Pacific Northwest NATIONAL LABORATORY

ACS Chemistry for Life®
American Chemical Society

PNNL@ ACS FALL 2024
ELEVATING CHEMISTRY
AUGUST 18–22 | DENVER, CO & HYBRID

ELEVATING CHEMISTRY | AGENDA

PNNL AT ACS FALL 2024

PRESIDENTIAL EVENT

PRESENTATION

Deepika Malhotra, Mariefel Olarte, Honghong Shi | 4113910 | Achievements in Elevating the Chemistry Enterprise: Advancement of Energy Transition & Smart Materials: Panel Discussion | **10:25 am, Tuesday**

GEOCHEMISTY

SYMPOSIA

Alexandra Nagurney, Emily Nienhuis-Marcial | The Role of Mineral-Water Interfaces in Carbon Mineralization & Critical Mineral Recovery | **2:00 pm, Tuesday**

Xin Zhang, Mineral Crystallization, Aggregation & Dissolution | **8:00 am, Wednesday and 8:00 am Thursday**

PRESENTATIONS

Mavis Boamah, John Loring, Zheming Wang, Kevin Rosso | 4095913 | Surface hydroxylation of magnesium oxide and forsterite | **9:25 am, Sunday**

Xiaoxu Li, Xin Zhang, Kevin Rosso | 4109302 | Orientated sliding during self-assembly of gibbsite nanoplates | **10:40 am, Sunday**

Michel Sassi, Winnie Liu, Kevin Rosso | 4085236 | Exploration of vivianite oxidation mechanisms from first principles | **4:00 pm, Sunday**

Madeline Bartels, Quin Miller, Nabajit Lahiri, Alexandra Nagurney, Emily Nienhuis-Marcial, Heath Stanfield, Herbert Schaef | 4110866 | Tracing carbonate mineralization in mafic-ultramafic rocks with thermogravimetric analysis-mass spectrometry | **2:25 pm, Tuesday**

Heath Stanfield, Madeline Bartels, Madeline Murchland, Nabajit Lahiri, Emily Nienhuis-Marcial, Alexandra Nagurney, Quin Miller, Herbert Schaef | 4082864 | Carbon mineralization, critical mineral, and olivine resource evaluation pathways for mafic-ultramafic assets | **3:05 pm, Tuesday**

Xin Zhang | 4109555 | Understanding particle aggregation-based crystallization pathways by using advanced transmission electron microscopy and X-ray scattering techniques | **3:30 pm, Tuesday**

Maria Sushko | 4107037 | Interfacial drivers for the formation of hierarchical architectures | **10:15 am, Wednesday**

Carolyn Pearce, Emily Nienhuis-Marcial, Trent Graham, Maxime Pouvreau, Mark Bowden, Lili Liu, Xin Zhang, Aurora Clark, Gregory Schenter, James De Yoreo, Kevin Rosso | 4108902 | Metastable intermediates facilitate aluminum transformations in concentrated alkaline electrolytes representative of radioactive waste | **11:30 am, Wednesday**

Zheming Wang, Xin Zhang, Xiaodong Zhao, Ping Chen, Trent Graham, Sebastian Mergelsburg, Zihua Zhu, Carolyn Pearce, Kevin Rosso | 4107033 | Rare-earth adsorption, incorporation and precipitation under basic solution conditions | **3:05 pm, Wednesday**

Xin Zhang, Zheming Wang, Carolyn Pearce, Kevin Rosso | 4078667 | Effect of trace metal or organic matter adsorption on aluminum mineral dissolution in caustic solutions | **3:40 pm, Wednesday**

Jim De Yoreo, Mingyi Zhang, Benjamin Legg, Elias Nakouzi, Lili Liu, Jaehun Chun, Gregory Schenter | 4105873 | In situ look at interfacially-driven mineralization | **8:30 am, Wednesday**

Duo Song, Lili Liu, Maria Sushko | 4109144 | Theoretical study on the role of interfacial dipolar interactions in directing growth pathways and dimensionality of the crystal | **9:20 am, Wednesday**

PHYSICAL CHEMISTRY

SYMPOSIUM

Karol Kowalski, Bo Peng | Addressing the Complexity of Correlated Quantum Many-Body Problems by Embedding & Downfolding | **8:00 am, Monday, Tuesday, Wednesday, and 2:00 pm, Wednesday**

