Science for our Nation's Energy Future

Energy Frontier Research Centers
Energy Innovation Hubs
Computational Materials and Chemical Sciences Projects

Principal Investigators' Meeting

August 11-12, 2025

U.S. DEPARTMENT OF ENERGY | Office of Science

Table of Contents

VIRTUAL PLENARY SESSION AGENDA

EFRC-Hub-CMS-CCS Virtual Principal Investigators' Meeting

Wed, August 6, 2025 from 11 – 4 pm ET
RSVP at https://www.zoomgov.com/webinar/register/WN_jCbRv87kQMez3xo_lVxyeg

11:00 – 11:15 am	**Welcome from the Office of Science** Harriet Kung, *Acting Director for the DOE Office of Science and Deputy Director for Science Programs*
11:15 – 12:00 pm	**Updates from Basic Energy Sciences** Bindu Nair, *Associate Director for Basic Energy Sciences*
12:00 -12:15 pm	**Break**
12:15 – 1:00 pm	**Impact of Science on the United States' Energy Mission** Cynthia Friend, *President and CEO of The Kavli Foundation*
1:00 – 1:45 pm	**AI for Science** Moderators: Claudia Mewes and Marat Valiev, *Program Managers for Basic Energy Sciences* • Maria Chan, *Scientist at Argonne National Laboratory* • Daniel O'Malley, *Team Lead at Los Alamos National Laboratory* • Pratyush Tiwary, *Millard and Lee Alexander Professor in Chemical Physics at the University of Maryland, College Park*
1:45 -2:15 pm	**Break**
2:15 – 3:00 pm	**Basic Energy Science at the Cutting Edge: New Discoveries and Insights** Moderator: Gail McLean, *Division Director for Basic Energy Sciences* • Dmtri Basov, *Director of the Programmable Quantum Materials EFRC* • Annie Greenaway, Senior Investigator in the Liquid Sunlight Alliance (LiSA) Hub • Carolyn Pearce, *Director of the Interfacial Dynamics in Radioactive Environments and Materials EFRC* • Mark van Schilfgaarde, *Director of the Hierarchical, Scalable Green's Function Modeling of Chemistry at Interfaces CCS* • R. Stanley Williams, *Director of the Reconfigurable Electronic Materials Inspired by Nonlinear Neuron Dynamics EFRC*
3:00 – 3:45 pm	**The Innovation Landscape: From Discovery to Deployment** Moderator: Andrew Schwartz, *Deputy Associate Director of Basic Energy*

Sciences

- Yet-Ming Chiang, *Senior Investigator in the Joint Center for Energy Storage Research (JCESR) Hub*
- Benny Freeman, *Director of the Center for Materials for Water and Energy Systems (M-WET) EFRC*
- Paul Kent, *Director of the Center for Predictive Simulation of Functional Materials CMS*
- LaShanda Korley, Director of the *Center for Plastics Innovation EFRC*

3:45 – 4:00 pm **Announce Winners of the Art of Science Image Contest**

IN-PERSON MEETING AGENDA

2025 EFRC-Hub-CMS-CCS Principal Investigators' Meeting

Bethesda North Marriott Hotel & Conference Center
To virtually listen to the Talk Sessions, RSVP at
https://www.zoomgov.com/meeting/register/dWCJPv_sQiibKrZXKGncJg
All Times Eastern

Sunday, August 10, 2025

7:00 pm – 9:00 pm	BES ECN Mixer for students and postdocs only at Owen's Tavern & Garden (11820 Trade St, North Bethesda, MD 20852)

Monday, August 11, 2025

9:00 - 9:10 am	BES welcome in each breakout room
9:10 - 10:30 am	Talk Session #1
10:30 – 10:40 am	Break
10:40 - 12:10 pm	Overview Poster Session
12:10 - 1:40 pm	Lunch
12:25 – 1: 25 pm	BES Early Career Network (ECN) Event: Networking Lunch with an Expert
1:40 - 3:20 pm	Talk Session #2
3:20 – 3:30 pm	Break
3:30 - 5:00 pm	Technical Poster Session #1
7:00 pm – 9:00 pm	BES ECN Sports Night for students and postdocs only Pinstripes Bethesda (11920 Grand Park Ave, North Bethesda, MD 20852)

Tuesday, August 12, 2025

9:00 - 10:20 am	Talk Session #3
10:20 - 10:30 am	Break
10:30 - 12:00 pm	Technical Poster Session #2
12:00 - 1:30 pm	Lunch
12:15 – 1:15 pm	BES Early Career Network (ECN) Event: Mission "in" Possible: A Lunchtime Journey into Collaborative Thinking
1:30 - 3:10 pm	Talk Session #4
3:20 – 3:30 pm	Break
3:20 - 5:00 pm	Technical Poster Session #3
4:50 – 5:00 pm	Announce Team Science Contest Winner

SPEAKER BIOGRAPHIES

WELCOME FROM THE OFFICE OF SCIENCE

Dr. Harriet Kung is Acting Director for the Office of Science in the U.S. Department of Energy (DOE). She also serves as the Deputy Director for Science Programs and is the senior career official providing scientific and management direction and oversight for the SC research programs, including Advanced Scientific Computing Research, Basic Energy Sciences, Biological and Environmental Research, Fusion Energy Sciences, High Energy Physics, and Nuclear Physics, as well as other supporting functions and offices. Dr. Kung served in various leadership roles in Basic Energy Sciences, the largest program in the Office of Science, from 2002-2020. She is the recipient of numerous awards including the Presidential Meritorious Executive Rank Award in 2009 and the Distinguished Executive Rank Award in 2022.

UPDATES FROM BASIC ENERGY SCIENCE

Dr. Bindu R. Nair is the Associate Director of Science for Basic Energy Sciences. In this role, she oversees the Department's investment in the fundamental research to understand, predict, and ultimately control matter at the electronic, atomic, and molecular levels. She is also responsible for the planning, construction, and operation of major scientific user facilities that serve researchers across the wide variety of fields supported by Basic Energy Sciences (BES). Prior to her appointment at the Department of Energy, Dr. Nair spent much of her career at the Department of Defense where she most recently served as the Director of Basic Research in the Office of the Under Secretary of Defense for Research and Engineering.

PLENARY: IMPACT OF SCIENCE ON THE UNITED STATES' ENERGY MISSION

Cynthia M. Friend, Ph.D, is the president and CEO of The Kavli Foundation. Prior to joining the foundation in January 2021, Dr. Friend was a member of the Harvard University faculty since 1982. At Harvard she served in numerous leadership positions, including Chair of the Department of Chemistry and Chemical Biology and Associate Dean of the Faculty of Arts and Sciences. She was the first female chair and the first female professor in chemistry at Harvard. Dr. Friend also served as Director of The Rowland Institute at Harvard from 2013 to 2019, a nonprofit conceived to advance science in a wide variety of fields. She also held the role of Associate Lab Director at SLAC National Accelerator Lab, a preeminent international facility for X-ray science.

AI FOR SCIENCE

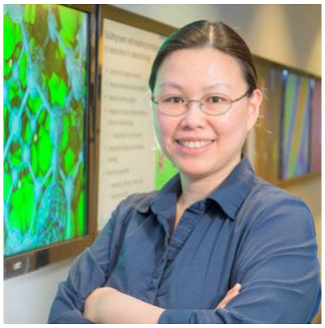
Moderators

Dr. Claudia Mewes joined the Materials Sciences and Engineering Division of the Office of Basic Energy Sciences at the U.S. Department of Energy in November 2021 as program manager for the Theoretical Condensed Matter Physics program. She is also a co-lead of the Computational Materials Science Program. Dr. Mewes was a professor of Physics and Material Science at the University of Alabama in Tuscaloosa, where she was a Leadership Board Fellow Professor from 2018 to 2021. In 2011 she was Visiting Fellow of the Center for Nanoscale Science and Technology in the Electron Physics group at the National Institute of Standards and Technology in Gaithersburg, MD.

Dr. Marat Valiev is the Program Manager for Quantum Information Sciences in the Chemical Sciences, Geosciences and Biosciences (CSGB) Division of the Office of Basic Energy Sciences, Office of Science, U.S. Department of Energy (DOE). Before joining DOE in April 2024, Dr. Valiev was a Computational Scientist at the Pacific Northwest National Laboratory (PNNL). He was also a Team Lead for Systems Modeling and Computational Sciences and later for Basic and Applied Molecular Foundations at PNNL and served as a detailee to Condensed Phase and Interfacial Molecular Science (CPIMS) Program in the CSGB Division. Dr. Valiev is one of the core developers of NWChem ab-initio computational chemistry software package and has extensive experience in the development and application of high-performance molecular simulation methods for the description of chemical transformations in large-scale chemical and biological systems.

Speakers

Maria Chan



Maria Chan is a scientist at the Center for Nanoscale Materials at Argonne National Laboratory who studies nanomaterials and renewable energy materials, including batteries, solar cells, and catalysts. Her particular focus is on using artificial intelligence/machine learning (AI/ML) for interfacing theoretical modeling with x-ray, electron, and scanning probe characterization. She is part of the Energy Storage Research Alliance (ESRA), a DOE Energy Innovation Hub, and the Midwest Integrated Center for Computational Materials (MICCoM), a Computational Materials Science Center.

Daniel O'Malley leads the Subsurface Flow and Transport Team within the Energy and Natural Resources Security Group at Los Alamos National Laboratory (LANL). He earned a B.S. in computer science and mathematics, an M.S. in mathematics, and a Ph.D. in applied mathematics, all from Purdue University. His research interests include computational science, quantum computing, and machine learning with an emphasis on applications to subsurface flow and transport. He has received numerous awards including a LANL Early Career Research award, a LANL Director's Postdoctoral Fellowship, the InterPore-Fraunhofer Award for Young Researchers from the International Society for Porous Media, a Charles C. Chappelle Fellowship from Purdue University, and a LANL Large Team Distinguished Performance Award.

Pratyush Tiwary is a Full Professor at the University of Maryland, College Park, where he holds the Millard and Lee Alexander Professorship in Chemical Physics. He maintains joint appointments in the Department of Chemistry and Biochemistry, the Institute for Physical Science and Technology, and the Institute for Health Computing, where he leads Therapeutics Discovery. His laboratory focuses on interdisciplinary theoretical and computational research, operating at the nexus of statistical mechanics, molecular simulations, and Artificial Intelligence, a field his lab terms "Artificial Chemical Intelligence." This work aims to model and predict thermodynamics and dynamics in complex real-world systems, including addressing challenges like the behavior of drug molecules, crystal formation, and protein flexibility, with significant implications for pharmaceutical, chemical, and materials sciences. Professor Tiwary also contributes as an Associate Editor for the Journal of Chemical Theory and Computation and is a member of the Scientific Advisory Board of Schrödinger, Inc.

BASIC ENERGY SCIENCE AT THE CUTTING EDGE: NEW DISCOVERIES AND INSIGHTS

Moderator

Dr. Gail McLean is the Director of the Chemical Sciences, Geosciences and Biosciences (CSGB) Division and the acting team lead for the Photochemistry and Biochemistry team in the Office of Basic Energy Sciences, Office of Science, U.S. Department of Energy. Dr. McLean joined the Chemical Sciences, Geosciences, and Biosciences Division in November 2008 as a program manager for Photosynthetic Systems. Prior to joining DOE, Dr. McLean was a National Program Leader for Plant Biology in the Competitive Programs Unit of the Cooperative State Research, Education, and Extension Service (now the National Institute of Food and Agriculture), United States Department of Agriculture (USDA).

Speakers

Dmitri N. Basov is the Higgins Professor and Chair of the Department of Physics at Columbia University. He also serves as the Director of the DOE Energy Frontiers Research Center on Programmable Quantum Materials and co-directs the Max Planck Society – New York Center for Nonequilibrium Quantum Phenomena. His research focuses on the physics of quantum materials, including superconductivity and two-dimensional materials, which he investigates using various nano-optical techniques developed in his laboratory. Dr. Basov's contributions have been recognized with numerous honors, including his election to the National Academy of Sciences.

Ann (Annie) Greenaway is a staff scientist in the Photochemistry and Chemical Processes group at NREL and a co-PI on the Photoactive Materials team of the Liquid Sunlight Alliance (LiSA). She joined NREL as a Director's Postdoctoral Fellow in 2018, working on the integration of emerging II-IV-N_2 semiconductors with established materials such as gallium nitride, and became a member of NREL's research staff in 2020. Her overall research portfolio focuses on the development of new photoelectrodes and photoelectrode architectures for photoelectrochemical carbon dioxide valorization and water splitting, including work in the BES Solar Photochemistry program and the SPECS EFRC. Within LiSA, Annie focuses on the discovery of new nitride semiconductors and the demonstration of cascade photoelectrochemical systems.

Dr. Carolyn Pearce re-joined PNNL in 2016 as a chemist specializing in geosciences. She works on the characterization of minerals relevant to radioactive waste storage and processing in order to determine reaction mechanisms and kinetics that affect radionuclide stability in waste forms and subsurface environments. In 2021, she was named Director of the Ion Dynamics in Radioactive Environments and Materials (IDREAM) Energy Frontier Research Center, which is led by PNNL for the U.S. Department of Energy Office of Basic Energy Sciences (BES) in the Office of Science. IDREAM researchers conduct fundamental science to support innovations in retrieving and processing of chemically hazardous and radioactive waste.

