization of N-quaternized ammonium pectin derivatives for tunable antimicrobial activity. **Presented by: Christina Diab**

8:00 AM [MW24] Strucural analysis of Crassostreas gigas OAZ RNA. **Presented by: Thong Tran**

8:00 AM [MW25] Optimization of a high-throughput FRET assay for the self-cleavage of the Bacillus cereus glmS riboswitch to identify potential antibiotic compounds. **Presented by: Josh Chandra**

8:00 AM [MW26] Cholesterol inhibition may alter the production and the molecular profile of microvesicles. **Presented by: Maddie Johnson, Myranda Griesert**

8:00 AM [MW27] WDR45: A beta-propeller protein associated neurodegeneration (BPAN) protein packaged in exosomes. **Presented by: Dawson Studer**

8:00 AM [MW28] Gene expression & structural analysis of OAZ RNA in Neurospora crassa. **Presented by: Billy Bettis**

8:00 AM [MW29] Optimization of a high-throughput FRET assay for identifying cleavage-inducing ligands for the glmS riboswitch in Staphylococcus aureus. **Presented by: Ivan Fedorchuk**

8:00 AM [MW30] Estrogenic signaling imposed by standard culture conditions. **Presented by: Myranda Griesert**

8:00 AM [MW31] *Withdrawn*

8:00 AM [MW32] RNA structure-based targeting of MALAT1 modulates triple-negative breast cancer cell behavior. **Presented by: Maddox Johnson**

8:00 AM [MW33] Computational and photophysical investigation of fluorogenic Pepper RNA aptamers. **Presented by: Gabriel Morrow**

8:00 AM [MW34] *Withdrawn*

8:00 AM [MW35] Structural characterization of the Homo sapiens ornithine decarboxylase antizyme (OAZ) RNA regulatory element. **Presented by: Taylor Ross**

Inorganic Chemistry

Time: 8:00 AM - 12:20 PM
Session type: Oral
Location: Room 206, Second Floor
Organizer(s): Tendai Gadzikwa
Presider(s): Tendai Gadzikwa

General oral session featuring inorganic chemistry research

Presentations:

8:00 AM [MW36] Surface organometallic chemistry as a synthetic tool for reactive ruthenium cations. **Presented by: Damien Culver**

8:20 AM [MW37] Phosphenium-controlled Pt(0) catalysts for regioselective alkyne hydrosilylation. **Presented by: Gayanethra Kaumini**

8:40 AM [MW38] Fe-Co-Ru-promoted Ni/CeO2 single-atom and nanocluster catalysts for dry reforming of methane at high space velocity. **Presented by: Samson Akorede Adeoye**

9:00 AM [MW39] Metal-metal bonded vanadium, chromium, and molybdenum complexes supported by redox-active tetradentate ligands. **Presented by: Scott R Daly**

9:20 AM [MW40] Demonstration of a thermodynamic cycle for interpreting cation-driven tuning of redox chemistry. **Presented by: Fynnegan Cooper**

9:40 AM Intermission.

10:00 AM [MW41] Reductive electrodeposition of uranium oxide materials from anhydrous uranyl triflate. **Presented by: Natalie Lind**

10:20 AM [MW42] Reversible rare earth cation capture by Zn–Al layered double hydroxides synthesized via deep eutectic solvent route. **Presented by: Mahmudul Islam Rain**

10:40 AM [MW43] Comparing the electronic properties of uranyl complexes featuring imine and amine ligands. **Presented by: Sunidhi Arora**

11:00 AM [MW44] Understanding the tunable properties of aza-crown complexes of the uranyl ion. **Presented by: Grant Arehart**

11:20 AM [MW45] Synthesis, preliminary characterization, and toxicity studies of three amino acid Schiff-base ligands and their potential binding sites to Ni (II) ion: Comparison with computational density functional theory (DFT) studies. **Presented by: James Titah**

11:40 AM [MW46] Engineering confined phosphonate pore environments in MOF-808 for selective rare-earth recovery. **Presented by: Shyam Chand Pal**

Machine Learning for Computational Chemistry

Time: 8:00 AM - 11:55 AM
Session type: Oral
Location: Cottonwood Room, Second Floor
Organizer(s): Saswata Dasgupta, Bin Liu
Presider(s): Saswata Dasgupta, Bin Liu
Sponsor(s): COMP, PHYS

This symposium will highlight recent advances in the development and application of machine-learning (ML) methods across chemical sciences, spanning molecular modeling, materials design, catalysis, and chemical discovery. It will bring together researchers who are developing new machine-learning methodologies as well as applying ML techniques to address fundamental and applied problems in chemistry and chemical engineering. Emphasis will be placed on the integration of machine learning with physical principles, first-principles simulations, and experimental data, as well as on challenges related to model interpretability, transferability, and reliability. By bringing together researchers working on diverse chemical problems, ranging from nonadiabatic dynamics and catalysis to chemoinformatics, biomolecular design, and materials discovery, this symposium aims to foster cross-disciplinary discussion and stimulate new collaborations within the regional chemical sciences community.

Presentations:

8:00 AM Opening Remarks.

8:05 AM [MW47] From reaction paths to free-energy landscapes: Exploring chemistry with machine-learned interatomic potentials. **Presented by: Joseph Gomes**

8:35 AM [MW48] Development of accurate and efficient machine-learned quantum dynamics methods for vibrational spectra. **Presented by: Md Omar Faruque**

8:50 AM [MW55] Applied machine learning for green catalysis. **Presented by: Kevin Charles Leonard** [note: time change from original program]

9:20 AM [MW51] DEL-GPT: Generative pretrained transformer to design targeted DNA-encoded libraries. **Presented by: Dmitri Kireev**

9:50 AM Intermission.

10:05 AM [MW52] From water to biomolecules: Predictive simulations through data-driven many-body models. **Presented by: Francesco Paesani**

10:35 AM [MW53] Transferable and accurate machine-learned potential for exploring the potential energy surfaces of gold chloride nanoclusters. **Presented by: Jonathan T Bvunzawabaya**

10:50 AM [MW54] What does a foundation model for atoms know? Running and reading Universal interatomic potentials, from nanocrystal precursors to oxide defects. **Presented by: Robert Bruce Wexler**

11:20 AM [MW49] AI-guided design of AshPhos-P3 ligand: A predictively engineered ligand for Pd-catalyzed amination of hindered primary amines. **Presented by: Mary Richardson** [note: time change from original program]

11:35 AM [MW50] Machine learning interatomic potentials for liquid alloy catalysts. **Presented by: Yao Du** [note: time change from original program]

11:50 AM Closing Remarks.

Organic Chemistry

Time: 8:00 AM - 12:00 PM
Session type: Oral
Location: Room 207, Second Floor
Organizer(s): Ryan J Rafferty
Presider(s): Aruni Peiris Malalasekera

General oral session featuring organic chemistry research

Presentations:

8:00 AM [MW56] Biocatalytic Oxa-Pictet-Spengler reactions. **Presented by: David C. Miller**

8:20 AM [MW57] Electrochemical and 13C NMR determination of Hammett substituent constants using a 2,6-azulenic π-linker. **Presented by: Rene Sabala**

8:40 AM [MW58] Biorenewable strategy for the synthesis of vinyl ethers via cobalt/photoredox decarboxylative eliminations. **Presented by: Colin Waller**

9:00 AM [MW59] Brocazine family of natural products: From total synthesis efforts to targeted chemical screening library construction. **Presented by: Vidya Dhamodharan Nadar**

9:20 AM [MW60] First total synthesis of Balgacyclamide C and new analog based upon computational docking. **Presented by: Meghan Hope Rice**

9:40 AM [MW61] Synthetic efforts towards Cahuitamycin. **Presented by: Matthew Barnett**

10:00 AM Intermission.

10:20 AM [MW62] Direct photochemical glycosylation via a fluorenol-based photoactive leaving group. **Presented by: Sepideh Asgari**

10:40 AM [MW63] Adapting organic reactions to flow chemistry: Synthesis of salen and octyl 3-phenylpropanoate. **Presented by: Sunita Khadka**

11:00 AM [MW64] Stereoselective α-sialylation through electrophilic peroxide–enabled etherification. **Presented by: Axel Matias Irianni**

11:20 AM [MW65] Structure and selectivity differences in the ring hydrogenation of furan 2,5-dicarboxylic acid by supported Pt catalysts. **Presented by: Alan M Allgeier**

11:40 AM [MW66] Generation of unnatural α-amino acids via photoredox-enabled radical decarboxylation. **Presented by: Aishwarya Singh**

Recent Progress in Electrochemical Sensing, Energy Storage, and Synthesis

Time: 8:00 AM - 12:05 PM
Session type: Oral
Location: Bluemont Room, Second Floor
Organizer(s): Takashi Ito, Jun Li
Presider(s): Takashi Ito, Jun Li
Sponsor(s): ANYL, ENFL, COLL

This symposium will provide an interdisciplinary forum for prominent researchers to present their recent achievements on broad electrochemical studies. The topics will include, but are not limited to: electrochemical measurements, electrochemical sensors, electrochemical energy storage devices, electrochemical material synthesis and characterization.

Presentations:

8:00 AM Opening Remarks.

8:05 AM [MW67] Is current always proportional to surface? Consequences in catalysis. **Presented by: Christophe Renault**

8:35 AM [MW68] Stripping-induced acidification accelerates zinc anode corrosion. **Presented by: Samantha Cullom**

8:55 AM [MW69] Driving uranium redox at positive potentials with crown ether chelation. **Presented by: James D Blakemore**

9:25 AM [MW70] Microscale surface ion conduction: Expanding the capabilities of porous biosensors. **Presented by: Robbyn K Anand**

9:55 AM Intermission.

10:15 AM [MW71] Ionic liquids for electrochemical gas sensing. **Presented by: Xiangqun Zeng**

10:45 AM [MW72] High-capacity lithium-oxygen batteries enabled by electrolyte engineering. **Presented by: Xianglin Li**

11:15 AM [MW73] Training-free data-driven prognosis of lithium-ion battery anomalies and thermal runaway. **Presented by: Lin Liu**

11:45 AM [MW74] One-pot versus two-step hydrothermal synthesis of PANI-modified Ni–Co sulfide/oxide electrodes: Mass loading effects on supercapacitor performance. **Presented by: Andrew Ouellette, Jocelyn Ouellette**

Synthesis and Applications of Functional Polymeric Materials

Time: 8:00 AM - 11:45 AM
Session type: Oral
Location: Flint Hills Room, Second Floor
Organizer(s): Patricia R Calvo, Aaron Teator
Presider(s): Patricia R Calvo, Aaron Teator
Sponsor(s): POLY, PMSE

This symposium will showcase recent advances in the design, synthesis, and application of functional polymeric materials that address challenges across science, engineering, and society. Topics will span innovative synthetic methodologies, precision macromolecular architectures, advanced characterization techniques, and emerging applications in areas such as biomedicine, energy, sustainability, electronics, and soft materials. By bringing together researchers working at the interface of chemistry, materials

science, and engineering, this symposium aims to foster interdisciplinary dialogue and highlight the transformative impact of functional polymers in modern technology.

