

Thought Leadership

Exhibitor Workshop:

Karl Mueller | Accelerating Scientific Discovery with HPC and AI Presented by Microsoft Corporation | 1:30 pm, Monday

The Kavli Lecture Series:

The Kavli Foundation Emerging Leader in Chemistry

Keynote Presentation:

Deepika Malhotra | Many flavors of carbon capture technologies | 5:00 pm, Monday

Colloid & Surface Chemistry

Symposium:

Jaehun Chun | Colloidal Forces: Connecting Molecular to Macroscopic Scales | 8:00 am and 2:00 pm, Sunday

Presentation:

Chunlong Chen | 3993108 | Bioinspired synthesis and assembly of nanoparticles through peptoid-based approaches | 11:30 am, Wednesday

Energy and Fuels

Symposium:

Bojana Ginovska | Fundamentals to Applications - Advances in Material-based Hydrogen Storage for Energy and Industry: Metal Hydrides for Hydrogen Storage | 8:00 am and 2:00 pm, Sunday

Dongping Lu | Solid State Batteries: Materials, Interfaces, and Cell Integration | 2:00 pm, Sunday

Bojana Ginovska | Fundamentals to Applications - Advances in Material-based Hydrogen Storage for Energy and Industry: New Materials for Hydrogen Adsorption Storage | 8:00 am, Monday

Bojana Ginovska | Fundamentals to Applications - Advances in Material-based Hydrogen Storage for Energy and Industry | 12:00 pm, Monday

Bojana Ginovska | Fundamentals to Applications - Advances in Material-based Hydrogen Storage for Energy and Industry: Insights into Materials for Hydrogen Economy | 2:00 pm, Monday

David Heldebrant, Keerti Kappagantula | Towards carbon-dioxide negative building composites | 2:00 pm, Monday

Presentations:

Abhi J. Karkamkar | 4002241 | Hydrogen infrastructure and storage - U.S. DOE hydrogen and fuel cell technologies Office Perspectives | 8:05 am, Sunday

Karthi Ramasamy, Mond Guo | 4002010 | Power-to-X: Sustainable aviation fuels via methanol intermediate | 9:25 am, Sunday

Uriah Kilgore, Tom Autry, Mark Bowden, Mi Yeon Byun | 3989417 | LOHC processes: First steps from laboratory to the real world | 3:50 pm, Sunday

Yuyan Shao | 3990291 | Tuning proton transfer and proton-couple electron transfer at heterogenous electrochemical interfaces for hydrogen reactions | 5:30 pm, Sunday

Bojana Ginovska, Peter Stephen Rice, Tom Autrey | 3995554 | Modulate properties of hydrogen storage materials using heteroatom doping configuration and lattice topology | 10:40 am, Monday

Chao Zeng, Soowhan Kim, Yucheng Fu, Yunxiang Chen, Jie Bao, Zhijie (Jay) Xu | 3994293 | Quantification of kinetics parameters for multiscale modeling in aqueous redox flow batteries | 2:45 pm, Tuesday

Johannes Lercher | 4001143 | Electrically heated reactor for steam methane reforming | 5:30 pm, Wednesday

Poster:

Mi Yeon Byun, Thuy Le, Mark Bowden, Tom Autrey | 3990793 | Role of palladium oxide as active site in Pd/C catalysts for formate dehydrogenation | 12:00 pm, Monday

Catalysis Science & Technology

Presentations:

Johannes Lercher | 4003397 | Reductive conversion of benzaldehyde on Pd/C in aqueous environments | 10:20 am, Sunday

Sten Lambeets, Mark Wirth, Daniel Perea, Shawn Kathmann | 3996865 | Influences of intense electric field on N₂ activation over Ru single nanoparticle revealed by Operando Atom Probe | 11:20 am, Sunday

Zdenek Dohnalek | 3992450 | Elementary steps in catalytic conversion of acetic acid on anatase TiO₂(101) single crystals and faceted nanoparticles | 3:15 pm, Monday

R. Morris Bullock, Ba Tran | 3997033 | Mechanistic and reactivity studies of copper-hydride monomer, dimer, and clusters | 4:20 pm, Monday