Mark van Schilfgaarde is the Chief Theorist at the National Renewable Energy Laboratory and the Director of the Hierarchical, Scalable Green's Function Modeling of Chemistry at Interfaces CCS. His research interests are centered around the theory of electronic structure, which is the key to understanding properties of materials at their most fundamental level, most notably the quasiparticle self-consistent GW approximation.

R. Stanley Williams, one of the initiators of neuromorphic computing, joined Texas A&M in 2019 as Professor of Electrical and Computer Engineering after 23 years at Hewlett Packard companies. Williams served in various technical and management roles at HP/HPE, including Laboratory Director, Senior Fellow and Senior Vice President. He previously served on the BES Advisory Committee. He is currently the Director of the Reconfigurable Electronic Materials Inspired by Nonlinear Neuron Dynamics (reMIND) EFRC.

THE INNOVATION LANDSCAPE: FROM DISCOVERY TO DEPLOYMENT

Moderator

Dr. Andrew Schwartz is the Deputy Associate Director of Science for Basic Energy Sciences. He also currently serves as Acting Division Director for Materials Sciences and Engineering and Scientific User Facilities. He served as Division Director for Materials Sciences and Engineering from 2022 to 2024, after serving as Acting Division Director since July 2020. From 2013 to 2022 he served as Senior Technical Advisor for Energy Frontier Research Centers (EFRCs), leading the team of BES Program Managers and support staff in management of the EFRC program. From 2008 to 2013 Dr. Schwartz was Program Manager for the BES Experimental Condensed Matter Physics program.

Speakers

Yet-Ming Chiang is a Taiwanese-American materials scientist and engineer, who is currently the Kyocera Professor at Massachusetts Institute of Technology. He has been influential in the development of new materials for energy storage, transfer, and power of a variety of different devices and vehicles. He is currently a Senior Investigator in the Joint Center for Energy Storage Research (JCESR) Hub. Professor Chiang is a Fellow of the Electrochemical Society, Materials Research Society, American Ceramic Society, and National Academy of Inventors.

Benny Freeman is the William J. (Bill) Murray, Jr. Endowed Chair in Engineering at The University of Texas at Austin. He is a professor of Chemical Engineering and has been a faculty member for 34 years. Dr. Freeman's research is in polymer science and engineering and, more specifically, in mass transport of small molecules in solid polymers. His research group focuses on discovery of structure/property relations for desalination and gas separation membrane materials, new materials for hydrogen separation, natural gas purification, carbon capture, and new materials for improving fouling resistance, permeation, and separation performance in liquid separation membranes. He is Director of the Center for Materials for Water and Energy Systems (M-WET).

Paul Kent is a distinguished research scientist at Oak Ridge National Laboratory (ORNL) and the Director of the Center for Predictive Simulation of Functional Materials CMS. At ORNL, he is a member of the Nanotheory Institute at the Center for Nanophase Materials Sciences (CNMS) and the Computational Chemical and Materials Science group in the Computational Science and Engineering Division. His is focused on predicting and explaining the properties of materials using computer simulation. He also led the development of the QMCPACK application for exascale computing as part of the Exascale Computing Project.

Prof. LaShanda T. J. Korley is a Distinguished Professor in the Departments of Materials Science & Engineering and Chemical & Biomolecular Engineering at the University of Delaware (UD). Her innovative research program utilizes a bioeconomy framework for the molecular design, manufac-ture, and valorization of polymeric systems with material complexity and hierarchical structure. Prof. Korley is the Director of an Energy Frontier Research Center – Center for Plastics Innova-tion (CPI) funded by the Department of Energy and also the Co-Director of a Materials Research Science and Center (MRSEC) – UD Center for Hybrid, Active, and Responsive Materials (UD CHARM) funded by the National Science Foundation. She is also the Associate Director of the Center for Research in Soft matter & Polymers (CRiSP) at UD.

BES EARLY CAREER ECN NETWORK (BES ECN) ORGANIZED EVENTS

About: The BES ECN is a group of graduate students, postdoctoral researchers, and early career scientists from current EFRCs, Hubs, and CMS/CCS projects. The goal is to share best practices between centers, provide workforce development opportunities, and create a network of early career scientists with a passion for energy science. See https://www.energyfrontier.us/bes-ecn.

SOCIAL EXCURSIONS

Organizers:

- Azim Haque, National Renewable Energy Laboratory, CHOISE EFRC (Co-lead)
- James Burrow, Argonne National Laboratory, ESRA Hub (Co-lead)
- Micheal Alowakennu, Michigan State University, BioLEC EFRC
- Elif Pinar Alsac, Georgia Tech, MUSIC EFRC
- Yunxia Chen, University of Florida, AIM EFRC
- Sheilah Cherono, North Carolina A&T, CEDARS EFRC
- Darci Collins, National Renewable Energy Laboratory, LiSA Hub
- Emma Daggett, Purdue University, QuPIDC EFRC
- John Dickenson, University of North Carolina, CHASE Hub
- Rachel Huang, University of Texas, M-WET EFRC
- Henry Kantrow, Georgia Tech, SPECS EFRC
- Elham Kianihaharchegani, Brown University, AIM EFRC
- Spela Kunstelj, University of Chicago, CD4DC EFRC
- Sharad Mahatara, National Renewable Energy Laboratory, APEX EFRC
- Ruby Manderna, University of North Carolina, MAPOL CCS
- Franziska Schmidt, Los Alamos National Laboratory, FUTURE EFRC
- Lauren Shepard, Pennsylvania State University, FaCT EFRC
- Salma Soliman, Georgia Tech, 3DFeM2 EFRC
- Arjun Yennemadi, Massachusetts Institute of Technology, CENT2 EFRC

NETWORKING MIXER

When: Sunday, Aug 10th 2025, 7 PM – 9 PM
Where: Owen's Tavern & Garden (11820 Trade St, North Bethesda, MD 20852)
Who: Students and postdocs only

Description: An evening for socializing and networking. The venue is located 0.5 miles from the hotel. The group will meet at Owen's Tavern & Garden near the high tables. Participants are responsible for their own food and drinks.

Contacts:
Azim Haque (mdazimul.haque@nrel.gov)
James Burrow (jnburrow@uchicago.edu)

SPORTS NIGHT

When: Monday, Aug 11th 2025, 7 PM – 9 PM
Where: Pinstripes Bethesda (11920 Grand Park Ave, North Bethesda, MD 20852)
Who: Students and postdocs only

Description: An evening for socializing and playing sports such as bowling and bocce. The venue is located 0.5 miles from the hotel. The group will meet at Pinstripes Bethesda near the bowling lanes. Participants are responsible for their own food and drinks.

Contacts:
Azim Haque (mdazimul.haque@nrel.gov)
James Burrow (jnburrow@uchicago.edu)

LUNCH EVENTS

NETWORKING LUNCH WITH AN EXPERT

When: Monday, August 11, 2025, lunch break
Where: Back right corner of the lunchroom (Salon D/E)
Who: All Meeting Attendees

Description: This networking luncheon is planned to promote focused interaction and discussion between the PIs/DOE members serving as mentors and early career scientists. The tables in the back right corner of the lunchroom will be designated for this event and arranged by common disciplinary interests or career paths (computational modeling, spectroscopy and electrochemistry, material design and synthesis, careers at DOE, careers in national labs, careers in academia). Each table will be led by designated PIs or DOE members (see list below), who will stay at their table for the duration of the lunch, acting as a dedicated point of contact for conversation and mentorship. Attendees will have the flexibility to move between tables as desired, allowing them to engage with various mentors and explore different areas of interest.

<u>Invited Experts:</u>

- Careers at DOE
  - **John Vetrano**, DOE BES Materials Science and Engineering Division, Program Manager, Mechanical Behavior and Radiation Effects and Batteries and Energy Storage Hub; EFRC Co-Lead

  - **Viviane Schwartz**, DOE BES Chemical Sciences, Geosciences, and Biosciences Division, Program Manager, Catalysis Science
- Careers in Academia
  - **Burcu Gurkan**, Kent H. Smith Professor II in the Department of Chemical and Biomolecular Engineering at Case Western Reserve University (BEES2 EFRC)
  - **Long-Qing Chen**, Donald W. Hamer Professor of Materials Science and Engineering and Professor of Mathematics and Engineering Science and Mechanics at The Pennsylvania State University (COMMS CMS)
- Careers at DOE National Labs
  - **Giulia Galli**, Senior Scientist at Argonne National Lab, Liew Family Professor of Electronic Structure and Simulations in the Pritzker School of Molecular Engineering and the Department of Chemistry at the University of Chicago (MICCoM CMS)
  - **James De Yoreo**, Battelle Fellow at Pacific Northwest National Laboratory, Affiliate Professor of Materials Science and Engineering and of Chemistry at the University of Washington (CSSAS EFRC)
- Material Design and Synthesis
  - **LaShanda T. J. Korley**, Distinguished Professor of Engineering in the Departments of Materials Science & Engineering and Chemical and Biomolecular Engineering at the University of Delaware (CPI EFRC)
- Electrochemistry and Spectroscopy
  - **Andrew Ferguson**, Senior Scientist in the Chemistry & Nanoscience Center and Group Leader for Spectroscopy and Photoscience at the National Renewable Energy Laboratory (reMIND EFRC)
  - **Neal R. Armstrong**, Regents Professor (Emeritus) in Chemistry/Biochemistry & Optical Sciences at the University of Arizona (SPECS EFRC)
- Computational Modeling
  - **Lucas K. Wagner**, Associate Professor of Physics at the University of Illinois Urbana-Champaign (QMC-HAMM CMS)
  - **Maria K. Chan**, Scientist at the Center for Nanoscale Materials at Argonne National Lab (ESRA Hub)

BES Early Career Network Organizers:

- Lauren Shepard, The Pennsylvania State University, FaCT EFRC (Lead)
- Emily Close, Pacific Northwest National Laboratory, CSSAS EFRC
- Saudagar Dongare, Case Western University, 4C EFRC
- Vaishali Khokhar, Case Western University, BEES2 EFRC
- Declan McCarthy, Lawrence Berkeley National Laboratory, CHiPPS EFRC
- Tawfiqur Rakib, University of Illinois Urbana-Champaign, QMC-HAMM CMS
- Vrindaa Somjit, Argonne National Laboratory, MICCoM CMS

Contact:
Lauren Shepard (lzs5735@psu.edu)

MISSION “IN” POSSIBLE: A LUNCHTIME JOURNEY INTO COLLABORATIVE THINKING

When: Tuesday, August 12, 2025, lunch break
Where: Salon G
Who: All Meeting Attendees

Description: Join us for a fun and interactive networking event designed to spark collaboration and creativity across disciplines! During lunch, participants will team up at round tables to tackle “impossible” missions—imaginative challenges that can only be solved by combining everyone’s diverse expertise. Whether you’re a chemist, physicist, engineer, lab manager, or beyond, bring your curiosity, meet new colleagues, and turn the impossible into possible! The goal of Mission “in” Possible event is to serve as a lunchtime icebreaker that encourages participants to connect across disciplines in a fun and low-pressure environment.

BES Early Career Network Organizers:
- Yunxia Chen, University of Florida, AIM EFRC (Lead)
- Elif Pinar Alsac, Georgia Institute of Technology, MUSIC EFRC
- Tim Chiang, Lawrence Berkeley National Laboratory, CCBC EFRC
- Robert Felsted, Pacific Northwest National Laboratory, IDREAM EFRC
- Elham Kianihaharchegani, Brown University, AIM EFRC
- Kate Matthews, University of California, San Diego, Q-MEEN-C EFRC
- Sharad Mahatara, National Renewable Energy Laboratory, APEX EFRC
- Linh Le, University of Chicago, CD4DC EFRC

Contact:
Yunxia Chen (yunxia.chen@ufl.edu)

Monday, August 11, 2025: Talk Session I from 9:00 – 10:30 am

	B. Catalysis I	**K. QIS II**	**D. Energy Storage I**	**E. Energy Storage II**	**F. Energy-Water**	**H. Microelectronics**	**J. QIS I**	**L. AI/ML**
Room	***Forest Glen***	***Glen Echo***	***Salon F***	***Salon H***	***Brookside B***	***Brookside A***	***Brookside C***	***Salon G***
Chair	***Viviane Schwartz***	***Athena Sefat***	***Andy Schwartz***	***Craig Henderson***	***Amanda Haes***	***Claudia Cantoni***	***Marat Valiev***	***Claudia Mewes***
9:00 AM	**BES Welcome**	**BES Welcome**	**BES Welcome**	**BES Welcome**	**BES Welcome**	**BES Welcome**	**BES Welcome**	**BES Welcome**
9:10 AM	**B-I-1** [**EFRC - CD4DC**] Rachel Getman; Joseph Hupp *Ohio State; Northwestern* Elucidating the Geometric and Electronic Structure of a Fully Sulfided Analog of an Anderson Polyoxomolybdate Cluster for photo-, electro-, and thermalcatalytic hydrogenation	**K-I-1** [**EFRC - CATS**] Su-Yang Xu *Harvard* Observation of the Axion Quasiparticle in Condensed Matter	**D-I-1** [**Hub - ESRA**] Y. Shirley Meng *ANL / U Chicago* New Perspectives on Ion-Matter Interactions	**E-I-1** [**EFRC - CABES**] Andrej Singer; David Muller *Cornell* Operando Characterization of Energy Materials and Devices	**F-I-1** [**EFRC - UNCAGE-ME**] Ryan Lively *Georgia Tech* Impacts of Acid Gases on Microporous Materials for Use in Polar/Non-Polar Gas Separations	**H-I-1** [**EFRC - CEEMag**] Xiaoqin (Elaine) Li *UT Austin* Exploring New Materials for Magnonics	**J-I-1** [**CMS - C2SEPEM**] Luna Liu[1]; Gurjyot Sethi[2,3]* *[1]Yale; [2]LBNL; [3]UC Berkeley* First-Principles Anatomy of Exciton Dynamics: From Dispersion to Quantum Transport	**L-I-1** [**CCS - CMSET**] Gregory Voth *U Chicago* Multiscale Computational Framework for Biomolecular Energy Transduction: from Electrons to the Mesoscale