Presentations:

8:00 AM Opening Remarks.

8:05 AM [MW75] Toward predictive design of functional polymeric materials: A three-phase interaction framework. **Presented by: Ji Qi**

8:30 AM [MW76] Multifunctional alginate-corn starch hydrogel beads for enhanced soil water retention and delivery of bioinoculants in agricultural soils. **Presented by: ASAD BIN ZAMAN**

8:55 AM [MW77] Engineered living hydrogels: Fundamental studies of microbe-material interactions in PEG-based matrices. **Presented by: Ryan Hansen, Jeffrey Reed, ASAD BIN ZAMAN**

9:20 AM [MW78] One-step method for the synthesis of bridged-functionalized pillararenes. **Presented by: Maggie He**

9:45 AM Intermission.

10:05 AM [MW79] Development of a thermoresponsive simvastatin prodrug for the treatment of periodontal bone defects. **Presented by: Dong Wang**

10:30 AM [MW80] Cationic polycatechol polymer coatings for multifunctional cardiovascular implants. **Presented by: Alessandro Francisco Martins**

10:55 AM [MW81] Dynamic polymers for energy, sustainability, and human health. **Presented by: Christopher B Cooper**

11:20 AM [MW82] Polymer architecture as a design tool for functional materials. **Presented by: Patricia R Calvo**

Undergraduate Research

Time: 8:00 AM - 11:50 AM
Session type: Oral
Location: Room 227, Second Floor
Organizer(s): Ryan J Rafferty
Presider(s): Ryan J Rafferty

This special oral session will highlight research performed by undergraduate students.

Presentations:

8:00 AM [MW83] Synthesis and characterization of novel aryl-cyanoximes. **Presented by: Thomas Banta**

8:15 AM [MW84] *Withdrawn*

8:30 AM [MW85] Computational modeling of aryl diazonium degradation products relevant to neuropeptide receptor protein labeling. **Presented by: Ryan Inman**

8:45 AM [MW86] Quantitative characterization of bromide- and bromate-dependent wave dynamics in the ferroin-catalyzed Belousov-Zhabotinsky reaction. **Presented by: Ray Guo**

9:00 AM [MW87] Determining the effect of coformer alkyl chain length on cocrystal melting points. **Presented by: Kaitlyn L Jewett**

9:15 AM [MW88] Synthesis of aspirin using FeCl3 in a variety of solvents. **Presented by: Aaron Paul Primrose**

9:30 AM [MW89] Preparation and characterization of two new cyclohexylamide-based cyanoxime ligands and their Pt(II) complexes. **Presented by: Charles Mitchell Lindner**

9:45 AM Intermission.

10:05 AM [MW90] Recovery and reuse of imide fragments from hemiaminal-based aryldifluoromethyl-transfer reagents. **Presented by: Evan Dickson**

10:20 AM [MW91] Alternative solvents to dichloromethane for ring closing metathesis of azamacrocycles. **Presented by: Rebecca McCreight**

10:35 AM [MW92] Evaluation of gold nanosphere-induced cytotoxicity in leukemia cells via MTT assay. **Presented by: Saahil Patel**

10:50 AM [MW93] Gold nanoparticle mediated delivery of FDI6 for targeted glioblastoma therapy. **Presented by: Elda Alsatam**

11:05 AM [MW94] Gold nanospheres as a novel drug delivery method for placenta. **Presented by: Hadiza Elhadji Oumarou Harouna**

11:20 AM [MW95] Co-occurrence of nitrate, nitrite, and arsenic in Lower Elkhorn Natural Resources District groundwater wells. **Presented by: Elizabeth Chhoeung**

11:35 AM [MW96] Critical developments towards using coaxial electrospun nanofibers for AgCl-based water disinfection in long-duration spaceflights. **Presented by: Luke Malone**

Chemical Education

Time: 8:30 AM - 10:05 AM
Session type: Oral
Location: Big 12 Room, Second Floor
Organizer(s): Christine M Aikens
Presider(s): Helena Malinakova

Presentations:

8:30 AM [MW01] Implications for dual-pathway course design in general chemistry. **Presented by: Julie Hamdi**

9:00 AM [MW02] Design and development of a reactive intermediates concept inventory. **Presented by: Sachin Nedungadi**

9:30 AM [MW03] Designing a student-driven environmental chemistry CURE: Integrating water quality research, community partnerships, and science communication. **Presented by: Kelsey Miles**

Biochemistry and Chemical Biology

Time: 10:20 AM - 12:00 PM
Session type: Poster
Location: Grand Ballroom, Second Floor
Organizer(s): Ping Li

General poster session featuring biochemistry and chemical biology research

Presentations:

10:20 AM [MW97] Thermodynamic characterization of naturally occurring RNA octaloops. **Presented by: Siyaanujan Panchalingam**

10:20 AM [MW98] Development of a reporter-based assay to identify VraSR inhibitors and enhance vancomycin activity in Staphylococcus aureus. **Presented by: TIMILEHIN DEMOLA ODERINDE**

10:20 AM [MW99] Discovery and development of novel quinoxaline analogs to treat hearing loss. **Presented by: Cassia Noah**

10:20 AM [MW100] Effects of agricultural biomass-derived hydrochar on soil fungal growth. **Presented by: Waqar Rasool Minhas**

10:20 AM [MW101] De novo mini-protein binders for TREM2 associated with Alzheimer's disease. **Presented by: Doniesha Perera**

10:20 AM [MW102] Improvement of copper and zinc affinity of thermostable green protein (TGP-E) by TGP-E E144H and TGP-E E144H A164H. **Presented by: Madison Guetzkow**

10:20 AM [MW103] Determining the role of acetylation on α-melanocyte stimulating hormone (α-MSH) neuropeptides. **Presented by: Luis Diego Resendiz**

10:20 AM [MW104] Probing the thermodynamics of ligand binding and pseudoknot formation of preQ1 riboswitch. **Presented by: Nusfa Lafir**

10:20 AM [MW105] RNAMotifDB: A hierarchical database of RNA secondary structure motifs for template-based tertiary structure prediction. **Presented by: Danyang Liu**

10:20 AM [MW106] Gamma-secretase modulators shift the cleavage site preference and Aβ trimming process of γ-secretase: Implications for Alzheimer's disease treatment. **Presented by: Tristan Sprague**

10:20 AM [MW107] Progress towards evaluating the modulation of receptor selectivity by amino acid isomerization across different phyla. **Presented by: Andy Elorm Agbakpo**

10:20 AM [MW108] Systematically improving the quality of atomically accurate RNA 3D structures. **Presented by: Kamshinen Joel Dewan**

10:20 AM [MW109] High-throughput analysis of purine riboswitch tertiary contact formation. **Presented by: Danushi Pathirage**

Organic Chemistry

Time: 10:20 AM - 12:00 PM
Session type: Poster
Location: Grand Ballroom, Second Floor
Organizer(s): Ryan J Rafferty

General poster session featuring organic chemistry research

Presentations:

10:20 AM [MW110] Catalytic C–O bond formation in Heck reactions through terminal C–O reductive elimination pathways. **Presented by: Oreoluwa Ayomide Adeyemo**

10:20 AM [MW111] Effect of N-amide substitution on the sensitivity of lysosome-targeted H2S sensors using 1,8-naphthalimide scaffold. **Presented by: Haishi Cao**

10:20 AM [MW112] *Withdrawn*

10:20 AM [MW113] Investigating intermolecular interactions via cocrystal synthesis between amidobenzoic acids and various pharmaceutical agents. **Presented by: Marina Wilson**

10:20 AM [MW114] Selective formation of 1- and 1,8-substituted fluorenones and synthesis of fluorenylspirocyclopropene compounds. **Presented by: John N. Brunn**

10:20 AM [MW115] Structure-guided design of broad-spectrum coronavirus protease inhibitors bearing a 1,3,2-oxazaphospholidin-3-one scaffold as a versatile design element. **Presented by: I.Kankanamge Ravindu Sachinthana Ilesinghe, Pulini Shanela Ranasinghe**

10:20 AM [MW116] Altering the physicochemical properties of benzoxazol derivatives through co-crystallization. **Presented by: Jordan Barb**

10:20 AM [MW117] From click chemistry to cocrystal synthesis. **Presented by: Ravindra W Pathinayaka**

10:20 AM [MW118] Acid-catalyzed non-reductive deoxygenation of biocrude. **Presented by: Espoir Victor Kwihangana**

10:20 AM [MW119] Design and in silico computational assessment of hydrocaffeic acid functionalized PAMAM derivatives for antimicrobial application: An integrated DFT, molecular docking, dynamics simulation and pharmacokinetic study. **Presented by: Mohammed Anowar Hosen**

10:20 AM [MW120] Tröger's base as a multifunctional platform for metallodrug and supramolecular design. **Presented by: Asanga Kasun Mannapperuma**

10:20 AM [MW121] Development of activated iodinated alkynyl esters for halogen-bond-driven crystal engineering. **Presented by: Arti Pujari**

10:20 AM [MW122] Mechanochemical control of divergent carboxylic acid activation: Selective formation of N-acylsuccinimides and anhydrides. **Presented by: Laxman Lamichhane**

10:20 AM [MW123] Arene-bridged polyvalent triazolium salts with antiseptic properties. **Presented by: Matthieu E Carter**

10:20 AM [MW124] One-step versus stepwise 2-electron electrochemical reduction of 6,6'-biazulenes. **Presented by: Ryan N Pierce**

10:20 AM [MW125] Investigating the importance of flexibility in antimicrobial quaternary ammonium surfactants using alkyne hydrogenation. **Presented by: Jackson Conrad Skuodas**

10:20 AM [MW126] Visible-light-driven defluorination of perfluoroalkyl carboxylic acids through an inner-sphere transition-metal photocatalytic pathway. **Presented by: Ashan S. Wickramaarachchi**

10:20 AM [MW127] Determining substituent effects on photodeprotection rates of antiseptic 1,2,3-triazolium salts. **Presented by: Alexis L. Murphy**

10:20 AM [MW128] *Withdrawn*

Leadership Panel and Workshop: Leap into Leadership

Time: 11:30 AM - 1:00 PM

Session type: Workshop

Location: JP's Union Station, First Floor

This workshop will bring together a diverse audience including current professionals, graduate students, K-12 educators, and other aspiring and emerging leaders, with the goal of fostering meaningful conversations about leadership, professional growth, overcoming challenges, and creating a positive impact within our communities and professions. Lunch will be provided. Pre-registration is required, $5.