PRESENTATIONS

Jingshan Du | 4094381 | Discovering plasmonic hetero-nanoparticles through combinatorial synthesis | **8:40 am, Sunday**

Bo Peng | 4097662 | Quantum embedding in excitation manifold | **9:35 am, Monday**

Karol Kowalski, Nicolas Bauman | 4107224 | Coupled cluster downfolding formalisms for simulating many-body systems | **10:25 am, Monday**

Jingshan Du, Jim De Yoreo | 4086609 | Molecular-resolution elucidation of ice defects formed by liquid water crystallization | **5:00 pm, Wednesday**

CATALYSIS SCIENCE & TECHNOLOGY

SYMPOSIUM

Vanessa Dagle, Huamin Wang | Catalysis for Renewable Fuels & Products: Scalable Processes for Biomass & Waste Carbon Valorization | **8:00 am and 2:00 pm, Sunday**

PRESENTATIONS

Mal-Soon Lee, Benjamin Jackson, Julia Moreira, Huamin Wang, Donald Camaioni, Johannes Lercher | 4104412 | Effect of pH and surface charge on electrocatalytic hydrogenation of benzaldehyde at solid/liquid interface | **8:50 am, Sunday**

Benjamin Jackson, Mal Soon Lee, Sungmin Kim, Donald Camaioni, Oliver Gutierrez, Johannes Lercher | 4104426 | Mechanistic studies on the role of solvent identity on alcohol dehydration in zeolite pores | **11:37 am, Sunday**

Benjamin Jackson, Mal Soon Lee, Liney Arnadottir, Simone Raugei, Zdenek Dohnalek | 4108623 | Structure and properties of single-atom catalyst Rh-Fe_{3O4}: The role of surface modification in Rh activation | **2:40 pm, Sunday**

Benjamin Moskowitz, Carrington Moore, Mark Engelhard, Libor Kovarik, Mal Soon Lee, Simone Raugei, Huamin Wang, Yong Wang | 4105131 | Geometry and stability of methanol adsorbates on anatase titania nanoshapes | **3:00 pm, Sunday**

Julia Moreira, Laura Meyer, Thuy Le, John Fulton, Sungmin Kim, Huamin Wang, Donald Camaioni, Udishnu Sanyal, Johannes Lercher | 4099732 | Metal electric potential influences non-faradaic hydrogenation in aqueous phase | **8:40 am, Monday**

Juan Lopez-Ruiz, Lyndi Strange, Bhanupriya Boruah, Shuyun Li, Nickolas Riedel | 4110427 | Sustainable wastewater electrolysis for H_2 and clean water generation | **2:50 pm, Monday**

Thuy Le, Julia Moreira, Donald Camaioni, Oliver Gutierrez, Abhijeet Karkamkar, Johannes Lercher | 4109714 | Effect of solvent on hydrogen-binding strength in the catalytic hydrogenation of benzaldehyde on rhodium | **4:20 pm, Monday**

Johannes Lercher | 4112995 | Hydrogenation addition reactions in aqueous environments | **5:20 pm, Monday**

Sungmin Kim, Oliver Gutierrez, Johannes Lercher | 4108462 | Solvent-aided upcycling of polyolefins into liquid alkanes on Ru/C-catalyzed hydrogenolysis | **10:20 am, Wednesday**

Mal-Soon Lee, Benjamin Jackson, Wei Zhang, Donald Camaioni, Sungmin Kim, Johannes Lercher | 4104421 | Reaction mechanisms of acid-catalyzed cracking and alkylation in the upcycling of polyethylene: AIMD study | **3:20 pm, Wednesday**

POSTER

Martin Affandy, Vanessa Dagle, Robert Dagle, Yong Wang | 4105015 | Single-step conversion of Ethanol into n-butene-rich olefins over promoted Cu supported on SiO_2 catalysts | **7:00 pm, Tuesday**

COLLOID & SURFACE CHEMISTRY

SYMPOSIUM

Dongsheng Li | Advanced In-Situ Imaging Methods for Colloidal Chemistry: Probing Interaction & Dynamics at the Nanoscale | **7:00 pm Sunday, 2:00 pm Tuesday, and 8:00 am Thursday**