	B. Catalysis I	**K. QIS II**	**D. Energy Storage I**	**E. Energy Storage II**	**F. Energy-Water**	**H. Microelectronics**	**J. QIS I**	**L. AI/ML**
9:30 AM	**B-I-2** [**EFRC - CEDARS**] Dhananjay Kumar; Brady Bruno *North Carolina A&T; Cornell* Conductive ruthenium oxide films with surface-orientation control as experimental models for oxygen evolution reaction studies	**K-I-2** [**EFRC - Pro-QM**] Xiaoyang Zhu *Columbia* Time-Lapsed Treasure Maps for Finding Programmable Quantum Materials	**D-I-2** [**Hub - ABC**] Yi Cui *Stanford; SLAC* Aqueous Battery Consortium	**E-I-2** [**EFRC - m2M#s**] Kenneth Takeuchi; Amy Marschilok; Esther Takeuchi *Stony Brook / BNL* High Entropy Oxides from the Molecular to the Mesoscale	**F-I-2** [**EFRC - M-WET**] Benny Freeman *UT Austin* Center for Materials for Water and Energy Systems (M-WET)	**H-I-2** [**EFRC - 3DFeM2**] Susan Trolier-McKinstry *Penn State* Switching in Wurtzite Ferroelectrics for Non-volatile Ferroelectric Memories	**J-I-2** [**EFRC - QuPIDC**] Zhaoyuan Zheng; Jonas Peterson* *Northwestern; Purdue* Strong Light–Matter Interaction in Plasmonic Arrays Enables Coherent Quantum Emission	**L-I-2** [**EFRC - AIM**] Alireza Zarei *U Delaware* Physically Constrained 3D Diffusion for Inverse Design of Fiber-Reinforced Polymer Composite Materials
9:50 AM	**B-I-3** [**CCS - BEAST**] Ravishankar Sundararaman *Rensselaer Polytechnic Institute* Beyond-DFT techniques for electrochemistry, accelerated by machine learning	**K-I-3** [**EFRC - QSQM**] Dipanjan Chaudhuri *UIUC* Measurement of the dynamic charge susceptibility near the charge density wave transition in $ErTe_3$	**D-I-3** [**Hub - CHASE**] Gerald Meyer; Jillian Dempsey *UNC Chapel Hill* Hybrid Photoelectrode Architectures for Liquid Solar Fuels	**E-I-3** [**EFRC - FaCT**] Xi Chelsea Chen *ORNL* Ion Transport Enhancement and Interfacial Reisistance in Polymer-Li-Garnet Composite Electrolytes	**F-I-3** [**EFRC - AMEWS**] Seth B. Darling; Kelsey B. Hatzell; Chong Liu *ANL / U Chicago; Princeton; U Chicago* Unifying Structure–Property Relationships in 2D Laminar Membranes: Insights from Phyllosilicates, TMDs, and MXenes	**H-I-3** [**CMS - COMMS**] Long-Qing Chen *Penn State* Stability and Dynamic Responses of Ferroelectric Polar Structures Under Light	**J-I-3** [**EFRC - CMQT**] Roel Tempelaar *Northwestern* Apparent Circular Dichroism for Improved Chiroptical Control	**L-I-3** [**EFRC - CABES**] Peter Frazier; Tomas Arias *Cornell* Machine Learning Approaches to Energy Materials and Devices
10:10 AM	**B-I-4** [**CCS - ExaPUC**] Matthew Hermes *U Chicago* Localized Active Space State Interaction Singles method	**K-I-4** [**EFRC - QuPIDC**] Souvik Biswas; Tongcang Li *Stanford; Purdue* Entanglement and Coherence from Quantum Emitters in hBN	**D-I-4** [**EFRC - MUSIC**] Jeff Sakamoto; Neil Dasgupta *U Michigan / UC Santa Barbara; U Michigan* Mechano-chemical Understanding of Solid Ion Conductors	**E-I-4** [**EFRC - BEES2**] Mark Tuckerman *NYU* Beating the Viscosity-Conductivity Inverse Relation Barrier to Create a Breakthrough Electrolyte for Emerging Battery Applications: Does Quantum Mechanics Hold the Key?	**F-I-4** [**EFRC - M-WET**] José Carlos Díaz1; Chuqiao (Elise) Chen[2]; Noah Wamble[1,3]* *[1]UT Austin; [2]UC Santa Barbara; [3]LBNL* Towards Rational Design of Tougher Snips Membranes for Water and Energy Systems	**H-I-4** [**CCS - Questc**] Mark van Schilfgaarde *NREL* High Fidelity Green's function theory for low dimensional systems	**J-I-4** [**EFRC - CHOISE**] David B. Mitzi *Duke* Using Chirality and Symmetry Breaking to Tailor Hybrid Metal Halide Perovskite Structures and Emerging Properties	**L-I-4** [**Hub - ESRA**] Maria Chan *ANL* Energy Storage Research Alliance - Accelerating Materials Discovery, Synthesis, Characterization, and Understanding with AI/ML and advanced characterization

* After the presenter names indicates a Team Science Contest talk.

Monday, August 11, 2025: Talk Session II from 1:40 – 3:20 pm

	B. Catalysis I	**C. Catalysis II**	**I. Nuclear**	**A. Advanced Manufacturing**	**F. Energy-Water**	**H. Microelectronics**	**J. QIS I**	**L. AI/ML**
Room	***Forest Glen***	***Glen Echo***	***Salon F***	***Salon H***	***Brookside B***	***Brookside A***	***Brookside C***	***Salon G***
Chair	***Jenny Roizen***	***Aaron Stone***	***Philip Wilk***	***Kate Brown***	***Chris Chervin***	***Patrick El-Khoury***	***Tim Mewes***	***Matthias Graf***
1:40 PM	**B-II-1** [**EFRC - BioLEC**] Kelly J. Gaffney *SLAC* Enhancing the Development of 3d transition metal photocatalysts with X-ray spectroscopies	**C-II-1** [**CCS - WFT2XC**] Paul Zimmerman *U Michigan* Pushing the Frontiers of Exchange-Correlation	**I-II-1** [**EFRC - FUTURE**] Franziska Schmidt; Saikumaran Ayyappan* *LANL; NC State* Metal Corrosion Under Irradiation – Explaining in Situ X-Ray Spectroscopy with Ex Situ Microscopy and Atom Probe Tomography	**A-II-1** [**EFRC - CSSAS**] Alex Berlaga; Renyu Zheng* *U Chicago; PNNL/U Washington* From Force-Field Parameters to Programmable Nanostructures: Integrated Simulation, Active Learning, and Experiment for Peptoid-Based Hierarchical Materials	**F-II-1** [**EFRC - CENT2**] Michael S. Strano *MIT* A New, Unified Theory of Confined Fluid Thermodynamics	**H-II-1** [**EFRC - Pro-QM**] Valentina Bisogni *BNL* Resonant Inelastic X-ray Scattering on programmable van der Waals materials	**J-II-1** [**CCS - MAPOL**] Jay Foley *UNC Charlotte* Active-space approaches for Ab initio Cavity Quantum Electrodynamics	**L-II-1** [**EFRC - 3DFeM2**] Ichiro Takeuchi *U Maryland* Autonomous Manufacturing and Automated Materials Exploration for 3D Ferroelectric Microelectronics Manufacturing
2:00 PM	**B-II-2** [**EFRC - EPN**] Justin B. Sambur; Shane Ardo *Colorado State; UC Irvine* Advanced Correlative Microscopy Reveals Links Between Nanoreactor Photosynthetic Properties and their Yields for Electronic Charge Separation	**C-II-2** [**EFRC - CEDARS**] Tanja Cuk; Shay McBride *U Colorado Boulder; Dartmouth College* Isolating intermediates of the photo-excited oxygen evolution reaction on titanium oxides	**I-II-2** [**EFRC - TETI**] Miaomiao Jin *Penn State* Multiscale Investigation of Defects in Oxide Fuels	**A-II-2** [**EFRC - REMAT**] Brandon R. Clarke; Pranav Krishnan* *Harvard; UIUC* Multi-Material 3D Printing with Frontally Polymerizable Resins	**F-II-2** [**EFRC - M-WET**] Lynn E. Katz *UT Austin* Structure and Dynamics of Water and Solutes Near Interfaces and in Solution	**H-II-2** [**EFRC - CEEMag**] Gregory Fuchs *Cornell* Magnon detection and function for next-generation energy efficient interconnects	**J-II-2** [**EFRC - CMQT**] Michael Wasielewski *Northwestern* Molecular Optical-Spin Interfaces for Quantum Information Applications	**L-II-2** [**EFRC - APEX**] Steven R. Spurgeon *NREL* Orchestrating Interfacial Control: AI-Driven Insights for Advanced Power Electronics

	B. Catalysis I	C. Catalysis II	I. Nuclear	A. Advanced Manufacturing	F. Energy-Water	H. Microelectronics	J. QIS I	L. AI/ML
2:20 PM	**B-II-3 [EFRC - SPECS]** Chad Risko; Erin Ratcliff *U Kentucky; Georgia Tech* Polarons report the composition of local nanoenvironments of the polymer–electrolyte interphase in soft semiconductor energy conversion and storage	**C-II-3 [CCS - FLOSIC]** Kushantha Withanage *UT El Paso* Advance Accuracy and Efficiency in Self-interaction-free Density Functional Theory	**I-II-3 [EFRC - FUTURE]** Blas Uberuaga *LANL* Developing and Validating Multiscale Models of Radiation-Modified Oxide Growth	**A-II-3 [EFRC - CSSAS]** Oleg Gang *Columbia / BNL* Controlling multiscale morphology of nanoscale self-assemblies with molecular clues and external fields	**F-II-3 [EFRC - AMEWS]** Yaguang Zhu; Qinsi Xiong* *Princeton; Northwestern* More than a Spectator: Critical Role of Water in Ion Transport through 2D Membranes	**H-II-3 [EFRC - ULTRA]** Robert Nemanich *Arizona State* Ultra Materials for a Resilient, Smart Electricity Grid (ULTRA)	**J-II-3 [EFRC - QuPIDC]** Alisa Javadi; Jonathan Hood *U Oklahoma; Purdue* Towards Scalable Generation of Indistinguishable Photons using Solid-State Platforms	**L-II-3 [CMS - MLAMD]** Cai-Zhuang Wang *Ames* Accelerating the discovery and design of advanced functional materials using AI/ML and exascale computing
2:40 PM	**B-II-4 [Hub - LiSA]** Matthew Salazar[1]; Aisulu Aitbekova[1]; Katherine Yan[2]* *[1]Caltech; [2]SLAC* A Solar-Driven Electrochemical/Photothermocatalytic Process for CO_2 Conversion to C_6 Oxygenates: An Assembly of Coupled Microenvironment	**C-II-4 [EFRC - CEDARS]** Cassius Boyd; Shay McBride; Sheilah Cherono* *U Colorado Boulder; Dartmouth College; NC A&T* Photo-electrochemistry of Titanium Oxides: A Platform for Assigning Visible Spectra to Oxygen	**I-II-4 [EFRC - MSEE]** Karen Chen-Wiegart *Stony Brook / BNL* Insights into Interfacial Morphological Evolution of Ni Binary Alloys in Molten Salts	**A-II-4 [EFRC - AIM]** Venkatesh Ananchaperumal; Elham Kiyani *Clemson; Brown* Modeling Crack–Void Interactions in Heterogeneous Composites Using Discrete Particle Dynamics and DeepONet Operator Learning	**F-II-4 [EFRC - CENT2]** Zuzanna S. Siwy *UC Irvine* Gating Nanofluidic Transport with Ions, Solvent, and Local Electric Potential	**H-II-4 [EFRC - APEX]** Satya K. Kushwaha; Jessica L. McChesney *Johns Hopkins; ANL* Floating Zone Crystal Growth and Characterization of Metallic Ceramics for Future Microelectronics	**J-II-4 [CMS - MICCoM]** Giulia Galli *ANL / U Chicago* Quantum simulations for quantum technologies	**L-II-4 [CMS - HeteroFAM]** Ting Cao; Peter Sushko *U Washington;PNNL* Learning at Scale: AI-Driven Design and Discovery of Moiré Superlattices and Complex Quantum Materials
3:00 PM	**B-II-5 [EFRC - EPN]** Olivia F. Bird; Faith A. Flinkingshelt* *U Colorado Boulder; UC Irvine* Extending Charge-Separated-State Lifetime in Nanocrystal–Molecule Hybrids via Rational Molecular Design	**C-II-5 [CCS - SPEC]** Sotiris S. Xantheas *PNNL / U Washington* Molecular Dynamics using highly correlated electronic structure methods driven by the Many-Body Expansion (MBE-MD)	**I-II-5 [EFRC - IDREAM]** Linda Young; Xiaosong Li *ANL; U Washington* Origin of Reactive Species in Solution Phase Radiolysis of Highly Concentrated Electrolytes	**A-II-5 [EFRC - REMAT]** Philippe Geubelle; Rafael Gómez-Bombarelli *UIUC; MIT* Manufacturing Patterned Materials Using Frontal Polymerization Instabilities: A Multiscale Mechanism-Based Model	**F-II-5 [EFRC - AMEWS]** Jeffrey W. Elam; Nicholas H.C. Lewis; George C. Schatz *ANL; U Chicago; Northwestern* Probing the Electrochemical Interface and Local Electrostatic Fields with Ultrafast IR Spectroscopy	**H-II-5 [EFRC - μ-ATOMS]** Jifeng Liu *Dartmouth College* Harnessing Atomic Ordering in Semiconductor Alloys Through Theory-Experiment Synergy	**J-II-5 [EFRC - M2QM]** Linqing Peng; Stephen Hill *Caltech; Florida State* 54 Ghz Clock Transition in a Ho^{3+} Spin Qubit Assembled Into a Metal-Organic Framework	**L-II-5 [CMS - QMC-HAMM]** Lucas Wagner *UIUC* QMC-HAMM: High accuracy multiscale models from quantum Monte Carlo

* After the presenter names indicates a Team Science Contest talk.