Mal-Soon Lee | 3995998 | Understanding the role dynamics entropy and confinement on the reaction energetics in nanopores | 4:30 pm, Monday

Mal-Soon Lee | 4000812 | Enhanced electrocatalytic hydrogenation of biomass-derived Organics at solid/liquid interface | 9:00 am, Tuesday

Fan Lin, Huamin Wang | 3989397 | High-temperature steam induced restructuring of the Lewis acid site on γ /Beta zeolite | 9:50 am, Tuesday

Jennifer Jocz, Vanessa Dagle | 3995325 | Liquid-phase catalytic conversion of 2,3-butanediol to jet fuel | 11:40 am, Tuesday

Xingyu (Xander) Wang, Xin Zhang | 3985279 | Observation of flat band in mesoscale ordered 2D hydrogen-bond organic framework | 10:05 pm, Thursday

Sten Lambeets, Daniel Perea | 3990444 | Real-time nanoscale observation by Operando Atom Probe of the Fe oxidation under the influence of intense electric fields | 10:03 am, Thursday

Inorganic Chemistry

Presentations:

Wilma Rishko, Jaehun Chun, Samantha I. Johnson | 3997090 | Correlating viscosity, molecular structure, and aggregation of DHP molecules for aqueous flow batteries using molecular dynamics simulations | 10:40 am, Sunday

Evan Patrick, Jeremy Erickson, R. Morris Bullock, Ba Tran | 3991386 | Synthesis of a bulky bidentate bis(NHC) ligand to support trigonal planar Cu(I) complexes | 8:00 am, Tuesday

Analytical Chemistry

Symposium:

Robert G. Ewing, Yehia Ibrahim, Thomas Metz, Simone Raugei, Bobbie-Jo Webb-Robertson | Progress in Mass Spectrometry: Unambiguous Identification for Small Molecules | 2:00 pm, Sunday and 2:00 pm, Monday

Presentations:

Christopher Anderton | 3990248 | Peak ambiguities and in-source fragmentation: Can we use all the peaks in mass spectrometry imaging approaches to increase biological meaning? | 3:55 pm, Sunday

Christopher Harrilal, Sean Colby, Peter Stephen Rice, Jessica Bade, Simone Raugei, Yehia Ibrahim | 4001624 | Towards leveraging gas-phase infrared spectra of cryocooled ions for the unambiguous identification of small molecules | 4:55 pm, Sunday

Katherine Schultz, Julia Nguyen, Chathuri Kombala, Kimberly Tyrrell, Vivian Lin, Adam Hollerbach, Jamie Rodriguez, Jonathan Foreman | 3987120 | Hydra: An in silico predictive tool for opioid crisis intervention | 9:10 am, Monday

Danielle Ciesielski | 3986469 | Targeted prediction of MS/MS spectra | 9:55 am, Monday

Adam Hollerbach, Yehia Ibrahim, Vivian Lin, Katherine Schultz, Thomas Metz, Robert Ewing | 3994407 | Reference-free identification of emerging fentanyl analogs using structures for lossless ion manipulations (SLIM) ion mobility Orbitrap mass spectrometry | 10:25, Monday

Samantha I. Johnson, Wilma Rishko, Sandilya Garimella, Adam Hollerbach, Marcel Baer, Simone Raugei | 3996781 | Multiscale computational modeling of evaporation and reactivity in acetonitrile-water-amino acid droplets for electrospray ionization | 4:25 pm, Monday

Sean Colby | 3995709 | Molecular vision: Multimodal, multitask retrieval of molecular structure from measured signatures for reference-free compound identification | 4:55 pm, Monday

Computers in Chemistry

Presentations:

Marcel Baer | 3995414 | Development and application of a systematic and extensible force field for peptoids (STEPS) | 3:55 pm, Sunday

Henry Sprueill, Mariefel Olarte, Udishnu Sanyal, Sutanay Choudhury | 3990839 | Integrating generative AI with computational chemistry for catalyst design in biofuel/bioprocess applications | 10:40, Monday

Marcel Baer | 3995466 | Structure prediction for sequence-defined polymers for electron transfer | 9:30 am, Thursday

Poster:

Henry Sprueill, Mariefel Olarte, Udishnu Sanyal, Khushbu Agarwal, Sutanay Choudhury | 3997655 | Extreme-scale heterogeneous inference with large language models and atomistic graph neural networks for catalyst discovery | 7:00 pm, Tuesday

Physical Chemistry

Presentations:

Sotiris Xantheas | 3995539 | Accurate modeling of many-body energies in water clusters and applications to liquid water and ice | 9:50 am, Monday

John Loring, Mark Bowden, Odeta Qafoku, Christopher Thompson, Sebastien Kerisit, Sebastian T. Mergelsberg | 3995113 | Surface passivation during carbonation under low water supercritical carbon dioxide | 8:05 am, Wednesday

Poster:

Joani Mato, Sotiris Xantheas | 3992298 | The back door to the hydrated electron | 7:00 pm, Tuesday

Polymeric Materials Science & Engineering

Presentations:

Shuai Zhang, Chunlong Chen, Jim De Yoreo | 3979798 | Hierarchical assembly of peptoids on van der Waals materials | 10:10 am, Monday

Chunlong Chen | 3993099 | Enzyme-mimetic catalysts based on assembly of sequence-defined polymers into crystalline nanomaterials | 9:32 am, Tuesday

Geochemistry

Symposium:

Sebastian T. Mergelsberg, Micah Prange | Intermediate and Disordered Phases in Natural Systems | 8:00 am and 2:00 pm, Tuesday

Presentations:

Daniel Perea, Sandra Taylor | 3996750 | Nanoscale insights into mineral-water interfaces using atom probe tomography | 9:25 am, Tuesday

Sebastian T. Mergelsberg, Sebastien Kerisit, Micah Prange, Nabajit Lahiri, Quin Miller | 3996158 | MN coordination in amorphous Ca/Mn carbonate solid solutions | 9:30 am, Tuesday

Micah Prange, Sebastian T. Mergelsberg, Sebastien Kerisit | 3988006 | Probing the composition dependence of local structure in amorphous carbonates with DFT-based molecular dynamics | 2:30 pm, Tuesday

Sebastien Kerisit, Micah Prange, Sebastian T. Mergelsberg | 3994799 | Atomic-scale mechanisms of metal incorporation in amorphous calcium carbonate | 2:50 pm, Tuesday

Maria Sushko, Duo Song, Lili Liu | 3996307 | Solvation directed morphological control in metal oxide nanostructures | 4:55 pm, Tuesday

Sebastien Kerisit, John Loring, Michel Sassi, Xinyi Shen, Christopher Thompson, Bavan Rajan | 3990122 | Fate of Ni and Co during carbonation of olivine | 8:30 am, Wednesday

John Loring, Bavan Rajan, Sebastian T. Mergelsberg, Christopher Thompson, Mark Wirth, Daniel Perea, Sebastien Kerisit | 3995193 | Carbonation of Ni- and Co-doped forsterite in humidified supercritical carbon dioxide | 10:40 am, Wednesday

Xinyi Shen, Sebastien Kerisit | 3990256 | Molecular simulation of carbonate nucleation during carbonation of Ni- and Co-bearing olivine | 10:00 am, Wednesday

Alexandra Nagurney, Nabajit Lahiri, Quin Miller, Herbert Schaef | 3994644 | CO₂ enhanced mineral recovery from ultramafic rocks for the mining of nickel | 11:00 am, Wednesday

Herbert Schaef, Quin Miller, Alexandra Nagurney, Emily Nienhuis, Nabajit Lahiri, Ross Cao | 3993608 | Bridging the gap between fundamental understanding of CO₂-related geochemical processes and practical applications | 2:05 pm, Wednesday

Environmental Chemistry

Presentation:

Winnie Liu, Zheming Wang, Mark Bowden, Odeta Gafoku, Kevin Rosso | 4002203 | Vivianite oxidation is not photocatalyzed | 8:50 am, Wednesday

Biological Chemistry

Presentation:

Sebastian T. Mergelsberg, Bojana Ginovska | 3996623 | REMD-informed SAXS tracks amelogenin structure in solution | 11:10 am, Thursday