Advances in Molecular Probes for Therapeutics

Time: 1:30 PM - 5:25 PM

Session type: Oral

Location: Cottonwood Room, Second Floor

Organizer(s): Ping Li

Presider(s): Ping Li, Pablo Sobrado

Sponsor(s): MEDI, Cambrex, Advion

This symposium will highlight recent advances in the design, synthesis, and application of molecular probes that are transforming research at the interface of chemical biology and medicinal chemistry. Topics will include innovative strategies for probing biological pathways, visualizing and modulating biomolecular targets, and accelerating the discovery of next-generation therapeutics. By bringing together researchers working across chemistry, biology, and drug discovery, the symposium will showcase the excitement and growing impact of molecular probe science in advancing human health.

Presentations:

1:30 PM Opening Remarks.

1:35 PM [MW129] Cholesterol metabolism and recycling in response to demyelination. **Presented by: Meredith D Hartley**

2:05 PM [MW130] Optimization of a small molecule inhibitor of complement protease C1s. **Presented by: Brian V Geisbrecht**

2:35 PM [MW131] Molecular probes for decoding NTMT1 biology: From substrate discovery to real-time targeted protein degradation. **Presented by: Ping Li**

3:05 PM [MW132] *Withdrawn*

3:25 PM Intermission.

3:45 PM [MW133] Flavin-dependent enzymes as antimicrobial targets: From mechanism to inhibitor discovery. **Presented by: Pablo Sobrado**

4:15 PM [MW134] Discovery of protein-binding peptides: From computational screening to biological applications. **Presented by: Xiaoqin Zou**

4:45 PM [MW135] Enzyme-activatable 5-ALA prodrugs for targeted photodynamic therapy. **Presented by: Karolina Rooney**

5:05 PM [MW136] *Withdrawn*

Analytical Chemistry

Time: 1:30 PM - 3:50 PM
Session type: Oral
Location: Bluemont Room, Second Floor
Organizer(s): Daniel A Higgins, Wenting Hu
Presider(s): Wenting Hu

General oral session featuring analytical chemistry research

Presentations:

1:30 PM [MW137] Quantitative glycomics reveals brain carbohydrate signatures associated with dairy-derived sialic acid and cognitive health. **Presented by: Han Peng**

1:50 PM [MW138] Continuous monitoring of tumor necrosis factor alpha using online affinity micro free-flow electrophoresis. **Presented by: Sandra Chinemerem Nwankwo**

2:10 PM [MW139] Stereochemical evaluation of cell-cell signaling peptides in Platynereis dumerilii. **Presented by: Ashley Clifton**

2:30 PM [MW140] Label-free single-molecule detection and machine learning classification of amino acids using a solid-state in-plane nanopore platform. **Presented by: Pramodi Kaushani Vithanage**

2:50 PM [MW141] Development of multiplex electrochemical biosensors for quantifying overexpressed proteases in cancer. **Presented by: Bingun Habarakadage**

3:10 PM [MW142] *Withdrawn*

3:10 PM [MW143] Protein analyses using novel divergent field ion mobility focusing (DIFIMOF) separations with high-resolution tandem MS. **Presented by: Adetayo S. Afolayan** [note: time has changed since original program]

Inorganic Chemistry

Time: 1:30 PM - 3:10 PM
Session type: Poster
Location: Grand Ballroom, Second Floor
Organizer(s): Tendai Gadzikwa

General poster session featuring inorganic chemistry research

Presentations:

1:30 PM [MW144] Design and development of Ln-MOF fluorophores for cellular multiplexing imaging applications. **Presented by: Brayden Schut**

1:30 PM [MW145] Design, synthesis, and characterization of mixed-linker Ln-MOFs with ligand and metal luminescence for cellular imaging applications. **Presented by: Ashlyn Erdmann**

1:30 PM [MW146] Synthesis of rigid quaternary ammonium compounds (QACs) for use as capping agents to create fluorescent lanthanide metal-organic framework (MOF) antimicrobial materials. **Presented by: Bradley Infield, Jackson Conrad Skuodas**

1:30 PM [MW147] Regioselective pyridine synthesis via an iron-catalyzed [2+2+2] cycloaddition. **Presented by: Michael Conk**

1:30 PM [MW148] New insights into iron β-diketiminato complexes for their group transfer and multicomponent reactions. **Presented by: Lillian Adams**

1:30 PM [MW150] Fabrication, characterization, and reactivity study of an FeIII-OMe complex. **Presented by: Marcus Fiedler**

1:30 PM [MW151] Synthesis, spectroscopy, and redox studies of Fe, Mn, and Co thiolate complexes supported by a triaryl tetradentate ligand. **Presented by: Dunya Sembukuttiarachchi**

1:30 PM [MW152] Synthesis of stable multinary MOFs. **Presented by: Yvonne Jongwe**

1:30 PM [MW153] Electronic properties of heterobimetallic complexes incorporating vanadyl and uranyl ions. **Presented by: Andrew Jacobs**

1:30 PM [MW154] Measuring and understanding how organic electrolytes impact molecular europium redox chemistry. **Presented by: Jared Schaeffer**

Midwest Awards Symposium

Time: 1:30 PM - 5:30 PM
Session type: Oral
Location: Big 12 Room, Second Floor
Organizer(s): Joshua Yuan
Presider(s): Joshua Yuan

This invited symposium highlights research by the Midwest Award winner and invited presenters.

Sponsor(s): St. Louis Local ACS Section

Presentations:

1:30 PM Opening Remarks.

1:35 PM [MW155] Defluorination of perfluorooctanesulfonate (PFOS) by vanadium carbide (V2C) mxenes catalyzed by hydrogen peroxide. **Presented by: Jessica Ray**

2:20 PM [MW156] Identifying key mechanisms for inhibiting calcium carbonate nucleation in reverse osmosis concentrate. **Presented by: Honghyun Kim**

2:45 PM [MW157] Crystal engineering for water: Molecular design meets artificial intelligence. **Presented by: Zhiling Zheng**

3:30 PM Intermission.

3:50 PM [MW158] Microbial and electro-microbial design for efficient carbon utilization. **Presented by: Joshua Yuan**

4:35 PM [MW159] Small Science, Big Impact. **Presented by: Young-Shin Jun**

5:25 PM Closing Remarks.

Organic Chemistry

Time: 1:30 PM - 5:30 PM
Session type: Oral
Location: Room 207, Second Floor
Organizer(s): Ryan J Rafferty
Presider(s): James Townsend

General oral session featuring organic chemistry research

Presentations:

1:30 PM [MW182] Phthalimide-derived hemiaminals and hemiaminolates as tunable aryldifluoromethyl-transfer reagents. **Presented by: Laxman Lamichhane**

1:50 PM [MW183] Hydrogen vs halogen bonding: The competition effect on thermal expansion in multicomponent solids. **Presented by: Jane Eilers**

2:10 PM [MW184] From chains to dimers: Structural motifs and co-crystal formation in benzothiazole amides. **Presented by: Bella Ginie**

2:30 PM [MW185] Programming molecular communication: From supramolecular design to functional materials. **Presented by: Christer B Aakeroy**

2:50 PM [MW186] *Withdrawn*

2:50 PM [MW187] Synthesis, characterization and evaluation of self-decontaminating cotton fabric for organophosphate detoxification. **Presented by: Shirin Mohammad Saeed** [note: time change from original program]

3:10 PM Intermission.

3:50 PM [MW188] Wavelength-selective photochemistry via distinct reactive intermediates. **Presented by: Logan Evans**

4:10 PM [MW189] Selective diamondoid functionalization using direct photochemical methodologies. **Presented by: Henry Thomas O'Callaghan**

4:30 PM [MW190] Can we predict photoreactivity. **Presented by: Madelyn Austin**

4:50 PM [MW191] Development of a self-sufficient biomass hydrothermal liquefaction process for the future biorefinery. **Presented by: Abdul Rashid Issifu**

5:10 PM [MW192] Covalent modification of Kevlar fabric with oxime for improved detoxification of organophosphates and its use in protective fabrics. **Presented by: Raghuram Gujjarappa**

Organic Chemistry

Time: 1:30 PM - 3:10 PM
Session type: Poster
Location: Grand Ballroom, Second Floor
Organizer(s): Ryan J Rafferty

General poster session featuring organic chemistry research

Presentations:

1:30 PM [MW160] Preparation of antiseptic polyvalent triazolium salts with bridging benzyl groups. **Presented by: Luke D. Abbott**

1:30 PM [MW161] Evaluating the substrate scope of an improved Blum aziridine synthesis. **Presented by: Hannah Cardenas**

1:30 PM [MW162] Novel enamine and imine analogs of 3-formylchromone and their cytotoxic effects. **Presented by: Sara Kimrey**

1:30 PM [MW163] Alkyl radical addition to activated vinyl imines. **Presented by: Ana Mendes**

1:30 PM [MW164] Radical synthesis of α-hydroxy allenes utilizing triethylborane. **Presented by: Gage Helm**

1:30 PM [MW165] Screening small molecule benzannulated indole libraries against sinonasal undifferentiated carcinoma (SNUC). **Presented by: Keith R Buszek**

1:30 PM [MW166] Total synthesis of the trikentrins and the trikentramides using one-pot tandem Bartoli syntheis/indole aryne Diels-Alder cycloaddition methodologies. **Presented by: An Nguyen**

1:30 PM [MW167] Computational investigation of demercuration mechanisms in alkylmercuric hydroxides. **Presented by: Donna K Jean**

1:30 PM [MW168] *Withdrawn*

1:30 PM [MW169] Transforming Reniochalistatin E into a modular drug delivery platform. **Presented by: Noah James Burgoon**

1:30 PM [MW170] Total synthesis of Reniochalistatin E analogs to enable drug delivery & potentiation. **Presented by: Jonathan Taylor Lora**

1:30 PM [MW171] Next generation of chemical screening libraries: From total synthesis of natural products to intermediate diversification: The story of Uvaretin and the Brocazine's. **Presented by: Gregory Evans**

1:30 PM [MW172] Photoswitch-enabled control of macrocyclic alkyne reactivity. **Presented by: Miles Mundorf**