Tuesday, August 12, 2025: Talk Session III from 9:00 – 10:20 am

	B. Catalysis I	**C. Catalysis II**	**D. Energy Storage I**	**E. Energy Storage II**	**G. Hydrogen**	**H. Microelectronics**	**J. QIS I**
Room	***Forest Glen***	***Glen Echo***	***Salon F***	***Salon H***	***Brookside B***	***Brookside A***	***Brookside C***
Chair	***Chris Bradley***	***Adam Kinney***	***Aaron Stone***	***Chris Chervin***	***Gail McLean***	***Tim Mewes***	***Jane Zhu***
9:00 AM	**B-III-1 [EFRC - iCOUP]** Anne LaPointe; Megan Fieser *Cornell; U Southern California* Functionalization of Post-Consumer Plastics into Novel Products	**C-III-1 [CCS - BEAST]** Sophi Gerits; Daniel Weinberg; Nima Karimitari* *U Colorado Boulder; LBNL; U South Carolina* Accurate Electrochemical Predictions with Many-Body and Machine-Learning Methods	**D-III-1 [EFRC - GMCS]** Chelsea Neil *LANL* Probing reactive fracture dynamics with experiments and modeling	**E-III-1 [EFRC - BEES2]** Thomas Zawodzinski *U Tennessee Knoxville* Tracking Behavior in Microemulsions from Bulk Structure and Transport to Interfacial Processes	**G-III-1 [EFRC - SPECS]** Seth Marder; Neal Armstrong *U Colorado Boulder; U Arizona* Tethering and Crosslinking Approaches to Build Resilient Multilayer Polymer Catalyst Architectures	**H-III-1 [EFRC - µ-ATOMS]** Paul C. McIntyre *Stanford/SLAC* Shining Light on Short-Range Ordering in Group-IV Semiconductor Alloys	**J-III-1 [EFRC - CMQT]** Iqbal B. Utama; Robert Classen; Srishti Pal; Hannah Christianson* *Northwestern; Ohio State; Cornell; UC Berkeley* Enabling Ambient Stability and Quantum Integration of Organometallic Magnonic Ferrimagnets via Atomic Layer Encapsulation
9:20 AM	**B-III-2 [EFRC - CPI]** Alex Balzer *U Delaware* Bridging the Gap: Experiments and Simulations of Polyethylene Transport in Catalytic Deconstruction	**C-III-2 [EFRC - CPEC]** Omar Abdelrahman *U Houston* Chemistry Beyond the Sabatier Limit: Programmable Photons for Accelerated Catalysis for Energy	**D-III-2 [EFRC - MUSIC]** David Kwabi; Mioafang Chi *Yale; ORNL* Mechano-chemical Understanding of Solid Ion Conductors (MUSIC) Selected topics	**E-III-2 [EFRC - FaCT]** Catalin Gainaru *ORNL* Controlling the Energy Barriers for Ion Transport in Polymers	**G-III-2 [EFRC - HEISs]** Ryan O'Hayre *Colorado School of Mines* Triple Play: Disentangling Protons, Oxygen Vacancies, and Holes and Their Role in the Electrocatalytic Activity of the $BaCo_xFe_{0.8-x}Zr_{0.1}Y_{0.1}O_{3-d}$ (BCFZY, $0.1 \leq x \leq 0.7$) Triple-Conducting Oxide System	**H-III-2 [EFRC - reMIND]** Patrick J. Shamberger *Texas A&M–TEES* Design of Dynamical Response in Electro-Thermal Neurons	**J-III-2 [EFRC - CHOISE]** Md Azimul Haque; Andrew Grieder* *NREL; U Wisconsin Madison* Chirality Transfer and Spin Selectivity in Hybrid Metal Halide Semiconductors

	B. Catalysis I	**C. Catalysis II**	**D. Energy Storage I**	**E. Energy Storage II**	**G. Hydrogen**	**H. Microelectronics**	**J. QIS I**
9:40 AM	**B-III-3** [**EFRC - CCBC**] Timothy K. Chiang *LBNL* Programming the Architecture of Self-Assembling Protein Nanomaterials	**C-III-3** [**EFRC - BioLEC**] Obadiah G. Reid *NREL / U Colorado Boulder* Photolysis of Nickel-Halide Bonds as a General Mechanism of Ni / Sensitizer Photocatalyst Activation	**D-III-3** [**EFRC - m2M#s**] Kenneth Takeuchi; Amy Marschilok; Esther Takeuchi *Stony Brook / BNL* Elucidating Productive Electrochemically Induced Dissolution/Deposition Systems	**E-III-3** [**Hub - ESRA**] Alae Eddine Lakraychi[1]; Harshan Reddy Gopidi[1]; Jiaqi Wang[2]; Zeqian Zhang[3]* *[1]U Houston; [2]ANL; [3]PNNL* Structure–Property Relationships for Multi-Electron Organic Positive Electrode Materials	**G-III-3** [**CMS - EPW**] Feliciano Giustino *UT Austin* Large Polarons and Exciton Polarons in Titanium Dioxide	**H-III-3** [**EFRC - Q-MEEN-C**] Duygu Kuzum *UC San Diego* Engineering Nanoelectronic Devices for Energy Efficient Neuromorphic Computing	**J-III-3** [**EFRC - M2QM**] Angel Albavera-Mata; Divya Kumar *U Florida; Florida State* Integrating Experiment, Theory and Artificial Intelligence for Discovery and Characterization of Advanced Spin Crossover Complexes
10:00 AM	**B-III-4** [**EFRC - CPI**] Zoé O. G. Schyns; Pedro A. R. Moura* *U. Delaware* Engineering Solutions for Complex Plastics Waste Using Polymer Science and Catalysis	**C-III-4** [**EFRC - iCOUP**] Wenyu Huang *Ames; Iowa State* Diverting Polyolefin Hydrogenolysis to Olefins with Low Gas Formation via Reactor and Catalyst Design	**D-III-4** [**EFRC - GMCS**] Haiying Huang *Georgia Tech* Geo-processes in mineral carbon storage - fundamental challenges	**E-III-4** [**Hub - CHASE**] James Cahoon *UNC Chapel Hill* Designing Silicon Coatings and Interfaces to Enable Efficient Charge Transfer to Molecule Catalysts, Impart Long-Term Stability, and Control Product Distributions	**G-III-4** [**EFRC - SPECS**] Henry Kantrow; Yael Tsarfati* *Georgia Tech; Stanford/LBNL* Understanding and Manipulating the Nanoenvironment of Ribbon-Like (Soft) Polymer Semiconductors to Enable Photoelectrochemistry	**H-III-4** [**EFRC - CHiPPS**] Ricardo Ruiz *LBNL* Hierarchical Materials for High Precision EUV Patterning: Directed Self-Assembly, Area-Selective Deposition and their Advanced Characterization	**J-III-4** [**EFRC - CATS**] Susanne Stemmer *UC Santa Barbara* Novel Topological States in Thin Films of Topological Matter

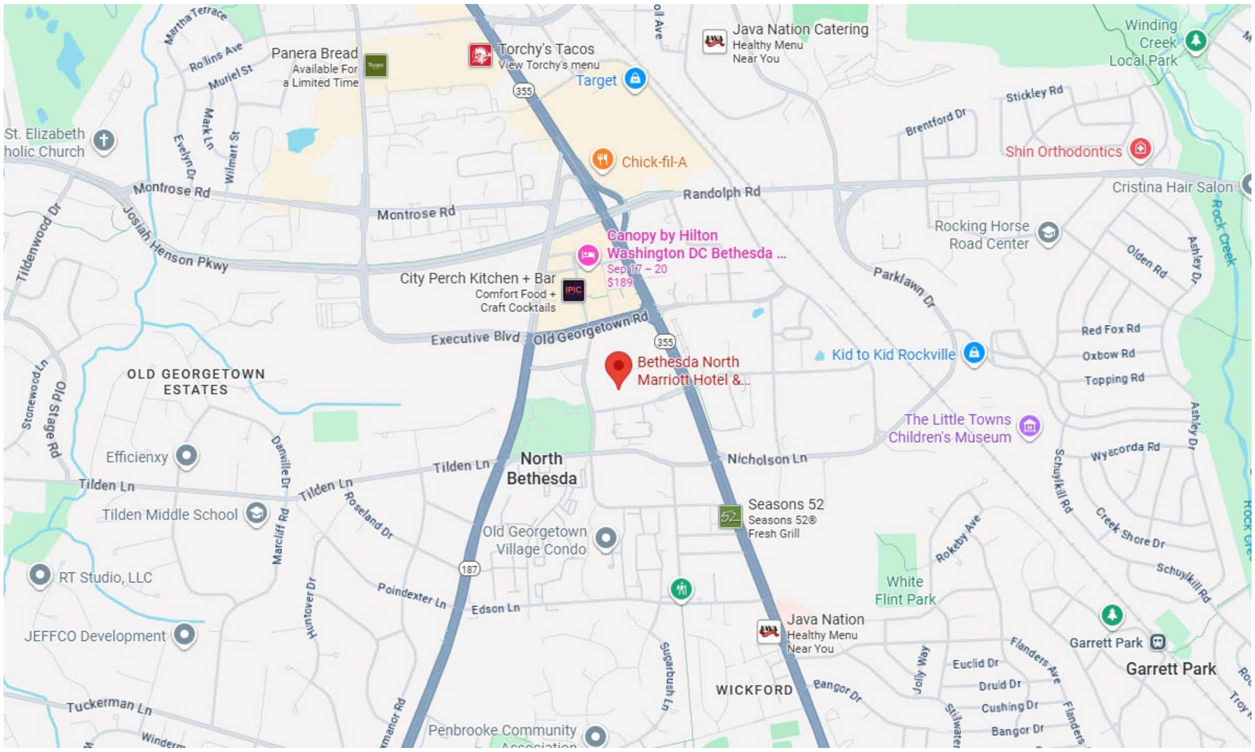
* After the presenter names indicates a Team Science Contest talk.

Tuesday, August 12, 2025: Talk Session IV from 1:30 – 3:10 pm

	B. Catalysis I	**C. Catalysis II**	**D. Energy Storage I**	**A. Advanced Manufacturing**	**I. Nuclear**	**H. Microelectronics**	**J. QIS I**
Room	***Forest Glen***	***Glen Echo***	***Salon F***	***Salon H***	***Brookside B***	***Brookside A***	***Brookside C***
Chair	***Chris Bradley***	***Viviane Schwartz***	***Craig Henderson***	***Jane Zhu***	***Philip Wilk***	***Shawn Chen***	***Claudia Mewes***
1:30 PM	**B-IV-1** [**Hub - LiSA**] Adam Nielander *SLAC* Exploring the basic science of durability and performance of CO$_2$ reduction solar fuels devices under diurnal operating conditions	**C-IV-1** [**EFRC - CPEC**] Paul Dauenhauer *U Minnesota* Implications and Methods of Programmable Catalysis for Energy	**D-IV-1** [**EFRC - FaCT**] Ji-young Ock; Amit Bhattacharya; Lauren B. Shepard* *ORNL; UC Santa Barbara; Penn State* Unlocking High Conductivity in Composite Electrolytes for Next Generation Energy Storage	**A-IV-1** [**EFRC - CHOISE**] Jinsong Huang *UNC Chapel Hill* Controlling the precise growth of halide perovskite crystals and interfaces	**I-IV-1** [**EFRC - TETI**] Saqeeb Adnan *Ohio State* Comprehensive Analysis of Thermal Transport in Defect-populated ThO$_2$	**H-IV-1** [**EFRC - reMIND**] R. Stanley Williams *Texas A&M–TEES* Discovery of Dynamical Electro-Thermal Transistors with High Signal Gain	**J-IV-1** [**CMS - C2SEPEM**] Steven G. Louie *LBNL / UC Berkeley* Study of novel phenomena in 2D materials with quantum many-body theories and exascale computing
1:50 PM	**B-IV-2** [**EFRC - CD4DC**] Massimiliano Delferro; Karena W. Chapman *ANL; Stony Brook* Metal-Organic Frameworks for the (de)Hydrogenation of Liquid Organic Hydrogen Carriers Enabled by Polarizable Metal Active Sites	**C-IV-2** [**EFRC - EPN**] Daniel V. Esposito; Rohini Bala Chandran *Columbia; U Michigan* Tuning Functional Properties of Oxide Coatings and their Influence on Nanoreactor Photosynthetic Redox Selectivity that is Crucial to Ensemble Performance	**D-IV-2** [**EFRC - BEES2**] Miguel Muñoz; Giselle de Araujo Lima e Souza; Michael Chen* *Case Western Reserve; Hunter College-CUNY; NYU* Quantum-Tuned Concentrated Hydrogen-Bonded Electrolytes for Enhanced Proton Transfer	**A-IV-2** [**EFRC - CHiPPS**] Christopher Ober *Cornell* Molecular design and its effects on high resolution patterning in EUV photoresists	**I-IV-2** [**EFRC - FUTURE**] Elena Romanovskaia *U Virginia* Overview of FUTURE Salt Effort	**H-IV-2** [**EFRC - Q-MEEN-C**] Alex Frano; Ivan K. Schuller *UC San Diego* Toward Efficient Neuromorphic Computing with Ion-Modified Quantum Materials	**J-IV-2** [**CMS - CPSFM**] Paul Kent *ORNL* Topology, band gaps, and magnetic structure of correlated 2D and quasi-2D quantum materials by exascale quantum Monte Carlo