PRESENTATIONS

Dongsheng Li | 4103134 | Understanding and controlling crystal growth and assembly via in situ techniques | **2:00 pm, Tuesday**

Jim De Yoreo, Chenyang Shi, Shuai Zhang | 4105920 | Self-assembly at the protein-materials interface | **9:00 am, Thursday**

COMPUTERS IN CHEMISTRY

PRESENTATIONS

Gihan Panapitiya, Peiyuan Gao, Emily Saldanha | 4109806 | FragNet: A graph neural network with four levels of interpretability for molecular property prediction | **11:00 am, Sunday**

Marcel Baer, Bradley Harris | 4107588 | Development and application of a systematic and extensible force field for peptoids in solution (STEPs-SOL) | **5:00 pm, Monday**

Michael LaCount, Scott Muller, Mohammadhasan Dinpajooh, Andrew Ritzmann | 4109398 | Evaluating machine learned potential for nitric acid solutions | **5:40 pm, Monday**

Michel Sassi, David Senor, Andrew Casella | 4085238 | Ab initio simulations of tritium diffusion in intermetallic Al12(TM)2.34 aluminide coating phases | **8:15 am, Thursday**

Hoshin Kim, Simone Raugei | 4105132 | Molecular insight into the active site chemistry of monoterpene synthase enzymes | **9:50 am, Thursday**

Gihan Panapitiya, Carter Knutson, Andrew McNaughton, Neeraj Kumar | 4109846 | Advancements in comparing deep learning models for cancer research | **10:40 am, Thursday**

Marcel Baer, Bradley Harris | 4107596 | Equilibrium and non-equilibrium simulations of water, solute, and ion transport in de novo designed membrane protein channels | **10:45 am, Thursday**

ENVIRONMENTAL CHEMISTRY

PRESENTATIONS

Allison Myers-Pigg, Morgan Barnes, Alan Roebuck, Joshua Torgeson, Emily Graham | 4102470 | Chemical composition drives carbon, nitrogen, and phosphorus mobilization across burn severities | **8:05 am, Monday**

Alan Roebuck, Allison Myers-Pigg | 4102595 | Spatio-temporal impacts of wildfire on organic matter chemistry through a stream network is related to watershed properties and burn severity | **4:45 pm, Monday**

Manish Shrivastava, Alla Zelenyuk | 4098415 | Modeling multiphase chemistry of biomass burning phenols and their potential to form secondary organic aerosols | **11:35 am, Thursday**

ENERGY AND FUELS

SYMPOSIUM

David Heldebrant, Deepika Malhotra | Advances in CO_2 Capture & Conversion: Mineralization, Direct Ocean Capture & Modeling | **7:00 pm, Tuesday, and 8:00 am and 2:00 pm, Wednesday**

PRESENTATIONS

Un-Hyuck Kim, Yaobin Xu, Jing Wu, Dahee Jin, Hongliang Xu, Mingi Jeong, Dongping Lu | 4113151 | Enhancing all-solid-state lithium batteries performance via external pressure optimization | **10:00 am, Sunday**

Huamin Wang | 4108472 | Co-processing wet waste hydrothermal liquefaction crudes with petroleum streams in refinery hydroprocessing | **3:40 pm, Sunday**

Emily Diaz, Uriah Kilogore, Yuan Jiang, Shuyun Li, Andrew Schmidt, Michael Thorson | 4103240 | De-risking HTL product separations through solvent processing | **4:20 pm, Sunday**

Krista Kulesa, Eric Wiedner, Tom Autrey, Aaron Appel | 4104292 | Atomically-defined metal carbon nitride electrocatalysts for long-duration energy storage | **8:50 am, Tuesday**

Peter Rice, Tom Autrey, Bojana Ginovska, Maria Sushko, Zdenek Dohnalek, Zbynek Novotny | 4103965 | Tuning liquid-organic hydrogen carrier interactions on supported and unsupported carbon sorbent materials | **11:30 am, Tuesday**