1:30 PM [MW173] Synthesis of Balgacyclamide C analogs in pursuit of discovering the biological pharmacophore: Retention of the upper heterocyclic ring system. **Presented by: Ryan Bachman**

1:30 PM [MW174] Modulating hole transport properties in PAHs: Substitution-driven optoelectronic tuning. **Presented by: Nico Spencer**

1:30 PM [MW175] Synthetic efforts towards a histidine analog of Reniochalistatin E for cancer drug delivery. **Presented by: Emma Rose Edwards**

1:30 PM [MW176] From total synthesis to chemical screening libraries: The story of Brocazine and new therapeutic agent discovery. **Presented by: Blessing Zvikomborero Kusena**

1:30 PM [MW177] Engineering dipole-parallel alignment in donor-acceptor organic molecular crystals. **Presented by: Max Markgraf, Gabrielle Thomas, Jacob Hidding**

1:30 PM [MW178] Synthesis of Balgacyclamide C analogs in pursuit of discovering the biological pharmacophore: Retention of the lower peptide fragment. **Presented by: Sicilei Redd**

1:30 PM [MW179] Unlocking Lagunamide C: Structure-activity-relationship studies of the polyketide and penetration investigations of the polypeptide backbone. **Presented by: Benjamin Clyde Rudeen**

1:30 PM [MW180] Investigation of a Tandem Indole 3-Sulfenylation/C2-C2' Coupling Reaction. **Presented by: Jonathon Scott Russel**

1:30 PM [MW181] Synthesis and characterization of hemiaminals and hemiaminolates as modular aryldifluoromethyl-transfer reagents. **Presented by: Evan Dickson**

Super-Resolved Spectroscopy: Physical Phenomena in Space and Time

Time: 1:30 PM - 5:30 PM
Session type: Oral
Location: Room 206, Second Floor
Organizer(s): Christopher G Elles, Daniel A Higgins
Presider(s): Christopher G Elles, Daniel A Higgins
Sponsor(s): PHYS, ANYL

This symposium will bring together prominent researchers developing and using state-of-the-art ultrafast and super-resolved spectroscopic and microscopic methods for studying physical and chemical phenomena in solution and near surfaces.

Presentations:

1:30 PM [MW193] Mapping molecular heterogeneity and interfacial anisotropy in biomolecular condensates using single-fluorogen imaging. **Presented by: Matthew D Lew**

2:10 PM [MW194] Vertically-stood anodic alumina membranes as unique platforms to study nanoconfined molecular diffusion and surface adsorption using single-molecule localization microscopy. **Presented by: Takashi Ito**

2:50 PM [MW195] Potential-modulated fluorescence approach for the determination of the electron transfer rate constant of electrode-tethered electroswitchable fluorophores. **Presented by: Anuththara D.G Karunarathna**

3:10 PM [MW196] Super-resolved single-molecule studies of Rhodamine B accumulation on fresh and aged polyethylene terephthalate. **Presented by: Sorour Salehi**

3:30 PM Intermission.

3:50 PM [MW197] Phasor assisted photon modulation for hyperspectral single-molecule microscopy. **Presented by: Bin Dong**

4:30 PM [MW198] Two-photon absorption spectroscopy in service of microscopy imaging and dynamics. **Presented by: Christopher G Elles**

5:10 PM [MW199] Two-photon excited fluorescence measurement of coumarin 153 using broadband two-photon absorption spectroscopy combined with sensitive fluorescence detection. **Presented by: Joohyun Lee**

Synthesis and Applications of Functional Polymeric Materials

Time: 1:30 PM - 5:15 PM
Session type: Oral
Location: Flint Hills Room, Second Floor
Organizer(s): Patricia R Calvo, Aaron Teator
Presider(s): Patricia R Calvo, Aaron Teator
Sponsor(s): POLY, PMSE

This symposium will showcase recent advances in the design, synthesis, and application of functional polymeric materials that address challenges across science, engineering, and society. Topics will span

innovative synthetic methodologies, precision macromolecular architectures, advanced characterization techniques, and emerging applications in areas such as biomedicine, energy, sustainability, electronics, and soft materials. By bringing together researchers working at the interface of chemistry, materials science, and engineering, this symposium aims to foster interdisciplinary dialogue and highlight the transformative impact of functional polymers in modern technology.

Presentations:

1:30 PM [MW200] Functionality for free: Interphases in composites. **Presented by: Frank Dennis Blum**

1:55 PM [MW201] Beyond the weighted average: Non-linear structure-property relationships in grafted polysaccharides. **Presented by: Cecile Chazot**

2:20 PM [MW202] Mechanically transparent seams and coatings: A solvent-free dual-network approach. **Presented by: Gabriela Moreira Lana**

2:45 PM [MW203] From dimerization to oligomerization through solid-state photochemistry. **Presented by: Kristin M Hutchins**

3:10 PM Intermission.

3:30 PM [MW204] Nitrogen insertion approaches to polymer backbone editing. **Presented by: Aaron Teator**

3:55 PM [MW205] Functionalization and crosslinking of brominated poly(lactic acid). **Presented by: Coleen Pugh**

4:20 PM [MW206] Room-temperature preparation of a luminescent crystalline gold chalcogenolate polymer. **Presented by: Kelly Powderly**

4:45 PM [MW207] Three-dimensional electrospun Zn/PCL and core–shell Zn/PCL@PCL scaffolds with tunable zinc release. **Presented by: Zhengtao Zhu**

5:10 PM Closing Remarks.

Theory, Modeling and Simulation of Biomolecular Systems

Time: 1:30 PM - 5:30 PM

Session type: Oral

Location: Room 227, Second Floor

Organizer(s): Jeffrey Robert Comer, Paul Edward Smith

Presider(s): Jeremy D. Schmit, Paul Edward Smith

Sponsor(s): COMP, PHYS

The session is aimed at bringing together a group of varied researchers who have a common goal of understanding biological systems through the use of theory and simulation, an important aspect of many biophysical studies.

Presentations:

1:30 PM [MW208] *Withdrawn;* Substitute talk: Absolute Binding Free Energy Calculations for Peptide Self-Assembly at Interfaces. **Presented by: Jeffrey Comer**

2:05 PM [MW209] Functionally-important protein dynamics are altered by amino acid changes at rheostat positions. **Presented by: Liskin Swint-Kruse**

2:40 PM [MW210] AI-driven peptide prediction integrated with molecular dynamics simulations for mechanistic insights into membrane selectivity. **Presented by: Nandan Kumar**

3:00 PM [MW211] *Withdrawn;* Substitute talk: TBA

3:20 PM Intermission.

3:40 PM [MW212] *Withdrawn*

4:15 PM [MW213] On the nature of ion atmospheres and rules for their formation. **Presented by: Elizabeth A Ploetz**

4:50 PM [MW214] Dynamic modulation and allosteric mechanisms underlying ACKR3-mediated arrestin2/3 activation. **Presented by: Xinqiu Yao**

5:10 PM [MW215] Simulations of ions diffusion with multilayer QM/MM adaptive partitioning methods. **Presented by: Emilie Brigitte Guidez**

Chemical Education

Time: 3:50 PM - 5:30 PM
Session type: Poster
Location: Grand Ballroom, Second Floor
Organizer(s): Christine M Aikens

Presentations:

3:50 PM [MW216] Get involved with the ACS Division of Chemical Education. **Presented by: Jennifer Boutte**

3:50 PM [MW217] Key role of students metacognitivie skills in learning organic chemistry. **Presented by: Helena Malinakova**

3:50 PM [MW218] Utilization of eye tracking to add to the validity of data obtained using the resonance concept inventory. **Presented by: Mary Simon**

3:50 PM [MW219] Utilization of chemical demonstrations as an experiential and collaborative learning strategy for general chemistry students. **Presented by: George P Nora**

3:50 PM [MW220] *Withdrawn*

3:50 PM [MW221] New training and professional development tools for bio/chemical analysis. **Presented by: Martha Dolan Morton**

3:50 PM [MW222] 3-D printing as a responsive tool to pedagogical and laboratory needs. **Presented by: Evan Vanable**

3:50 PM [MW223] Assessment of an open-source stopped flow system. **Presented by: Finley Hall**

3:50 PM [MW224] Spectroscopic characterization and extraction optimization of catechins in green tea. **Presented by: Zach McKinley**

3:50 PM [MW225] Synthesis and characterization of sodium trioxodinitrate (Na2N2O3; Angeli's salt). introduction to nitroxyl (HNO) chemistry in upper-division undergraduate laboratory. **Presented by: Daniel Pham**

3:50 PM [MW226] Integration in upper-division chemistry laboratories: Synthesis and characterization of oxovanadyl(IV) compounds. **Presented by: Natalie Gonzalez Pacheco**

3:50 PM [MW227] Controlled release of oxygen from hydrogen peroxide using recycled HotHand packet solid. **Presented by: Aaron Paul Primrose**

3:50 PM [MW228] Lipid oxidation and effect of antioxidants in food matrices of varying water activity level: A model for food chemical education. **Presented by: Gerald Joseph Buonopane, Daniel Francis, Nicholas Battista**

Inorganic Chemistry

Time: 3:50 PM - 5:30 PM
Session type: Poster
Location: Grand Ballroom, Second Floor
Organizer(s): Tendai Gadzikwa

General poster session featuring inorganic chemistry research

Presentations:

3:50 PM [MW149] Lewis acid effects on the reduction of a monometallic vanadyl complex. **Presented by: Noah Tucker**

3:50 PM [MW229] Interpretation of the electronic structure from experimental X-ray absorption spectra (XAS) using computational methods. **Presented by: Rhoda Cherotich Komen**

3:50 PM [MW230] Flow synthesis of cryptomelane (KMn8O16): A greener alternative to conventional batch synthesis. **Presented by: Sunita Khadka**

3:50 PM [MW231] Design of NiMoO4/Ni-Mo-S MOF composite electrodes for supercapacitor applications. **Presented by: Quoc Bao Le**

3:50 PM [MW232] Measuring Hammett substituent constants with a sensitive organometallic 13C NMR reporter. **Presented by: Jonathan Joel Davis**

3:50 PM [MW233] Comparing the thermodynamic properties and reactivity of FeIII- and MnIII-hydroxo complexes. **Presented by: Anagha Puthiyadath**

3:50 PM [MW234] Spectroscopic and mechanistic study of a manganese cerium adduct: Effect of electron-donating ligand on selectivity. **Presented by: Purti Patel**