	B. Catalysis I	**C. Catalysis II**	**D. Energy Storage I**	**A. Advanced Manufacturing**	**I. Nuclear**	**H. Microelectronics**	**J. QIS I**
2:10 PM	**B-IV-3** [**EFRC - 4C**] Jenny Yang *UC Irvine* Co-designing Sorbents and Catalysts for Integrated CO_2 Capture and Conversion	**C-IV-3** [**CCS - ECC**] Judit Zádor *SNL* Resolving the Coverage Dependence of Surface Reaction Kinetics with Machine Learning and Automated Quantum Chemistry Workflows	**D-IV-3** [**EFRC - HEISs**] Yan-Yan Hu *Florida State / National High Magnetic Field Laboratory* Atomic Insights into Proton Conduction in Phosphosilicate Glass	**A-IV-3** [**EFRC - REMAT**] Jeremiah A. Johnson *MIT* Efficient Manufacturing of Multigenerational Thermosets	**I-IV-3** [**EFRC - IDREAM**] Aurora Clark; Kevin Rosso *U Utah; PNNL* Radiation Enhances Gibbsite Dissolution Through Disruption of Ion Networks and Changes to Interfacial Speciation	**H-IV-3** [**EFRC - 3DFeM2**] Ece Gunay[1]; Drew Behrendt[2]; Albert Suceava[3]; Ian Mercer3; Quyen Tran[3]* *[1]Carnigie Mellon; [2]U Pennsylvania; [3]Penn State* Forging the Future of Ferroelectric Memory	**J-IV-3** [**CMS - NPNEQ**] Jacopo Simoni; Jonah Haber *U Wisconsin Madison; Stanford* Real-Time Excitation Dynamics in Out-Of-Equilibrium-Driven Materials with the INQ Code
2:30 PM	**B-IV-4** [**Hub - LiSA**] Theodor Agapie *Caltech* Impact of Organic Films on Electrocatalytic CO_2 Reduction with Metal Electrodes	**C-IV-4** [**EFRC - CCBC**] Josh Vermaas *Michigan State* Feeding the furnace: molecular-scale permeability and catalysis within bacterial microcompartments	**D-IV-4** [**Hub - ABC**] Linda Nazar *U Waterloo* Challenges and Opportunities for Aqueous Batteries	**A-IV-4** [**EFRC - CPI**] Brent Sumerlin *U Florida* Cross-Disciplinary Solutions for Plastics Circularity: Tailored Triggers and Thermal Depolymerization Mechanisms	**I-IV-4** [**EFRC - MSEE**] Santanu Roy *ORNL* Structure and Dynamics of Molten Salts: From Reactivity and Speciation to Network Formation	**H-IV-4** [**EFRC - reMIND**] John Ponis[1]; Kenna Ashen[1]; Michelle Smeaton2; Jialu Li[3]* *[1]Texas A&M; [2]NREL; [3]LBNL* Mapping Atomistic Structure to Neuromorphic Function Through Single-Crystal Neuronal Oscillators	**J-IV-4** [**CCS - ADEPTs**] Yuan Ping *U Wisconsin Madison* First-principles open quantum dynamics and transport for solids based on density-matrix formalism
2:50 PM	**B-IV-5** [**EFRC - 4C**] Francois Nkurunziza; Saudagar Dongare *U Louisville; Case Western Reserve* Alkali Cation Inhibition of Imidazolium-Mediated Electrochemical CO_2 Reduction on Silver		**D-IV-5** [**EFRC - UNCAGE-ME**] Janani Sampath *U Florida* Understanding Hydroxide Transport in Anion Exchange Membranes using Molecular Simulations	**A-IV-5** [**EFRC - CSSAS**] James J. De Yoreo *PNNL / U Washington* Fundamentals of Protein Assembly at the Materials Interface	**I-IV-5** [**EFRC - IDREAM**] Ryan Beck; Simantini Paul; Amita Bedar; Greg Felsted* *U Washington; U Utah; Notre Dame; PNNL* Understanding How Radiation Uniquely Transforms the Physicochemical Properties of Electrolytes	**H-IV-5** [**EFRC - Q-MEEN-C**] Pavel Salev; Elliot Kisiel; David Alspaugh* *UC San Diego* Inhomogeneities of Electrically Triggered Metal-Insulator Transitions in Neuromorphic Devices	**J-IV-5** [**CCS - NEREST**] Edward Valeev *Virginia Tech* Numerically-Exact Treatment of Dirac and Schrodinger Electrons in Molecules and Solids

HOTEL MAPS



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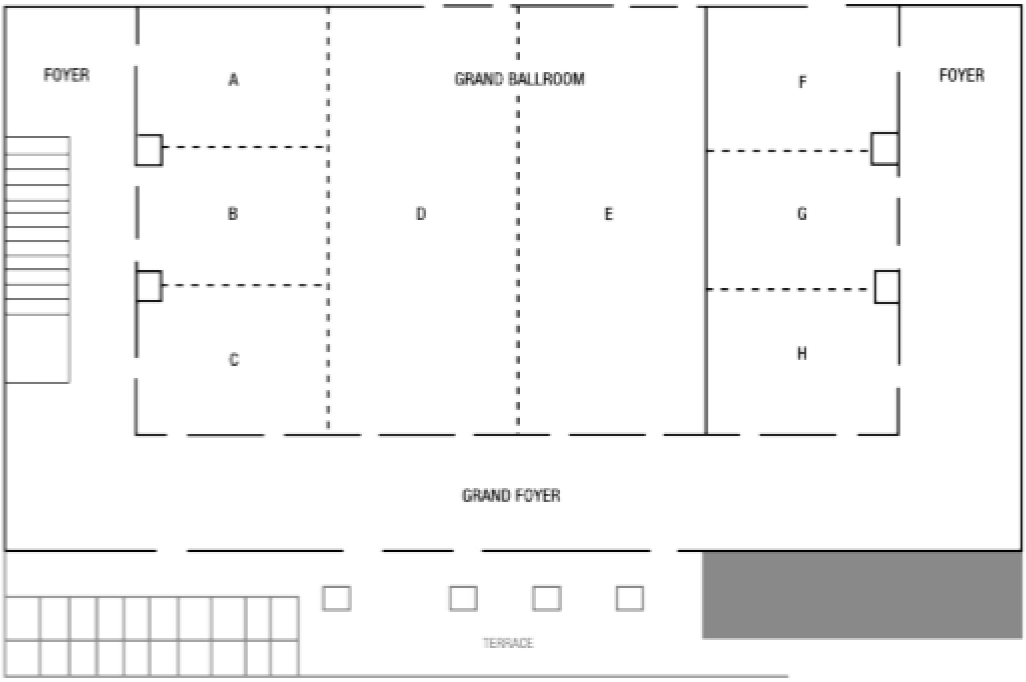
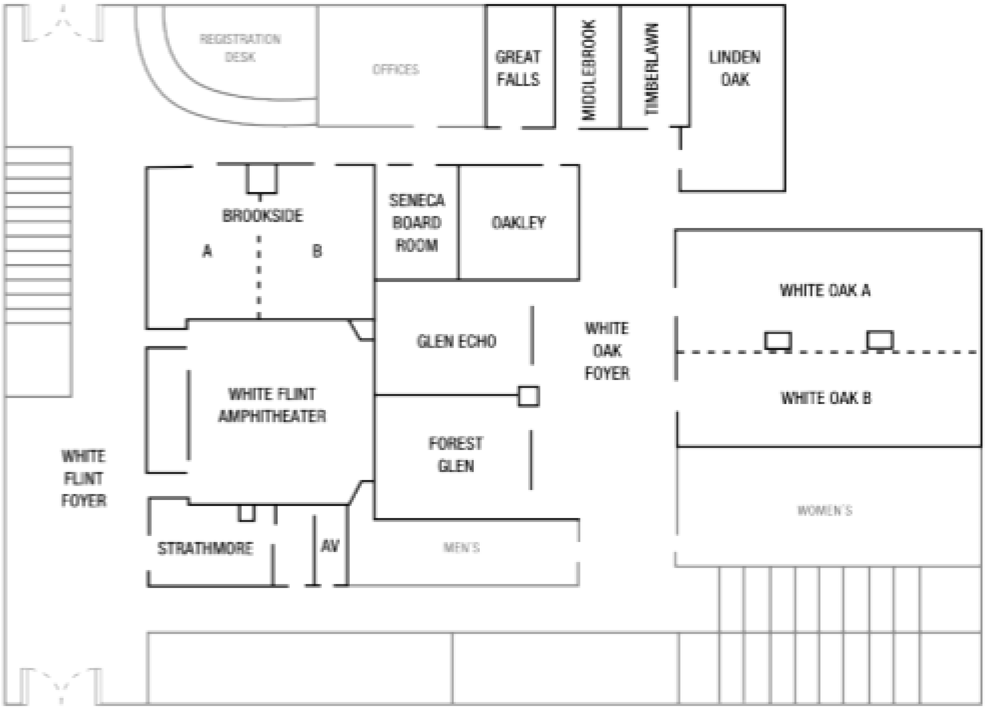
Meeting Rooms:
Brookside A, Brookside B, Brookside C, Forest Glen, Glen Echo, Grand Ballroom (Salon D/E), Salon F, Salon G, Salon H

MAIN LEVEL



LOWER LEVEL



*Note: the White Flint Amphitheater is now called Brookside C

TECHNICAL TALK ABSTRACTS

A. Advanced Manufacturing

Session II: Monday, August 11, 2025, 1:40 – 3:20 PM, Salon H

1:40 PM – Team Science Finalist

A-II-1: FROM FORCE-FIELD PARAMETERS TO PROGRAMMABLE NANOSTRUCTURES: INTEGRATED SIMULATION, ACTIVE LEARNING, AND EXPERIMENT FOR PEPTOID-BASED HIERARCHICAL MATERIALS

[EFRC - CSSAS] Alex Berlaga[1], Renyu Zheng[2,3], Kaylyn Torkelson[2], Xin Qi[2], Christopher D. Lowe[2], Helen Larson[2], Brandi M. Cossairt[2], Jim Pfaendtner[4], Chun-long Chen[2,3], Andrew L. Ferguson[1]
[1]University of Chicago; [2]University of Washington; [3]Pacific Northwest National Laboratory; [4]North Carolina State University

In CSSAS, we use sequence-defined peptoids to extrapolate principles from complex biomacromolecules to simplified sequence-defined molecular building blocks and precisely predict and control their assembly into hierarchical materials. We first introduce MoSiC-CGenFF-NTOID, a modular, CHARMM-compatible force field that ports 20 natural and 13 synthetic peptoid sidechains without bespoke parameterization, enabling routine all-atom molecular-dynamics (MD) studies of peptoids and hybrid systems at microsecond time scales (**Fig. A**). Building on this platform, we deploy an active-learning loop that couples MD-derived stability metrics with Gaussian-process regression and Bayesian optimization to identify sequences that mimic known self-assembling peptides (e.g., collagen-mimetic peptides) but whose peptoid substitutions raise triple-helical melting temperatures beyond natural Pro-Pro-Gly analogues. Results establish a hierarchical design framework to provide transferable force fields that furnish reliable energetics, promote active learning that accelerates sequence exploration for peptoids, and demonstrate multiscale simulations to bridge molecular chemistry to higher-order assembly and tertiary and quaternary structure engineering. In a parallel effort, we use DFT and MD calculations, along with experimentally derived design principles, to understand the molecular level peptoid interactions that give rise to the emergence of order, and to synthesize supramolecular hybrid nanostructures. Guided by simulation, we design a series of amphiphilic peptoid regulators that co-assemble with oleate-coated CdS quantum dots (QDs) to precisely tune the formation of peptoid-QD superlattices in non-aqueous solvents (**Fig. B**). We also manipulate the intramolecular folding of multiblock peptoids to control their assembly into Janus 2D nanosheets that template the growth of silica nanoparticles (**Fig. C**). In summary, we use peptoids to unravel the principles that orchestrate the self-assembly of high-information-content molecular building blocks across scales, from the molecular-level emergence of order to supramolecular hybrid hierarchies.