Dhruba Jyoti Deka, Yong Wang, Kenneth Rappe | 4099561 | Ammonia inhibition of selective catalytic NOx reduction on Cu-CHA catalyst: Insights into the roles of redox half cycle kinetics and Cu-site diffusion | **5:10 pm, Tuesday**

David Heldebrant, Manh Thuong Nguyen, Jian Liu | 4099016 | Direction-specific diffusion of CO_2 augmented by polygonal rifling in chiral B-N nanotubes | **8:05 am, Wednesday**

Wendy Shaw, Emily Saccuzzo, Regina Trevino | 4102995 | Using nature as inspiration for Energy Solutions | **9:25 am, Wednesday**

Paul Marsh, Peter Valdez, Scott Edmundson, Chinmayee Subban | 4104851 | Integrated development of marine carbon dioxide removal strategies for maximum CO_2 capture | **9:30 am, Wednesday**

Uriah Kilgore, Tom Autrey, Mark Bowden, Mi Yeon Byun, Tanmayi Bathena | 4101923 | Liquid organic hydrogen carrier technology: progressing from lab to pilot | **10:00 am, Wednesday**

Tom Autrey, Mark Bowden | 4108841 | Energy storage in chemical bonds: Coupling hydrogen production to hydrogen utilization | **10:25 am, Wednesday**

CHEMICAL TOXICOLOGY

PRESENTATION

Vivian Lin, Tong Zhang, Chathuri Kombala, Madelyn Berger, Leo Gorham, John Melchior | 4097295 | Activity-based protein profiling strategies for identifying highly sensitive protein targets of organophosphate pesticides | **3:45 pm, Tuesday**

INORGANIC CHEMISTRY

SYMPOSIUM

Aaron Appel, Ba Tran | Electrocatalysis & Sustainable Chemistry Based on Metal Hydrides: Symposium in honor of Morris Bullock | **8:00 am and 2:00 pm, Monday**

PRESENTATIONS

Ajay Karakoti, Kevin Thangaraj, Tanmayi Bathena, Shannon Lee, Karthi Ramasamy, Vijay Murugesan | 4106082 | Multi-modal in situ characterization for unraveling the structure-property-function co-relations in functional materials | **10:35 am, Sunday**

Evan Patrick, Jeremy Erickson, Morris Bullock, Ba Tran | 4100707 | Effects of geometry at Cu(I) complexes on hydrogen activation and beta-elimination reactions | **8:55 am and 2:00 pm, Monday**

Simone Raugei, Jack Fuller, Gregory Schenter, Bojana Ginovska | 4109721 | Toward the control of metal hydrides reactivity for CO_2 reduction | **9:35 am, Monday**

Wendy Shaw, Regina Trevino, Bojana Ginovska | 4099449 | How does the protein scaffold of an artificial enzyme contribute to catalysis for hydrogen and CO_2 chemistry? | **10:00 am, Monday**

ANALYTICAL CHEMISTRY

PRESENTATION

Fanny Chu, Eva Brayfindley, John Zapanta, Andy Lin, Abdullah Shouaib, Joshua Chong, Shannon Schrader | 4086228 | How similar is "similar"? Quantifying sample similarity for chemical forensics | **10:45 am, Monday**

POSTER

Abhishek Kumar, Ji-Hye Seo, Yingzhe Wu, Eirik Krogstad, Kyle Makovsky, Dushyant Barpaga, Kelly McHugh | 4084762 | Metal-organic frameworks-derived nanoporous ion emitters for picogram level analysis of actinides | **12:00 pm, Wednesday**

NUCLEAR CHEMISTRY AND TECHNOLOGY

PRESENTATIONS

John Ducilon, Aaron Nicholas, Robert (Gian) Surbella | 4108588 | Structural characterizations of neptunyl coordination with multidentate acyclic ligands | **8:45 am, Tuesday**

Jose Veleta, Ean Arnold, Staci Herman, Chelsie Beck | 4105472 | Magnetic Particles as extractants for radionuclides | **9:25 am, Wednesday**

POSTER

Staci Herman, Dana Arbova, Bethany Lawler, Ean Arnold, Chelsie Beck | 4104986 | Separation of divalent transition metal activation products | **7:00 pm, Sunday**

U.S. DEPARTMENT OF ENERGY

PCSD_0860