3:50 PM [MW235] Characterization of the oxidation of an Fe(II)-aqua complex via a hydrogen atom transfer reaction. **Presented by: Haley Sellmeyer**

3:50 PM [MW236] Synthesis, isolation, and redox chemistry of heterobimetallic uranium/europium complexes. **Presented by: Ty OJanovac**

3:50 PM [MW237] Spectroscopic properties and reactivity of a MnIII-hydroperoxo complex that is stable at room temperature. **Presented by: Zahra Aghaei**

3:50 PM [MW238] Facile linking of lanthanide cations with soft metals via thiosulfate. **Presented by: Braeden D Barry**

3:50 PM [MW239] Synthesis and crystal structures of heavy metal thiosalicylate complexes. **Presented by: Ava R Zimmerman**

3:50 PM [MW240] *Withdrawn*

3:50 PM [MW241] Functionalizing nanoporous metal-organic supercontainers for environmental remediation of illicit substances. **Presented by: MaKenna King**

3:50 PM [MW242] Designing metal-organic supercontainers for direct air capture. **Presented by: Taylor Kragel**

3:50 PM [MW243] Chiral bifunctional urea-based MOF catalyst with simultaneous basicity and dual-hydrogen-bond-donor activation for the Henry reaction. **Presented by: Lamontain Udube**

3:50 PM [MW244] Uranium redox at very positive potentials with oxygen-donor crown ethers. **Presented by: Chad Lakin**

3:50 PM [MW245] Electrochemical studies of lanthanide complexes supported by a di-aza crown ether ligand. **Presented by: Aubrey Brown**

3:50 PM [MW246] Experimental studies of platinum heterobimetallic complexes to probe Lewis acid effects. **Presented by: Dermot O'Connor**

Governance Reception

Time: 5:30 PM - 6:30 PM
Session type: Social Event
Location: Grand Ballroom, Second Floor

All MWRM ACS attendees are invited to attend this reception.

Awards Banquet

Time: 7:00 PM - 9:00 PM
Session type: Social Event
Location: Bluemont Room, Second Floor

Tuesday, October 27, 2026

Registration

Time: 6:30 AM - 5:00 PM
Session type: Registration
Location: Second Floor Lobby

Badge pick-up and onsite registration.

Midwest Regional Board breakfast

Time: 7:30 AM - 11:00 AM
Session type: Board Meeting
Location: JP's Union Station, First Floor

Advancement in Electrocatalytic Materials for Energy and Fuel Productions

Time: 8:00 AM - 12:05 PM
Session type: Oral
Location: Bluemont Room, Second Floor
Organizer(s): Jun Li, Bin Liu
Presider(s): Jun Li, Bin Liu
Sponsor(s): Shimadzu, ANYL, PHYS

This symposium will provide a forum for researchers to present their recent achievements in electrocatalysis studies. A mix of experimental and theoretical/modelling studies on topics related to electrocatalysis are planned. The symposium will include areas such as the development of electrocatalysts, architectures and systems for energy and fuel production, including fuel cells, electrolyzers, sensors, electrosynthesis, electrochemical energy storage, environmental remedies, etc. This symposium will enhance interactions among researchers who are working on materials synthesis, characterization, modeling and system integration related to electrocatalytic systems.

Presentations:

8:00 AM Opening Remarks.

8:05 AM [MW247] Improving Li-S battery performance by incorporating a set of MoSx/rGO electrocatalysts in the S/C cathode and interlayer. **Presented by: Zahirul Islam Saddam**

8:35 AM [MW248] Unusual reactivity of 2D transition metal carbides (MXenes). **Presented by: Vadym Mochalin**

9:05 AM [MW249] Influence of groundwater contaminates on electrocatalytic nitrate reduction. **Presented by: Mukhtiar Ali**

9:25 AM [MW250] Unravelling the impact of interfacial pH swings on nitrate electroreduction selectivity. **Presented by: Karthik Mamandur Gopalakrishna**

9:45 AM [MW251] Integration of thermoelectric generators and solid oxide electrolysis cells for efficient waste heat recovery in green hydrogen production. **Presented by: Hamza Fakhsy, Youssef Naimi, Hassan Mabrak**

10:05 AM Intermission.

10:25 AM [MW252] Investigation of low-dimensional materials as potential Li-ion anode materials: A case study of quasi-1D NbTe4. **Presented by: Jian Wang**

10:55 AM [MW253] Sodium versus lithium: How solvation improves battery behavior. **Presented by: Rachel Carter**

11:25 AM [MW254] *Withdrawn*

11:25 AM [MW255] Flower-like Fe-based metallogel as a durable electrocatalyst for oxygen evolution reaction. **Presented by: Mita Dutta** [Note time change from original program]

Advances in Catalysis and Methods for Organic Synthesis

Time: 8:00 AM - 12:00 PM
Session type: Oral
Location: Big 12 Room, Second Floor
Organizer(s): Socrates B. Munoz, Jon A Tunge
Presider(s): Socrates B. Munoz, Florence J Williams
Sponsor(s): ORGN, FLUO, Cambrex, Advion

This symposium honors recent Cope Scholar, Prof. Thomas Lectka

Presentations:

8:00 AM Opening Remarks.

8:10 AM [MW256] Atropdiastereomerism in metacyclophane macrocycles. **Presented by: Junqi Li**

8:45 AM [MW257] From oxaboranes to oxaborole catalysts: Modular synthesis of and regioselective catalysis with non-benzofused boron heterocycles. **Presented by: Levi M Stanley**

9:20 AM [MW258] Controlling ambident reactivity in organic synthesis via catalysis. **Presented by: Douglas Edward Frantz**

9:55 AM Intermission.

10:15 AM [MW259] Molecules, molecular diagnostics, and the interplay between organic synthesis and functionalized electrodes. **Presented by: Kevin David Moeller**

10:50 AM [MW260] New strategies for photocatalytic bond activation of strong C-H bonds. **Presented by: David Martin**

11:25 AM [MW261] Leveraging multi-component reactions toward xylochemical decarboxylative functionalization. **Presented by: Jon A Tunge**

Analytical Chemistry

Time: 8:00 AM - 12:00 PM
Session type: Oral
Location: Room 206, Second Floor
Organizer(s): Daniel A Higgins, Wenting Hu
Presider(s): Wenting Hu

General oral session featuring analytical chemistry research

Presentations:

8:00 AM [MW262] Infrared quantification of siloxanes in synthetic biogas in the presence of carbon dioxide. **Presented by: Kayla McCreary**

8:20 AM [MW263] Results of a regulatory assignment to determine opiate alkaloids on imported poppy seeds. **Presented by: Erica L. Bakota**

8:40 AM [MW264] Enhancing capacitive deionization performance through safe polymeric binders. **Presented by: Sanjeev Billa**

9:00 AM [MW265] Textural property evaluation of mesoporous silica induced by acid, solvent, thermal treatment and methylene blue uptake. **Presented by: Resham Lal Shrestha**

9:20 AM [MW266] Engineering AgCl-loaded nanofiber membranes for sustained antimicrobial water treatment in long-duration space missions. **Presented by: Vijay Nathan Somasundaram**

9:40 AM [MW267] Investigation of electrodeposited Cu-MOF for enzyme immobilization at electrode interfaces. **Presented by: Helen Qin**

10:00 AM Intermission.

10:20 AM [MW268] Super-resolved single molecule detection and tracking studies of Rhodamine B adsorption on fresh and aged polyethylene terephthalate and polystyrene microplastic models. **Presented by: Mohammad Motiur Rahman**

10:40 AM [MW269] Quantitative analysis of pesticides in potatoes. **Presented by: Lydia Wilson**

11:00 AM [MW270] Hybrid MXene and metal organic framework for electrochemical nitrate sensing. **Presented by: Aarthi Kannan**

11:20 AM [MW271] Occurrence, spatial distribution, and dietary risk assessment of cypermethrin and glyphosate residues in environmental matrices from agricultural settlements in southwestern Nigeria. **Presented by: Omolara Jemimah Jemimah Ojezele**

11:40 AM [MW272] Establishing EPA Method 1633A as the primary analytical tool for PFAS analysis of agricultural samples in Kansas. **Presented by: Kushan Kompalage**

Chemistry under Nanoconfinement

Time: 8:00 AM - 11:45 AM
Session type: Oral
Location: Flint Hills Room, Second Floor
Organizer(s): Saswata Dasgupta, Tendai Gadzikwa, Takashi Ito
Presider(s): Saswata Dasgupta, Tendai Gadzikwa, Takashi Ito
Sponsor(s): INOR, ANYL, PHYS

This symposium will highlight recent advances in understanding chemical phenomena in confined and porous environments. This symposium will bring together researchers working on the synthesis, experimental characterization, and computational modeling of porous and low-dimensional materials, including metal-organic frameworks (MOFs), porous organic crystals, zeolites, nanotubes, and two-dimensional materials. Emphasis will be placed on how nanoconfinement alters structure, dynamics, transport, and reactivity at solid-liquid and electrode-electrolyte interfaces, with applications spanning electrocatalysis, electrochemical sensing, energy storage, separations, and confined fluids. By integrating experimental and theoretical research, ranging from advanced spectroscopy and electrochemical measurements to quantum chemistry and molecular simulations, this symposium aims to foster cross-disciplinary discussion and collaboration.

Presentations:

8:00 AM Opening Remarks.

8:05 AM [MW273] Mesopore-confinement enhances selective polyolefin hydrogenolysis. **Presented by: Wenyu Huang**

8:35 AM [MW274] Confinement-driven catalysis in metal–organic frameworks. **Presented by: Subhajit Acharya**

8:55 AM [MW275] Solute diffusion in nanoconfined partially miscible n-butanol/water mixtures. **Presented by: Safoura Asadi**

9:15 AM [MW276] Correlating solvent structure and single-molecule transport in nanoconfined ethanol–water–salt mixtures using confocal Raman and fluorescence correlation spectroscopy. **Presented by: Kumar Amgain**

9:35 AM [MW277] Dynamics of water in mesoporous silica. confinement and interfacial effects. **Presented by: Ward H. Thompson**

10:05 AM Intermission.