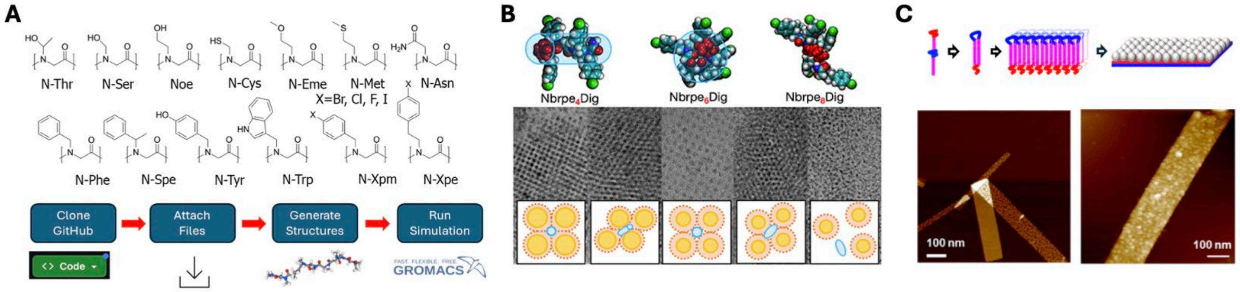


Figure* (*A*)** *Force field models peptoid-specific interactions.* (B***) *Peptoid-control of QD superlattice formation in chloroform. (C) Janus nanosheet formed by multiblock peptoids templates silicification.*

Contributions: A.B. and K.T. developed the peptoid force field. A.B. developed the active learning framework. R.Z. synthesized peptoids, characterized their assembly, and developed the Janus nanosheet system. X.Q. conducted DFT and MD calculations of peptoid structure in non-aqueous solvents. C.D.L. and H.L. co-assembled peptoids and QDs into superlattices.

2:00 PM – Team Science Finalist

A-II-2: MULTI-MATERIAL 3D PRINTING WITH FRONTALLY POLYMERIZABLE RESINS

[EFRC - REMAT] Brandon R. Clarke[1], Pranav Krishnan[2], Connor D. Armstrong[2], Yun Seong Kim[2], Ignacio Arretche[2], Derrick Sanders[2], Jeffrey S. Moore[2], Sameh H. Tawfick[2], Nancy S. Sottos[2], Jennifer A. Lewis[1]
[1]Harvard University; [2]University of Illinois Urbana-Champaign

This work is part of the U.S. Department of Energy's Energy Frontier Research Center (EFRC) for Regenerative Energy-Efficient Manufacturing of Thermoset Polymeric Materials (REMAT), a cross-institutional initiative aimed at revolutionizing the production, performance, and end-of-life management of thermoset polymers. Our collaborative research unites experts in mechanical engineering, polymer chemistry, and polymer physics at Harvard University and the University of Illinois Urbana-Champaign to develop next-generation additive manufacturing (AM) materials and platforms.

Our AM research is driven by the design and deployment of frontally polymerizable (FP) resins, particularly those incorporating dicyclopentadiene (DCPD) and cyclooctadiene (COD), which form low-energy, rapid-curing thermoset systems. These materials polymerize through self-sustaining reaction fronts which require a small thermal activation energy to initiate, significantly reducing cure energy consumption compared to traditional thermoset manufacturing. However, this resin system poses challenges for AM, including short working time and spontaneous polymerization. We address these hurdles through precise control of polymerization kinetics, catalyst/inhibitor ratios, and gelation behavior. Our team leverages copolymer chemistries to modulate network structure, achieving extended pot lives and printable gel states suitable for extrusion-based AM processes.

Our copolymer resin systems have been utilized in three novel multi-material AM platforms: Rotational Direct Ink Writing (DIW), Active Mixing DIW, and Morphogenic Growth Printing (**Figure 1a-c**). These FP AM techniques are capable of efficiently forming complex geometries with orders of magnitude thermomechanical property tunability (*e.g.* glass transition temperature, Young's modulus, and elongation at break) over multiple length scales through a single stream process. Multi-material FP AM offers a promising avenue for fabrication of functional, gradient-rich structures such as tendon-like hinges for soft robotic actuation and shape-memory components for biomedical devices, demonstrating performance tailored by design.

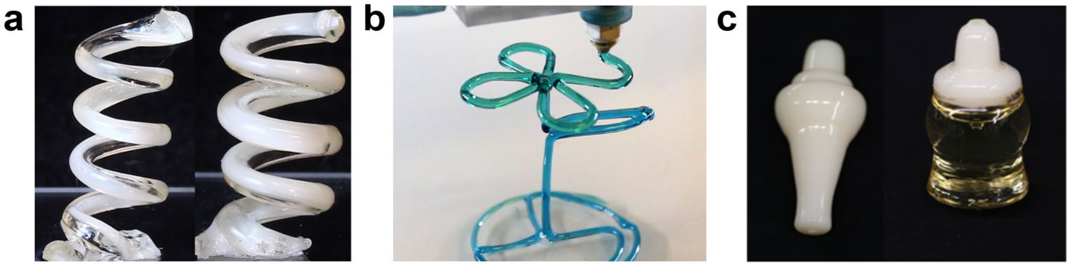


Figure 1. Multi-material parts fabricated using copolymer resin chemistries and additive manufacturing systems developed in REMAT. **(a)** Rotational DIW (R-DIW), **(b)** Active mixing DIW, **(c)** Multimaterial morphogenic growth printing (MMGP). Each manufacturing method allows varied modes of FP resin printing, providing access to a wide variety of possible structures using the same chemistries.

Contributions*:* J.A.L., S.H.T, N.R.S., and J.S.M. supervised the research. B.R.C., P.K., C.D.A., J.A.L., S.H.T., and N.R.S. conceptualized this work. B.R.C., P.K., C.D.A., Y.S.K., I.A., and D.S. conducted all experiments. All worked to draft figures and presentation of the work. J.A.L, S.H.T., N.R.S., and J.S.M. provided funding to graduate students and postdoctoral researchers.

2:20 PM

A-II-3: Controlling multiscale morphology of nanoscale self-assemblies with molecular clues and external fields

[EFRC - CSSAS] Oleg Gang[1,2], Daphne Shen[1], Daniel McKeen[1], Zohar Arnon[1], Yifeng Cai[3], Huat Thart Chiang[3], Nick Herringer[4], Feiyue Teng[2], Shuai Zhang[3,5], Lilo Pozzo[3], Andrew L. Ferguson[4], François Baneyx[5]

[1]Columbia University; [2]Brookhaven National Laboratory; [3]University of Washington; [4]University of Chicago; [5]Pacific Northwest National Laboratory

A wide range of optical, biological, electronic, and mechanical materials require precise 3D organization at the nanoscale. However, current bottom-up approaches are limited in architectural control, material diversity, and multiscale organization. Conventional nanofabrication is often costly and inefficient at generating 3D nanomaterials, and incompatible with many desired material classes. Our research explores the use of DNA-programmable self-assembly to create large-scale, hierarchically organized nano-architectures. We investigate control across multiple scales, from nanoscale to macroscale, tuning thermodynamic factors and molecular interactions to achieve desired morphology and reconfigure material states. We also explore how to guide material formation and its dynamic behavior via external fields (magnetic, acoustic) and surface patterning. For example, we developed a DNA-guided nanoparticle assembly approach using mobile DNA strands embedded in lipid bilayers on silica particles. Cholesterol-functionalized DNA anchors within the bilayer drive assembly, while maintaining lateral mobility. Using machine learning, we identified DNA design motifs that predict thermally tunable interparticle spacing and assembly outcomes. To enable thermally reconfigurable systems, we designed DNA-peptide hybrid shells with opposing thermal responses, allowing reversible control over nanoparticle interactions. We also established methods to grow arbitrarily shaped 3D DNA architectures over large areas via patterned guided nucleation and studied how 3D lattice morphology depends on surface properties. Additionally, we incorporated external fields by assembling DNA lattices on magnetic beads and aligning them using acoustic fields into macroscopic strings. These structures function as magnetically active fibers and exhibit programmable locomotion, combining mechanical responsiveness with DNA lattices that can incorporate nano-cargo with diverse functional applications.

2:40 PM

A-II-4: Modeling Crack–Void Interactions in Heterogeneous Composites Using Discrete Particle Dynamics and DeepONet Operator Learning

[EFRC - AIM] Venkatesh Ananchaperumal[1], Elham Kiyani[2], Gang Li[2], Srikanth Pilla[3], George Em Karniadakis[2]

[1]Clemson University; [2] Brown University; [3]University of Delaware

In this work, we address the challenge of modeling crack propagation in materials with varying geometries, a critical problem in predicting structural failure. We employ Constitutively informed Particle Dynamics (CPD), a particle-based simulation method that naturally captures crack initiation and propagation without relying on continuum approximations. The high-fidelity simulation data generated by CPD is used to train Deep Operator Networks (DeepONets), specifically the vanilla and Fusion DeepONet variants. These architectures are well-suited for learning mappings between function spaces, making them ideal for modeling complex, time-dependent phenomena such as fracture evolution.

We investigate two DeepONet variants (vanilla and Fusion) for predicting time-evolving crack propagation in specimens with varying geometries. Three representative cases are studied: (i) varying notch height without active fracture, and (ii)–(iii) combinations of notch height and hole radius where dynamic fracture occurs on irregular discrete meshes. The models are trained on 32 to 45 samples, using geometric inputs in the branch network and spatial-temporal coordinates in the trunk network.

Results show that Fusion DeepONet consistently outperforms the vanilla variant, providing more accurate predictions, particularly in non-fracturing scenarios. These findings underscore the power of combining physics-informed simulations like CPD with data-driven operator learning, enabling faster, geometry-aware predictions of crack propagation in composite materials and their interaction with voids and reinforcement.

3:00 PM

A-II-5: Manufacturing Patterned Materials Using Frontal Polymerization Instabilities: A Multiscale Mechanism-Based Model

[EFRC - REMAT] Donald Bistri[1], Anna Cramblitt[1], Ignacio Arretche[1], Lauren Chua[2], Philippe Geubelle[1], Rafael Gómez-Bombarelli[2]

[1]University of Illinois Urbana-Champaign; [2]Massachusetts Institute of Technology

Materials with hierarchical architectures that combine soft and hard material domains with coalesced interfaces possess superior properties compared to their homogeneous counterparts. In REMAT, we harnessed frontal polymerization spin-mode dynamics to autonomously fabricate patterned stiff crystalline and soft amorphous domains in poly(cyclooctadiene) with multiscale organization (Paul et al., Nature 2024). These front mode instabilities are associated with the processing conditions (e.g., initial temperature) and the chemistry (e.g., monomer-to-catalyst ratio) of the resin. While some success was achieved in the modeling of this process using a reaction-diffusion model, the phenomenological nature of the thermo-chemical model used in that work prevented the unified capture of the impact on the FP-driven instabilities of the relative concentration of monomer, catalyst and inhibitor present in the resin. We developed a multiscale mechanism-based 3-step model of FP that captures accurately the inhibition, initiation, and propagation steps of the ring-opening metathesis polymerization (ROMP) process and investigate the ability of the model to capture the effects of both the initial temperature and chemical composition of the resin on the thermo-chemical FP-driven instabilities (Bistri et al., JACS, 2024 & PNAS, 2025). While the propagation of the polymerization front is modeled at the continuum level by combining the reaction model with a thermal diffusion relation that incorporates the enthalpy of the exothermic polymerization reaction, some of the parameters entering the multiscale 3-step model are extracted from Density Functional Theory (DFT). The model is validated against experiments conducted with a resin system composed of cyclooctadiene, Grubbs initiator, and tributyl phosphite inhibitor.

Session IV: Tuesday, August 12, 2025, 1:30 – 3:10 PM, Salon H

1:30 PM

A-IV-1: Controlling the precise growth of halide perovskite crystals and interfaces

[EFRC - CHOISE] Jinsong Huang[1], Yanfa Yan[2], Adrienne Stiff-Roberts[3], Matthew C. Beard[4], Joseph M. Luther[4], Kai Zu[4], Volker Blum[3], David B. Mitzi[3]

[1]University of North Carolina at Chapel Hill; [2]University of Toledo; [3]Duke University; [4]National Renewable Energy Laboratory

Perovskite crystals serve as a platform for CHOISE to understand their fundamental properties and are also needed in applications including solar cells, light emitting diodes and detectors.

Solution growth of metal halide perovskites has enabled the development of these applications, but the crystal growth mechanism remains unclear, and the fundamental structure of conformal interface or quantum well has not been demonstrated. In a collaborative effort at CHOISE, we studied the mechanism of crystallization process at liquid-solid interface by examining two reported theorems, i.e. monomer (ions) attachment and cluster attachment. Our study identified a cooler interfacial region 1.5-4 micrometers from the crystal edge serving as a protective layer to hinder the attachment of particles with random orientations, which enables maintained crystal facet orientation. Using ligand-controlled facet growth, we synthesized perovskite crystals with record low point defect density, which showed record long spin lifetime. By understanding the temperature dependent solubility of cations, we demonstrated the formation of heterojunctions and quantum wells, and superlattices with coherent interfaces made of 4AMP-$MA_2Pb_3I_{10}$ (n=3) and 4AMP-$MAPb_2I_7$ (n=2) with various barrier thickness and well thickness. Type I band alignment at 4AMP-$MA_{n-1}Pb_nI_{3n+1}$ (n=2/n=3) heterojunction is confirmed by both computation and optical studies. The quantum wells have 2 to 10 times stronger emission than free-standing bulk crystals of the same composition.

1:50 PM

A-IV-2: Molecular design and its effects on high resolution patterning in EUV photoresists

[EFRC - CHiPPS] Christopher Ober[1], Chenyun Yuan[1], Kas Andrle[2], Sam Blau[2], Brett Helms[2], Frances Houle[2], Honggu Im[2], Oleg Kostko[2], Nitesh Kumar[2], Bernhard Luttgenau[2], Declan McCarthy[2], Cheng Wang[2], Qi Zhang[2], Maxx Muller[3], Dayhun Oh[3], Aung Paing[3], Kevin Zhao[3], Stacey Bent[4], Jacqueline Lewis[4], Long Viet Than[4], Cameron Adams[5], Rachel Segalman[5]

[1]Cornell University; [2]Lawrence Berkeley National Laboratory; [3]San Jose State University; [4]Stanford University; [5]University of California, Santa Barbara

Traditionally, photoresists have been made from polymers involving multiple components. As advanced, high-resolution patterning has moved to using shorter wavelength, EUV (13 nm) radiation two issues (chemical stochastics and secondary electron generation) have revealed significant limitations to this approach. As polymers have been traditionally produced, they consist of a mixture of molecules of different size, composition and sequence. Starting a decade ago metal oxide complexes have been explored and shown that the use of chemically identical patterning moieties with superior chemical stochastics that also explore sections of the periodic table with higher z elements that lead to improvement in secondary electron generation. This report describes three approaches to producing and controlling these characteristics in photoresists through: 1) the preparation and study of sequence defined, molecularly identical polypeptoids as patterning materials, 2) perovskite systems that alternate layers of organic and inorganic materials and 3) dry deposited alucones and related materials. Metals and organic components are being explored in these motifs in common. The most recent understanding of their patterning mechanism and their lithographic performance will be described.

2:10 PM

A-IV-3: Efficient Manufacturing of Multigenerational Thermosets

[EFRC - REMAT] Kwangwook Ko[1], Zhenchuang Xu[2], Xuyi Luo[3], Yasmeen AlFaraj[1], Edgar B. Meija[2], Hayden E. Fowler[4], Suong T. Nguyen[1], Yuyan Wang[1], Kecheng Wang[2], Benjamin A. Suslick[2], Shuyi Zhang[1], Yong Min Kim[3], MJ Lee[2], Yuran Shi[3], Yan Xia[3], Jeffery W. Baur[2], Jeffrey S. Moore[2], Samuel C. Leguizamon[4], Nancy R. Sottos[2], Jeremiah A. Johnson[1]
[1]Massachusetts Institute of Technology; [2]University of Illinois Urbana–Champaign; [3]Stanford University; [4]Sandia National Laboratories

Polydicyclopentadiene (pDCPD) thermosets are valuable for high-performance structural applications, yet their permanent covalent network structures have historically precluded chemical recycling, which limits circularity and contributes to energy- and resource-intensive waste. Addressing these challenges, we introduce a suite of strategies that enable low-energy manufacturing and multi-cycle chemical recycling of pDCPD thermosets without compromising thermomechanical performance. Central to this approach is Frontal Ring-Opening Metathesis Polymerization (FROMP)—a self-propagating, energy-efficient curing process compatible with additive manufacturing workflows. We integrate cleavable additives, including cleavable comonomers (CCs) and strand-fusing cross-linkers (SFCs), with activatable repeat units to achieve deconstructability of pDCPD thermosets at minimal additive loadings. These functionalities allow for targeted bond cleavage and recovery of soluble oligomeric fragments. Through one-pot deconstruction-reactivation protocols, functional groups such as norbornenes and furans are retained or installed in situ, enabling reincorporation of recycled fragments into new thermoset formulations. Incorporation of 40–45 wt. % recycled content per cycle has been demonstrated across three to five generations, with full retention of thermomechanical properties including glass transition temperature and stiffness. Overall, this material platform could significantly reduce energy demand during both manufacturing and end-of-life processing, contributing to decarbonization of industrial materials and promoting circular economy models. The combined advances in molecular design, energy-efficient curing, and chemical reusability establish a scalable pathway for next-generation thermosets that meet stringent performance requirements while improving sustainability metrics.

2:30 PM

A-IV-4: Cross-Disciplinary Solutions for Plastics Circularity: Tailored Triggers and Thermal Depolymerization Mechanisms

[EFRC - CPI] Rhys W. Hughes[1], Tanmoy Maity[1], Timothée Sergent[1], Alex H. Balzer[2], Isabella S. Zastrow[1], Mansi S. Patel[1], Leah M. Baker[1], Payson M. Keown[1], Lexie Handlin[3], Frank A. Leibfarth[3], LaShanda T. J. Korley[2], Brent S. Sumerlin[1]
[1]University of Florida; [2]University of Delaware; [3]University of North Carolina at Chapel Hill

Advancing the chemical transformation of plastic waste into valuable building blocks requires new approaches to overcome the intrinsic stability of commodity plastics. Strategies that allow for controlled depolymerization under milder conditions offer promising routes for converting plastic waste into monomer feedstocks for manufacturing. We explore integration of latent triggers at

the ends of polymer backbones or as pendent functionalities to promote efficient depolymerization. By embedding thermally labile comonomers into polystyrene, we generate backbone radicals upon heating that drive unzipping and monomer recovery. This method achieves up to 91% conversion to styrene under solvent-free conditions and at substantially lower temperatures than those typically required for pyrolysis. Additionally, modification of commercial poly(methyl methacrylate) with decarboxylative triggers enables closed-loop depolymerization and monomer reuse, extending these strategies to high-molecular-weight materials and networks. Ongoing work seeks to lower the energetic barrier to depolymerization further, with new triggering chemistries emerging from molecular design efforts. These advances benefit from a multidisciplinary approach, drawing on small-molecule reactivity, polymer synthesis, and rigorous materials characterization, to design responsive systems that interface performance with sustainability. This modularity of trigger placement and mechanism emphasizes two key tenets of our program: designing plastics with their end-of-life in mind and developing new chemistry-centric approaches to deal with existing plastic waste. This capability diverts waste from disposal and enables the regeneration of key monomers that can re-enter manufacturing streams. These depolymerization pathways represent a compelling strategy for recovering monomers from existing plastics and highlight the role of synthetic control in creating sustainable inputs for future materials production.

2:50 PM

A-IV-5: Fundamentals of Protein Assembly at the Materials Interface

[EFRC - CSSAS] James J. De Yoreo[1,2], Ying Xia[2], Zhiyin Zhang[3], Chenyang Shi[1], Hao Shen[2], Charlotte Zhao[4], Timothy C. Moore[4], Haoyuan Shi[1], Mingyi Zhang[1], David Baker[2], Christopher. J. Mundy[1,2], Sharon Glotzer[4], Shuai Zhang[1,2], F. Akif Tezcan[3]
[1]Pacific Northwest National Laboratory; [2]University of Washington; [3]University of California, San Diego; [4]University of Michigan

From harvesting solar energy, to purifying water, to capturing CO_2, living organisms have solved some of the most vexing challenges now facing humanity. They have done so by creating a vast library of proteins that can assemble into hierarchical structures to control the transport and transformation of matter and energy and direct the formation and organization of inorganic components to form hybrid materials. While the high information content contained within the intricate sequences of proteins is crucial for accomplishing these tasks, both assembly and the formation of hybrid materials are nonetheless constrained to proceed according to the physical laws that govern all such processes. One of the key challenges in producing hybrid materials for energy technologies, is that of understanding how to manipulate those laws to create coherent protein-inorganic interfaces by design. Using a combination of in situ atomic force microscopy and coarse grain simulations, we investigate the assembly of both de novo designed proteins and natural proteins engineered to assemble into extended structures at the interface with an inorganic crystal surface. The results reveal the importance of surface charge, facet-specific binding, solvent organization, and, more generally, the balance of protein-substrate-solvent interactions in determining how proteins assemble at inorganic surfaces. These findings demonstrate the vast potential of protein design and engineering in materials science and elucidate the mechanisms by which the interactions between biomolecules and materials leads to unique materials and morphologies.

B. Catalysis I

Session I: Monday, August 11, 2025, 9:10 – 10:30 AM, Forest Glen

9:10 AM

B-I-1: Elucidating the Geometric and Electronic Structure of a Fully Sulfided Analog of an Anderson Polyoxomolybdate Cluster for photo-, electro-, and thermalcatalytic hydrogenation

[EFRC - CD4DC] S. M. Gulam Rabbani[1], Zhihengyu Chen[2], Jingyi Sui[3], Joseph T. Hupp[3], Karena W. Chapman[2], Rachel B. Getman[1]
[1]The Ohio State University; [2]Stonybrook University; [3]Northwestern University

The catalytic activity of transition metal sulfide (TMS) clusters in small molecule activation, redox transformations, and charge transfer has inspired the design of novel TMS-based materials for energy-related catalysis and chemical applications. Polyoxometalates (POMs), known for their structural diversity, can in principle be transformed into TMS clusters; however, fully sulfided analogs are rarely isolated, likely due to the strong tendency of uncapped TMS clusters to agglomerate. Here, we report the geometric and electronic structure of a capping ligand-free fully sulfided analog of heptamolybdate Anderson POM $[Mo^{VI}_7O_{24}]^{6-}$, synthesized through the sulfidation of a nanoconfined POM secured within a porous Zr-metal organic framework (NU-1000). A combined computational and experimental analysis indicates that the sulfided counterpart of the Anderson POM is geometrically and electronically more sophisticated than the parent POM. Comparison of experimental pair distribution function (PDF) data with molecular simulations confirms that, unlike the oxygen-only $[Mo^{VI}_7O_{24}]^{6-}$ cluster, the $[Mo^{IV}_7(m_3\text{-}S)_6(m_2\text{-}SH)_6(S_2)_6]^{2-}$ polythiometalate (PTM) exhibits a diverse array of sulfur anions (S^{2-}, HS^-, S_2^{2-}). DFT calculations indicate that H_2S acts as a reducing agent, and together with terminal disulfide (S_2^{2-}) ligands in the PTM structure, facilitates the complete reduction of all seven Mo^{VI} centers in the parent POM to Mo^{IV}. These findings are supported by X-ray photoelectron spectroscopy (XPS), which confirms exclusive Mo^{IV}, and elemental analysis, which shows quantitative sulfur incorporation. Difference envelope density (DED) mapping further reveals that the PTM clusters are spatially confined within the MOF pores, preventing agglomeration and preserving molecular integrity.

9:30 AM

B-I-2: Conductive ruthenium oxide films with surface-orientation control as experimental models for oxygen evolution reaction studies

[EFRC - CEDARS] Mengxin Liu[1], Brady Bruno[2], Austin Reese[2], Ghanshyam Gyawali[1], Ikenna Chris-Okoro[1], Lei Zhang[3], Swapnil Nalawade[1], Sheilah Cherono[1], Simon Gelin[4], Maria Maalouf[4], Soyoung Kim[5], Jin Suntivich[2], Shyam Aravamudhan[1], Geoffroy Hautier[3], Ismaila Dabo[4], Junko Yano[5], Ethan Crumlin[5], Yang Shao-Horn[6], Tanja Cuk[7], Dhananjay Kumar[1]

[1]North Carolina A&T State University; [2]Cornell University; [3]Dartmouth College; [4]Carnegie Melon University; [5]Lawrence Berkeley Laboratory; [6]Massschusettes Institute of Technology; [7]University of Colorado Boulder

This presentation reports on a study of ruthenium oxide (RuO_2) films from the perspectives of synthesis, structure-property connection, and electrocatalytic properties. The goal of CEDARS is to understand the oxygen evolution reaction (OER) mechanism on metal oxides by aligning the synthesis, electrochemistry, in-situ spectroscopy, and first-principles modeling toward fundamental studies. RuO_2 is one of the well-known OER electrodes. However, understanding their OER mechanism has not been straightforward, as material variation affected the characterization outcomes. The Center for Electrochemical Dynamics and Reactions on Surfaces (CEDARS) utilizes thin-film syntheses to build a well-characterized RuO_2 model. Pulsed laser deposition, molecular beam epitaxy, and atomic layer deposition methods were used to grow RuO_2 films with controlled thicknesses, orientation, and crystallinity. Transport and electrocatalytic measurements show that the conductivity, nature of charge carriers, and electrochemistry are strongly dependent on the films' orientations. Select RuO_2 films were studied using electrochemical atomic force microscopy and non-linear spectroscopy. The surface symmetry of the RuO_2 film was found to depend on the applied potential. This observation was rationalized through surface water polarization and dissociation on RuO_2, a picture that was verified via the first-principles modeling of the dehydrogenation of water. This collaborative effort enables the assignment of the electrochemical and spectroscopic response of RuO_2 to interfacial water activation, a step that precedes the OER cycle. The presentation will conclude by highlighting the broader impact of CEDARS workforce development.