10:25 AM [MW278] Chemistry under nanoconfinement: From MAX phase etching to functional MXenes. **Presented by: Alexander Sinitskii**

10:55 AM [MW279] Unravelling the driving forces behind confined water dynamics in nanoscale silica slit pores. **Presented by: Thanuja Jayawardena**

11:15 AM [MW280] Aqueous electrolytes in nanoscale slit pores: Structure, dynamics, and ion-pairing thermodynamics. **Presented by: Saswata Dasgupta**

Physical Chemistry

Time: 8:00 AM - 10:20 AM
Session type: Oral
Location: Room 207, Second Floor
Organizer(s): Christine M Aikens
Presider(s): Sadish Karunaweera

General oral session featuring physical chemistry research

Presentations:

8:00 AM [MW281] Beyond benzenoid aromatics' comfort zones. **Presented by: Mikhail V Barybin**

8:20 AM [MW282] Thermodynamic kinetics of gold ion retrieval by linear and branched cross-linked polyethyleneimine networks. **Presented by: Merina Sah**

8:40 AM [MW283] Crystallographic insights into ionic-liquid phase behavior: σ-hole interactions, melting, and supercooling. **Presented by: Patrick Hillesheim**

9:00 AM [MW284] Activation energies from single-temperature simulations: Insights into water dynamics. **Presented by: Elizabeth R. Bartlett**

9:20 AM [MW285] Activation energies and activation volumes for water dynamics in cryoprotectant solutions. **Presented by: Anjali Radhakrishnan**

9:40 AM [MW286] Infrared study of partially hydrated lithium thiocyanate salts: Insight into hydration structure and geometry. **Presented by: Herman Richard Krueger**

10:00 AM [MW287] Size-dependent effects of a hydrophobic solute on water structure and dynamics. **Presented by: Nnamdi K. Uzoukwu**

Polymer Chemistry

Time: 8:00 AM - 11:45 AM
Session type: Oral
Location: Cottonwood Room, Second Floor
Organizer(s): Patricia R Calvo
Presider(s): Dean Afsar, Anna M. Luke

General oral session featuring polymer chemistry research

Presentations:

8:00 AM [MW288] Alternating ADMET as a platform for precision polymer design. **Presented by: Digambar Bhandari**

8:20 AM [MW289] Single-site bismuth alkoxide catalysts for the stereoselective ring-opening polymerization of rac-lactide. **Presented by: Anna M. Luke**

8:40 AM [MW290] From chains to cycles: Nitrilium-driven cyclization in secondary polyacrylamides. **Presented by: Pranay Bonagiri**

9:00 AM [MW291] Structure-property relationships in glycerol-crosslinked and HMDS-modified soybean oil-based polyurethane coatings. **Presented by: Mayankkumar Chaudhary**

9:20 AM [MW292] High-throughput microwave synthesis and machine-learning optimization of covalent organic framework (COFs). **Presented by: Reid Augustyn Coyle**

9:40 AM Intermission.

10:05 AM [MW293] Diblock copolymers with LCST behavior for conformance control in carbonate reservoirs. **Presented by: Sara McCauley**

10:25 AM [MW294] Trojan terephthalates for scalable depolymerization. **Presented by: Dhananjay Dileep**

10:45 AM [MW295] Chemical vapor deposition synthesis of hydrazone-linked covalent organic framework (COF-42) thin films. **Presented by: Gurunanthanan Vijayakumar**

11:05 AM [MW296] Microstructural diversity through Brook rearrangement polymerization. **Presented by: Alec Lininger**

11:25 AM [MW297] Controlled aqueous RAFT polymerization of amino-functional polymers for antimicrobial applications. **Presented by: Dean Afsar**

Polymer Chemistry

Time: 8:00 AM - 9:40 AM
Session type: Poster
Location: Grand Ballroom, Second Floor
Organizer(s): Patricia R Calvo

General poster session featuring polymer chemistry research

Presentations:

8:00 AM [MW298] Inositol-derived stiff methacrylates for sustainable high-temperature polymer applications. **Presented by: Tyler Schepanski**

8:00 AM [MW299] Synthesis of aliphatic poly(ester carbonate) copolymers using novel chloroformates and their hydrolytic and enzymatic degradation. **Presented by: Mahrokh Moradi**

8:00 AM [MW300] Benzimidazolum salts from renewable sources for antibacterial applications. **Presented by: Charles J Neef**

8:00 AM [MW301] Backbone editing via the Beckmann rearrangement. **Presented by: Peace Adelowokan**

8:00 AM [MW302] Contact lens modification & microparticles production for ocular drug delivery. **Presented by: Jetty Lynn Duffy-Matzner**

8:00 AM [MW303] Imidazolium salts from renewable sources for antibacterial applications. **Presented by: Charles J Neef**

8:00 AM [MW304] Antibacterial testing of hyaluronic acid derivatives. **Presented by: Charles J Neef**

8:00 AM [MW305] Skeletal editing of diene rubbers for controlled depolymerization. **Presented by: Keith Huang**

8:00 AM [MW306] Selective nitrogen insertion functionalization of styrenic polymers. **Presented by: Kezia Jacob**

8:00 AM [MW307] Sequential post-polymerization modification via amide activation and click chemistry. **Presented by: Dinesha Madhuwanthi Kande Vidanalage**

8:00 AM [MW308] Investigation of structure and performance in alginate–hemp composite films for sustainable packaging. **Presented by: Aditya Goyal**

8:00 AM [MW309] Ctrl-X, Ctrl-V, Ctrl-PET: Rapid, selective, and mild depolymerization of poly(ethylene terephthalate). **Presented by: Benjamin Heiderscheit**

8:00 AM [MW310] rPET at large: Smuggling sustainable Trojan units at scale. **Presented by: Will Teggatz**

8:00 AM [MW311] Polymer infiltration in UiO MOFs monitored by NMR: Exploring the role of polymer chain length. **Presented by: Colton Rhoads**

8:00 AM [MW312] Synthesis of PLB-g-PMMA by grafting MMA from PLB. **Presented by: Parisa Jahangiri**

8:00 AM [MW313] Formulation and fabrication of a fluorinated polymer based material loaded with 6Li for neutron shielding applications. **Presented by: Abegel Freedman**

8:00 AM [MW314] Injectable microgels for wound healing applications. **Presented by: Brenden Draney**

8:00 AM [MW315] Design and synthesis of multifunctional bio-inspired polymers for metal chelation. **Presented by: Destinee Shaffer**

8:00 AM [MW316] No time to waste: Rapid, selective, and mild depolymerization of poly(ethylene terephthalate). **Presented by: Dhananjay Dileep**

Theory, Modeling and Simulation of Biomolecular Systems

Time: 8:00 AM - 12:00 PM
Session type: Oral
Location: Room 227, Second Floor
Organizer(s): Jeffrey Robert Comer, Paul Edward Smith
Presider(s): Jeffrey Robert Comer, Elizabeth A Ploetz
Sponsor(s): COMP, PHYS

The session is aimed at bringing together a group of varied researchers who have a common goal of understanding biological systems through the use of theory and simulation, an important aspect of many biophysical studies.

Presentations:

8:00 AM [MW317] Towards a consistent framework for efficient simulation of phase transitions of proteins, nucleic acids and metabolites. **Presented by: Jianhan Chen**

8:35 AM [MW318] Palm-reading for your phase diagram: Disentangling multi-phase effects in biomolecular condensates. **Presented by: Jeremy David Schmit**

9:10 AM [MW319] Osmotically induced shape changes in membrane vesicles. **Presented by: Buddhapriya Chakrabarti**

9:45 AM Intermission.

10:10 AM [MW320] Polarizable constant pH molecular dynamics of proteins in aqueous and crystalline environments. **Presented by: Michael J. Schnieders**

10:45 AM [MW321] Predicting oncogenic mutants of epidermal growth factor receptor in lung cancer by molecular dynamics simulation with machine learning. **Presented by: Chung Fun Wong**

11:20 AM [MW322] Selective degradation of the SARS-CoV-2 main protease (Mpro) through the application of proteolysis-targeting chimeras (PROTACs). **Presented by: Kavinayashri Chidambaranathan**

11:40 AM [MW323] Development and validation of a physiologically based pharmacokinetic (PBPK) model for dihydrocaffeic acid, a pharmacologically active antioxidant metabolite. **Presented by: Christopher L Basel**

Polymer Chemistry

Time: 10:20 AM - 12:00 PM
Session type: Poster
Location: Grand Ballroom, Second Floor
Organizer(s): Patricia R Calvo

General poster session featuring polymer chemistry research

Presentations:

10:20 AM [MW324] Evaluating the efficacy of aggregation propensity as a predictor of oligopeptide dimerization in redox-active conditions. **Presented by: Pranav Kolli**

10:20 AM [MW325] Understanding polymer-metal interactions through amino acid-functionalized polymers. **Presented by: Graham Moran**

10:20 AM [MW326] Investigating the effect of polymer composition on metal chelation thermodynamics. **Presented by: Justin Garrit Pickering**

10:20 AM [MW327] Comparative assessment of the environmental degradation of polylactic acid (PLA) and starch-based bioplastics under simulated environmental conditions using mass loss and ATR-FTIR analysis. **Presented by: Florence Fifteen, Hunter Anderson**

10:20 AM [MW328] Rapid photoiniferter strategy for the synthesis of hyperbranched polymers. **Presented by: Ayesha Imiya Mudiyanselage**

10:20 AM [MW329] N-acetylcysteine-modified chitosan/tannin-based coatings for titanium surface engineering. **Presented by: Alessandro Francisco Martins**

10:20 AM [MW330] Characterizing microplastic pollution in Midwestern farmlands through farmer engagement. **Presented by: Md Jamiun Noor Shadman**

10:20 AM [MW331] Designing antimicrobial polymers to combat antibiotic-resistant bacteria. **Presented by: Marie Kerschen**

10:20 AM [MW332] Ground state destabilization as a means to access transformable poly(acrylamides). **Presented by: Alexis Redwine**

10:20 AM [MW333] Investigation of adsorption of naphthalene and pyrene by pentafluorostyrene-based homopolymer, copolymers, and nanoparticles. **Presented by: Bibaran Gautam**

10:20 AM [MW428] Integrated filtration and analytical evaluation of multi-mixed matrix membranes for water purification. **Presented by: May Moe Thu Han**

Theoretical and Computational Chemistry

Time: 10:20 AM - 12:00 PM
Session type: Poster
Location: Grand Ballroom, Second Floor
Organizer(s): Christine M Aikens

General poster session featuring theoretical and computational chemistry research

Presentations:

10:20 AM [MW335] Development of a free, open-source Python kinetic simulation package for modeling, fitting, and mechanism discovery. **Presented by: Taylor Paez**

10:20 AM [MW336] Data-efficient energy correction for quantum-informed molecular dynamics using Gaussian process delta learning. **Presented by: Vibhav Chinta**

10:20 AM [MW337] Comparing machine-learned interatomic potentials for diamond stability in liquid metals. **Presented by: Amin Ahmadisharaf**

10:20 AM [MW338] Geometrical and electronic structure, stability, and optical absorption spectra comparisons between thiolate- and hydroxide-stabilized gold nanoclusters. **Presented by: Dushmanthi Anuradha Wasalamudali Wasala Mudiyanselage**

10:20 AM [MW339] Simplified TDDFT in CP2K: Efficient optical spectra of thiolate-protected gold nanoclusters. **Presented by: Paul Javed**

10:20 AM [MW340] Optical rotation calculations on 1D periodic systems at coupled cluster with single and double excitations level. **Presented by: Julia Abdoullaeva**

10:20 AM [MW341] Spin-phonon driven decoherence of molecular qubits in an open quantum system. **Presented by: Ilana Berlin**

10:20 AM [MW342] Computational study of how molecular structure governs energy absorption, storage, and release in organic chromophores for quantum battery applications. **Presented by: Muhammad Khan**

10:20 AM [MW443] Exploring photophysical effects of linker modifications of MOF-76 via computational and experimental methods. **Presented by: Blen Lemma**

Analytical Chemistry

Time: 1:30 PM - 3:10 PM
Session type: Poster
Location: Grand Ballroom, Second Floor
Organizer(s): Daniel A Higgins, Wenting Hu

General poster session featuring analytical chemistry research

Presentations:

1:30 PM [MW343] Development of a reactive Py-GC/MS methodology for the mass quantification of microplastics in water samples. **Presented by: Tashfiqul Islam**

1:30 PM [MW344] Development and validation of an UHPLC/MS/MS method for quantitative measurements of per- and polyfluoroalkyl substances using a linear ion trap. **Presented by: Gavin White**

1:30 PM [MW345] Plasma lipidomics reveals melanoma and treatment-dependent remodeling in a mouse model. **Presented by: Aminul Islam**

1:30 PM [MW346] Quantifying DNA loading density on biolayer interferometry probes using quantitative PCR. **Presented by: Maya Lozano**

1:30 PM [MW347] Acetylcholine electrochemical assay derived from biohybrid cyclophane-based organic semiconductor frameworks for point-of-care testing to aid Alzheimer's disease diagnosis. **Presented by: Layla Sheta**

1:30 PM [MW348] Investigating bulk graphite crystal growth through silicon doping and isotope enrichment. **Presented by: Ishika Thakur**

1:30 PM [MW349] Peptide identification from exopeptidase-generated amino acids. **Presented by: Niki Ahmadian**

1:30 PM [MW350] Label-free detection and identification of epitranscriptomic modifications using XToF nanofluidic device. **Presented by: Minaza Yahiya**

1:30 PM [MW351] Multi-field spin-matrix workflow for measuring and interpreting carbohydrate 1H NMR spectra. **Presented by: Ceceilia Hedrick**

1:30 PM [MW352] Optimization of gold nanotriangle arrays for localized surface plasmon resonance-based biosensing. **Presented by: Gayanika Jayarathne**

1:30 PM [MW353] Self-assembly of gold-binding peptides on graphite. **Presented by: Hashitha Tharakee Degambadage**

1:30 PM [MW354] Improved in-channel microchip electrophoresis with electrochemical detection for catecholamine analysis. **Presented by: Hayden Bush**

1:30 PM [MW355] Cu(II) adsorption behavior of an organic nanotube having inner amine groups. **Presented by: Mikynzie Tatro**

1:30 PM [MW356] Fabrication of spatially aligned gold nanotriangle–silver nanodot arrays using optimized nanosphere lithography masks. **Presented by: Nimodi Uduwela**

1:30 PM [MW357] Hierarchical bimodal nanoporous gold-enhanced molecularly imprinted polymer sensor for point of care real-time monitoring of salivary cortisol. **Presented by: Naila Haroon**

1:30 PM [MW449] Electronic transitions of copper oxide in the 15,000 – 16,000 cm-1 Region. **Presented by: Leah Christine O'Brien**

Biochemistry and Chemical Biology

Time: 1:30 PM - 5:10 PM
Session type: Oral
Location: Room 207, Second Floor
Organizer(s): Ping Li
Presider(s): James W. Checco, Kainan Chen

General oral session featuring biochemistry and chemical biology research

Presentations:

1:30 PM [MW358] Evaluating the functional selectivity of endogenous D-amino acid-containing neuropeptides in Aplysia californica. **Presented by: Alisha Doda**

1:50 PM [MW359] Alpha-synuclein interaction with gedunin. **Presented by: TONY NYABAYO**

2:10 PM [MW360] DNA origami–chitosan hybrid nanocarrier enables sustained intracellular antioxidant delivery for protection against oxidative stress in early cataract. **Presented by: Chikadibia Edward**

2:30 PM [MW361] Slower motions and dramatic conformational populations present in A:G mismatched DNA phosphates. **Presented by: Theodora Osborne**

2:50 PM Intermission.

3:10 PM [MW362] Metabolism-guided design of integrated electro-biomanufacturing systems. **Presented by: Kainan Chen**

3:30 PM [MW363] *Withdrawn*

3:50 PM [MW364] Next-generation plasmonic nanoparticles: Transforming biosensors and targeted therapeutics. **Presented by: Moustafa R.K. Ali**

4:10 PM [MW365] Monomeric antigen-CD22l conjugates temporarily deplete cognate B cell subsets. **Presented by: Kyle Apley**

4:30 PM [MW366] Virtual screening for modulators of the J-domain of DNAJA1. **Presented by: David Johnson**

4:50 PM [MW367] S. cerevisiae and L. plantarum co-fermentation improves fig wine quality: Identification of key aroma compounds via molecular docking and dynamics simulation. **Presented by: Jiaqi Song**

Chemistry under Nanoconfinement

Time: 1:30 PM - 5:25 PM
Session type: Oral
Location: Flint Hills Room, Second Floor
Organizer(s): Saswata Dasgupta, Tendai Gadzikwa, Takashi Ito
Presider(s): Saswata Dasgupta, Tendai Gadzikwa, Takashi Ito
Sponsor(s): INOR, ANYL, PHYS

This symposium will highlight recent advances in understanding chemical phenomena in confined and porous environments. This symposium will bring together researchers working on the synthesis, experimental characterization, and computational modeling of porous and low-dimensional materials, including metal organic frameworks (MOFs), porous organic crystals, zeolites, nanotubes, and two-dimensional materials. Emphasis will be placed on how nanoconfinement alters structure, dynamics, transport, and reactivity at solid liquid and electrode electrolyte interfaces, with applications spanning electrocatalysis, electrochemical sensing, energy storage, separations, and confined fluids. By integrating experimental and theoretical research, ranging from advanced spectroscopy and electrochemical measurements to quantum chemistry and molecular simulations, this symposium aims to foster cross-disciplinary discussion and collaboration.

Presentations:

1:30 PM [MW368] Tuning ion association via surface interactions: When bulk-centric pictures may disappoint. **Presented by: Ryan Jorn**

2:00 PM [MW369] Ring opening mechanism of epichlorohydrin in Sn-Beta: A DFT and microkinetic modelling study. **Presented by: Ying-Ge Chen**

2:20 PM [MW370] Polarizable Drude force field for gas adsorption. **Presented by: Yiling Nan**

2:50 PM [MW371] Data-driven predictive synthesis of metal–organic frameworks. **Presented by: Zhiling Zheng**

3:20 PM Intermission.

3:40 PM [MW372] Electrochemistry-induced deposition for formation of mixed metal ZIF thin films. **Presented by: Elise Skinner**

4:00 PM [MW373] Impact of nanoconfined water upon irradiation of metal-organic nanotubes. **Presented by: Tori Forbes**

4:30 PM [MW374] *Withdrawn*

4:30 PM [MW375] Insights into metal-organic framework and polymer infiltration for membrane applications. **Presented by: Angela Devlin** [note: time change from original program]

5:00 PM Closing Remarks.

Materials Science

Time: 1:30 PM - 3:30 PM
Session type: Oral
Location: Room 206, Second Floor
Organizer(s): Christine M Aikens
Presider(s): Vijay Nathan Somasundaram

General oral session featuring materials chemistry research

Presentations:

1:30 PM [MW376] Improving fast-charging performance and durability of graphite anodes for lithium-ion battery. **Presented by: Emily Espino-Mendoza**

1:50 PM [MW377] Dual lithiophilic promotors for dendrite-less lithium metal batteries. **Presented by: Senthil Chenrayan**

2:10 PM [MW378] Electrochemical and computational analysis of organic cathodic corrosion inhibitors: The effect of polarizability on corrosion inhibition. **Presented by: Adam Willett**

2:30 PM [MW379] Engineering lithium storage in PAN- and PVP-derived carbon anodes through carbonization, nanofiber architecture, and C60 reinforcement. **Presented by: Arijit Roy, Emily Espino-Mendoza**

2:50 PM [MW380] Metal-doped semiconducting polymer nanoparticles for bioanalysis and cancer treatment. **Presented by: Xu Wu**

3:10 PM [MW381] Engineering plasmonic nanoparticles for quantitative surface-enhanced Raman spectroscopy. **Presented by: Sujan Subba**

Polymer Chemistry

Time: 1:30 PM - 4:50 PM
Session type: Oral
Location: Cottonwood Room, Second Floor
Organizer(s): Patricia R Calvo
Presider(s): Alec Lininger, Graham Moran
General oral session featuring polymer chemistry research

Presentations:

1:30 PM [MW382] Functionalized chitosan as a polymeric chelator for targeted radionuclide delivery. **Presented by: Dilanka N B D Dassanayake Mudiyanselage**

1:50 PM [MW383] Synthesis of a quaternized polyampholytic pectin derivative and Tanfloc-based multilayer coatings for antimicrobial biomedical interfaces. **Presented by: Alessandro Francisco Martins**

2:10 PM [MW384] Going bananins: A sugary solution to stiff engineering thermoplastics. **Presented by: Dhananjay Dileep**

2:30 PM [MW385] Engineering a reprocessable and self-healable boronic ester vitrimer derived from epoxidized soybean oil and eugenol. **Presented by: MD YEASIN ARAFAT**

2:50 PM [MW386] Pressure-tunable CO2-H2O media for enhanced hydrolytic depolymerization of polyethylene terephthalate waste. **Presented by: Apoorva Mahendra Ranjekar**

3:10 PM Intermission.

3:30 PM [MW387] Carboxamide-containing crosslinkers in soybean oil-based polyurethane adhesives. **Presented by: Rutu Patel**

3:50 PM [MW388] Antioxidant cannabinoids and polycannabinoids enable low temperature additive manufacturing of oxidation-free copper. **Presented by: Alex Chortos**

4:10 PM [MW389] Microfluidic mixing of the high viscosity urethane forming reaction of PTMEG and H12-MDI. **Presented by: John P Styers**

4:30 PM [MW390] Dynamics of microplastics occurrence in residential environments following Southern California wildfires: A multi-matrix assessment. **Presented by: Hrithik Nath**

Theoretical and Computational Chemistry

Time: 1:30 PM - 5:30 PM
Session type: Oral
Location: Room 227, Second Floor
Organizer(s): Christine M Aikens
Presider(s): Emilie Brigitte Guidez

General oral session featuring theoretical and computational chemistry research

Presentations:

1:30 PM [MW391] Multicomponent constrained nuclear-electronic orbital wavefunction methods: Development and applications of CNEO-MP2 and CNEO-CCSD. **Presented by: Gabrielle Brieanna Tucker**

1:50 PM [MW392] Phonon flux as a nonequilibrium mechanism for modulating biomolecular function. **Presented by: Ryan Alan Riskowski**

2:10 PM [MW393] Mechanistic study of propene metathesis on heterogenous catalyst. **Presented by: Shreyaa Brahmachari**

2:30 PM [MW394] Adsorption models of superheavy elements and their chemical homologs. **Presented by: Matthew Anmar Romaya**

2:50 PM [MW395] Predicting LaFeO3 solid-state synthesis pathways using cellular automaton simulations and first-principles thermodynamics. **Presented by: Nabanita Mondal**

3:10 PM [MW396] At-scale data-driven exploration of high-voltage cathode materials for sodium batteries. **Presented by: Suchona Akter**

3:30 PM Intermission.

3:50 PM [MW397] Finite-resolution identifiability of molecular conformers from vibrational spectroscopy. **Presented by: Megan Simons**

4:10 PM [MW398] Graph theory analysis of DNA adsorption mediated by alkaline earth metal ions. **Presented by: Makenzie Long**

4:30 PM [MW399] Probing phase transfer catalysis with oriented external electric fields at liquid-liquid interface. **Presented by: Emmanuel Forson**

4:50 PM [MW400] Ion pairing in confined aqueous electrolytes. **Presented by: Rajapaksha Thewage Dilshan Kavinda bandara Karunachandra**

5:10 PM [MW401] Anatomy of vapor-liquid interfacial structure formed by pentafluoroethane (HFC-125) using molecular dynamics simulations. **Presented by: Akshay Malik**

Theoretical and Computational Chemistry

Time: 1:30 PM - 3:10 PM
Session type: Poster
Location: Grand Ballroom, Second Floor
Organizer(s): Christine M Aikens

General poster session featuring theoretical and computational chemistry research

Presentations:

1:30 PM [MW402] Multiscale modeling of the NarK nitrate/nitrite antiporter using adaptive-partitioning algorithms based on hierarchical truncated many-body expansion (PAP-HMBE). **Presented by: Julia Roma**

1:30 PM [MW403] Structural responses of pea protein to low urea concentrations: Molecular dynamics study. **Presented by: Xuhuan Chen**

1:30 PM [MW404] Leucine-rich arrestin loop and receptor phosphosite spacing modulate membrane engagement in ACKR3–arrestin2/3 molecular dynamics simulations. **Presented by: Cece Hedrick**

1:30 PM [MW405] In silico modeling of bispecific dual-affinity re-targeting (DART) molecules targeting PD-1 and LAG-3 for solid tumor and hematologic cancers immunotherapy. **Presented by: Gopikaashri Chidambaranathan**

1:30 PM [MW406] Structure-guided computational modeling of molecular tweezers targeting histone proteins in pediatric high-grade glioma. **Presented by: Pahul Kaur**

1:30 PM [MW407] Identification of potential PDGFRA-targeting therapeutics for glioblastoma using diffusion and structure-based drug discovery. **Presented by: Dhruv Mogenahalli**

1:30 PM [MW408] Assessing the impact of AlphaFold3-derived structures on molecular docking accuracy. **Presented by: Hadiza Elhadji Oumarou Harouna**

1:30 PM [MW409] AI-guided optimization and structure-based virtual screening identify novel dual-state KRAS G12D candidate binders. **Presented by: Rakin Khan**

1:30 PM [MW410] Analysis of a novel decoupled relaxation method for estimating condensed-phase water dipoles. **Presented by: Joel Adkins**

1:30 PM [MW411] Crystallization kinetics and structural signatures of phase transition in supercooled water. **Presented by: Christopher Zhou**

1:30 PM [MW412] Using activation energies to elucidate the effects of osmolytes on water dynamics. **Presented by: Abigail Kerr**

1:30 PM [MW413] Balancing divalent ions–functional group interactions for condensed phase simulation in the polarizable Drude force field. **Presented by: Bishal Lamichhane**

1:30 PM [MW414] Molecular dynamics modeling of concentrated aqueous solutions at salt surfaces: The role of explicit polarizability. **Presented by: Khusbu Rai**

1:30 PM [MW415] Enhanced sampling approaches to Li-ion transport across the solid electrolyte interphase. **Presented by: Hiruni Wimalasiri**

1:30 PM [MW416] Computational study of CO2 solubility in the ionic liquid [bmim][PF6] using Monte Carlo simulations. **Presented by: Rund Al-Kofahi**

Advances in Catalysis and Methods for Organic Synthesis

Time: 2:00 PM - 5:10 PM
Session type: Oral
Location: Big 12 Room, Second Floor
Organizer(s): Socrates B. Munoz, Jon A Tunge
Presider(s): Jon A Tunge
Sponsor(s): ORGN, FLUO, Cambrex, Advion

This symposium honors recent Cope Scholar, Prof. Thomas Lectka

Presentations:

2:00 PM [MW417] From molecular innovation to manufacturing impact: Catalysis for sustainable chemical production. **Presented by: Sachin Handa**

2:35 PM [MW418] Boron triiodide: A new reducing agent. **Presented by: Florence J Williams**

3:10 PM [MW419] Advances in catalytic acylations and fragmentative generation of [ArCF2-] synthons from accessible precursors. **Presented by: Socrates B. Munoz**

3:45 PM Intermission.

4:00 PM [MW420] Metal ion-induced large fragment deactivation: A new strategy for site-selective fluorination in complex molecules. **Presented by: Thomas Lectka**

5:00 PM Closing Remarks.

Analytical Chemistry

Time: 3:50 PM - 5:30 PM
Session type: Poster
Location: Grand Ballroom, Second Floor
Organizer(s): Daniel A Higgins, Wenting Hu
General poster session featuring analytical chemistry research

Presentations:

3:50 PM [MW421] Surrogate reference standards for RP-HPLC quantification of paracetamol: Influence of structural variability on assay values. **Presented by: Japhat Opoku Ofosu**

3:50 PM [MW422] Analyzing the role of microplastic size, surface area and chemical composition on PFAS sorption in sanitary water samples: A case study of the Galesburg area. **Presented by: Lumala Nelum Naullage**

3:50 PM [MW423] Correlation of high molecular weight-glutenin subunit allele Glu-B1-al with seed, milling, dough, and baking characteristics in hard winter wheat. **Presented by: Bruna Mattioni**

3:50 PM [MW424] University of Kansas nanofabrication facility: Equipment and capabilities. **Presented by: Haider Warraich**

3:50 PM [MW425] Gas-phase ion-molecule reactions of protonated oxime compounds with 2-methoxypropene in a linear quadrupole ion trap mass spectrometer. **Presented by: Bright Harrison Adu**

3:50 PM [MW426] *Withdrawn*

3:50 PM [MW427] *Withdrawn*

3:50 PM [MW429] Optimization of acrylamide roadblocks for the recovery of high-molecular-weight DNA. **Presented by: Logan Funk, Francisco Cantillo, Kristy Kounovsky-Shafer**

3:50 PM [MW430] Protecting long DNA molecules with an agarose-based inverted insert. **Presented by: Mason Taylor, Kristy Kounovsky-Shafer**

3:50 PM [MW431] Optimization of insert geometry for enhanced recovery of high-molecular-weight DNA. **Presented by: Samantha Bursaw, Megan Miller, Avery Lowther, Kristy Kounovsky-Shafer**

3:50 PM [MW432] Recovery of high-molecular-weight DNA using a 3D-printed concentration device. **Presented by: Samantha Bursaw, Kristy Kounovsky-Shafer**

3:50 PM [MW433] Investigation of pH and metal coordination effects on natural phenolic compounds using UV-visible spectroscopy. **Presented by: Griffin Whitehill, Carl Malvo**

3:50 PM [MW434] Fourier transform infrared spectrometric quantification of volatile organic compounds emitted by common commercial 3D printers. **Presented by: Daphne Hedrick**

3:50 PM [MW435] Quantitative assessment of the burden of per- and polyfluoroalkyl substances (PFAS) in South Dakota water systems via EPA Method 1633. **Presented by: Nashrifa Israt Khanom**

3:50 PM [MW436] High-resolution lipidomic profiling identifies distinct metabolic dysregulation following traumatic brain injury in a mouse model. **Presented by: Sanjida Afroz Mitu**

3:50 PM [MW437] *Withdrawn*

3:50 PM [MW438] Method-dependent variability in μ-FTIR microplastic analysis: Effects of scan area, spectral resolution, and library composition. **Presented by: Atif Bashir**

Physical Chemistry

Time: 3:50 PM - 5:30 PM
Session type: Poster
Location: Grand Ballroom, Second Floor
Organizer(s): Christine M Aikens
General poster session featuring physical chemistry research

Presentations:

3:50 PM [MW439] *Withdrawn*

3:50 PM [MW440] Autonomous movement of Belousov-Zhabotinsky droplets enclosed by diverse surfactants. **Presented by: Izabela Carlson**

3:50 PM [MW441] *Withdrawn*

3:50 PM [MW442] *Withdrawn*

3:50 PM [MW444] Spectroscopic investigation of the role of acid-base sites toward C-C bond formation on TiO2-based nanomaterials. **Presented by: Dilip K Paul**

3:50 PM [MW445] Comparative photochemical oxidation behavior for different aldehydes over mixed oxide nanoparticles. **Presented by: Dilip K Paul**

3:50 PM [MW446] Uniformity from disorder in electrochemical reaction networks. **Presented by: Olivia Underwood**

3:50 PM [MW447] Ultrafast study of a pH-sensitive azobenzene photoswitch in basic conditions. **Presented by: Jaden Riddle**

3:50 PM [MW448] Characterizing piezoelectric motion for the construction of a micro Fabry-Pérot cavity. **Presented by: Trevor Ottman**