9:50 AM

B-I-3: Beyond-DFT techniques for electrochemistry, accelerated by machine learning

[CCS - BEAST] Michelle Kelley[1], Josh Quinton[1], Jacob Clary[2], Taylor Aubry[2], Daniel Weinberg[3], Cooper Tezak[4], Sophie Gerits[4], Andrew Diggs[4], Ben Rich[4], Abdulaziz Alherz[4], Nima Karimitari[5], Teerchote Pakornchote[5], Christopher Sutton[5], Charles Musgrave[4], Mauro Del Ben[3], Derek Vigil-Fowler[2], Ravishankar Sundararaman[1]

[1]Rensselaer Polytechnic Institute; [2]National Renewable Energy Laboratory; [3]Lawrence Berkeley National Laboratory; [4]University of Colorado Boulder; [5]University of South Carolina

First-principles calculations for electrochemistry require both accurate electronic structure beyond density-functional theory (DFT) and treatment of the electrochemical environment including the effects of solvation and electrode potential. We have developed efficient, well-

scaling implementations of the random-phase approximation (RPA) for accurate electronic structure, capable of handling simulations of hundreds of atoms necessary for simulating electrochemical surfaces. We have prototyped a universal neural network functional approximation technique for learning nonlocal classical and electronic density-functionals, establishing a pathway towards first-principles liquid structure simulations for the electrolyte environment. Since this combination of accurate electronic and liquid structure simulations is computationally expensive for high-throughput electrocatalyst design, we have also developed a suite of data-driven and machine learning approaches to accelerate their application. We released BEAST DB with an initial dataset of over 20,000 grand-canonical DFT simulations of solvated adsorbates on surfaces spanning several classes of catalysts and electrochemical reaction pathways, and we are currently calculating an expanding subset of these systems with RPA. We have developed a graph neural network technique to predict higher-level electronic structure using DFT electronic structure as an input, which will enable rapid estimation of beyond-DFT energies using the DFT inputs available for the entire BEAST DB. Finally, we are also leveraging these large datasets of electrochemical simulations to fine tune machine-learned interatomic potentials for electrochemistry to enable even more rapid exploration of reaction pathways.

10:10 AM

B-I-4: Localized Active Space State Interaction Singles method

[CCS - ExaPUC] Matthew Hermes[1], Valay Agarawal[1], Rishu Khurana[1,2], Cong Liu[2], Christopher Knight[2], Laura Gagliardi[1]

[1]University of Chicago; [2]Argonne National Laboratory

When modeling multimetallic transition metal compounds, the active space can quickly become intractable. Fragmentation methods such as localized active space self-consistent field (LASSCF) express the active space wavefunction as an antisymmetrized product of product wavefunctions. The price of approximation is the lack of any interfragment correlations, which is necessary to low-lying electronic structure of multimetallic compounds. We introduce an automated method for recovering such interfragment correlation, and producing density matrix renormalization group quality wavefunctions, while retaining wavefunction interpretability.

Session II: Monday, August 11, 2025, 1:40 – 3:20 PM, Forest Glen

1:40 PM

B-II-1: Enhancing the Development of 3d transition metal photocatalysts with X-ray spectroscopies

[EFRC - BioLEC] Kelly J. Gaffney[1], Amy A. Cordones-Hahn[1], Reagan Hooper[1], Sumana Raj[1], Ben Poulter[1], Kacie Nelson[1], Sujia Dong[2], Felipe Curtolo[2], Elena Jakubikova[3], Marwa Al Rammal[3], Mariam Barakat[3]

[1]SLAC National Accelerator Laboratory; [2]Northeastern University; [3]North Carolina State University

The BioLEC EFRC focuses on developing and improving light-powered catalysts, and the reactions they facilitate, to generate specific and valuable chemical products from more stable and abundant starting materials. The development of photocatalysts with first-row transition metals has been an important component of this mission. A key distinction between 3d transition metal photocatalysts, and the more prevalent 4d and 5d analogues, is the central role of metal-centered (MC) electronic excited states in their photophysics and photochemistry. These MC states often lead to quenching of the optically generated charge transfer (CT) excited states used in photoredox catalysis, reducing their effectiveness. These MC states also provide new pathways to photocatalytic activity, as demonstrated by BioLEC studies of Co and Ni based photocatalysts. I will provide an update on research efforts to understand the role MC excited states play in determining the photocatalytic activity of Fe, Co, and Ni based photocatalysts. I will focus on two topics: (1) X-ray resonance Raman Spectroscopy studies of the MC electronic excited states of Fe carbene photocatalysts and (2) combined time-resolved X-ray Solution Scattering and X-ray Emission Spectroscopy investigations of the photophysical dynamics of Ni cross-coupling photocatalysts. The investigation of Fe carbene complexes clearly shows that the CT excited state lifetime is poorly correlated with the energy of the MC excited states and the Ni photocatalyst studies have characterized the yield and structure of the triplet MC excited state formed from the optically generated MLCT excited state.

2:00 PM

B-II-2: Advanced Correlative Microscopy Reveals Links Between Nanoreactor Photosynthetic Properties and their Yields for Electronic Charge Separation

[EFRC - EPN] Justin B. Sambur[1], Shane Ardo[2]
[1]*Colorado State University;* [2]*University of California, Irvine*

EPN EFRC aims to understand, predict, and control the ensemble activity, selectivity, and stability of inorganic nano-to-micro-particles driving photosynthetic reactions. Causes of electronic charge separation relevant to real-world, low-photon-flux operation are being revealed with the help of operando multimodal microscopies. Correlative optical, electron, scanning-probe, and photoelectrochemical microscopies have indicated the importance of lattice, dopant, surface, and cocatalyst properties. Operando mid-infrared scattering-type scanning near-field optical microscopy (SNOM) was used in conjunction with scanning photoelectrochemical microscopy (SPCM) to map water adsorption to distinct lateral facets of individual $BiVO_4$ particles that are also, in general, the most active for light-driven water oxidation. Transmission electron microscopy (TEM) measurements spanning energy dispersive X-ray spectroscopy (EDS), electron energy loss spectroscopy (EELS), and 4D scanning TEM uncovered dopant site occupation in $SrTiO_3$ particles at the single atom-level and mapped charge polarization near Pt cocatalysts, which each correlate with activity for light-driven water reduction. Moreover, EELS methods were developed to deconvolute photoinduced thermal versus electronic ultrafast dynamics revealing light-driven charge accumulation at surface trap sites. Single-molecule fluorescence microscopy was additionally coupled to kinetic Monte Carlo data analysis to reveal that energy transfer yields from ZnO to surface-bound molecules vary greatly between particles. Together, these efforts showcase our ability to resolve charge separation and transport in individual particles, which will help to clarify how charge sequentially accumulates at well-defined reaction centers to impart overall multiple-electron/proton-transfer reactions of relevance to meeting EPN aims.

2:20 PM

B-II-3: Polarons report the composition of local nanoenvironments of the polymer–electrolyte interphase in soft semiconductor energy conversion and storage

[EFRC - SPECS] Chad Risko[1], Erin Ratcliff[2], Megan R. Brown[1], Zhiting Chen[3], Shuya Li[4], Jonathan R. Thurston[5], William P. Kopcha[4], Joel Bombile[1], Sa Suo[6], Bo Dong[6], Arianna Magni[7], Obadiah G. Reid[5], Neal R. Armstrong[3], Alberto Salleo[7,9], Tianquan Lian[6], Michael F. Toney[5], Andrew J. Ferguson[4], Elisa M. Miller[4], Ann L. Greenaway[4], Hong Li[3], Jean-Luc Bredas[3], Matthew Bird[8]
[1]University of Kentucky; [2]Georgia Institute of Technology; [3]University of Arizona; [4]National Renewable Energy Laboratory; [5]University of Colorado Boulder; [6]Emory University; [7]Stanford University; [8]Brookhaven National Laboratory; [9]SLAC National Accelerator Laboratory

The Center for Soft Photoelectrochemical Systems (SPECS) focuses on understanding the fundamental factors that control charge and matter transport processes that underpin energy conversion and storage technologies across spatiotemporal scales in scalable, durable, π-conjugated polymer materials. As part of our efforts, SPECS is providing significant advances in revealing the nature of polarons in semiconducting polymers as a function of the varying chemical environment of the polymer–electrolyte interphase, a longer length scale description than discrete interfaces due to polymer swelling and dynamics in the presence of an electrolyte. The interphase stores charge with long lifetimes due to Coulombic interactions between polarons and supporting counterions and solvent from the electrolyte, where physicochemical variables such as the dielectric field, chain (chromophore) structure, interactions of polarons with counterions of varying hardness and valency, and polymer microstructure each can impact the nature and transport of polarons. Efforts that will be described in this talk include multiple spectroelectrochemical methods and theoretical efforts to reveal the impact of electrochemical doping and ultimately serve as signatures to drive charge transfer reactions such as solar fuel production. A key point of consideration is catalytic site attachment to the polymer, towards understanding charge transfer between a polymer and a catalyst. Significant challenges remain, however, to provide the appropriate understanding of the factors that control that efficiency, so as to provide design guidelines for future energy conversion platforms, and pathways to manipulate soft matter that might be integrated into other photoelectrochemical platforms.

2:40 PM – Team Science Finalist

B-II-4: A Solar-Driven Electrochemical/Photothermocatalytic Process for CO_2 conversion to C_6 oxygenates: An Assembly of Coupled Microenvironments

[Hub - LiSA] Matthew Salazar[1,2], Aisulu Aitbekova[1,2], Katherine Yan[1,3], Jonas C. Peters[1,2], Thomas F. Jaramillo[1,3], Harry A. Atwater[1,2], Theodor Agapie[1,2], Alexis T. Bell[1,4]
[1]Liquid Sunlight Alliance; [2]California Institute of Technology; [3]SLAC National Accelerator Laboratory; [4]Lawrence Berkeley National Lab

Coupling CO_2 electrolysis to a thermocatalytic process is a promising approach to convert CO_2 into products beyond C2 hydrocarbons. Herein, we demonstrate the use of a co-design approach to coupled microenvironments to generate sustainable liquid fuels, advancing LiSA's mission. Specifically, we present a solar-driven, two-step process that converts CO_2 into 2-Methyl-2-pentenal, a C6 oxygenate and food additive, and a flavoring additive (***Figure 1***). In the first step, a photovoltaic-driven membrane electrode assembly (MEA) with a catalyst area of 5 cm^2 converts CO_2 and water into a mixture of carbon monoxide, hydrogen, and ethylene. In the second step, the MEA outlet stream is sent to a photothermocatalytic reactor where it is converted into 2-Methyl-2-pentenal. To obtain the desired product distribution from the CO_2 electrolyzer, we designed a copper/silver (Cu/Ag) tandem electrode. CO_2 is first reduced to CO on Ag, and CO is subsequently reduced further on Cu to C_2H_4. From the CO_2RR coupled assembly, factors such as varying Ag and Cu ratios and operating parameters (e.g., membrane type, cell compression, and cell pressure) were considered. To perform the photothermocatalytic step, we developed a dual-bed catalyst consisting of phosphine ligand functionalized rhodium (Rh) on SBA-15 and titania (TiO_2). The Rh catalyst converts ethylene, carbon monoxide, and hydrogen to propanal via ethylene hydroformylation. Different co-impregnation hydroformylation catalysts were screened under simulated MEA outlet streams to maximize ethylene conversion to propanal. The best-performing ligand suppresses the formation of undesired ethane and yields an average ethylene-to-propanal conversion of 15 % with propanal selectivity > 95% (< 5% selectivity to ethane). The TiO_2 catalyst converts propanal to 2-Methyl-2-pentenal with an average yield of 3.2%. The development of the photothermocatalytic microenvironment involved tailoring catalyst architectures to match operating pressure and temperature. Our team has successfully demonstrated the solar-driven operation of such a system. To increase the production of 2-methyl-2-pentenal, a larger production of ethylene is needed. As such, we scaled up the MEA area from 5 cm^2 to 25 cm^2. With this larger cathode area, issues such as pressurization and anode degradation were more evident than in the 5 cm^2 MEA. More investigation is needed to address challenges with scale-up within the context of taking a co-design approach to couple electrocatalytic and thermocatalytic processes.

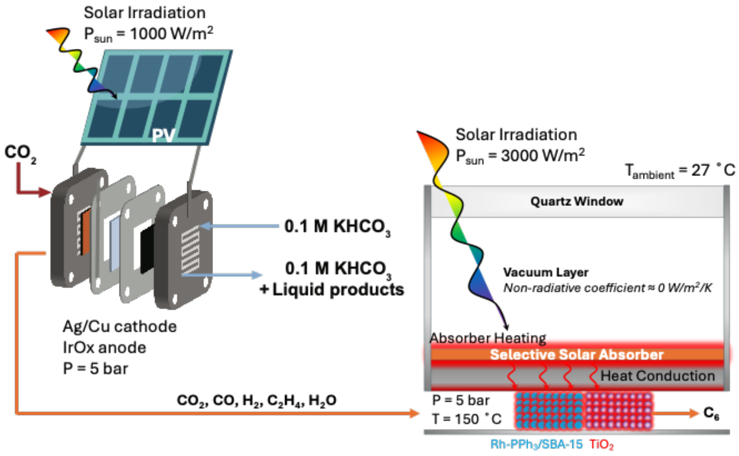


Figure 1. A solar-driven tandem system converts CO_2 into a C_6 oxygenate.

Contributions: M.S., A.A., and K.Y. contributed equally to this work.

3:00 PM – Team Science Finalist

B-II-5: EXTENDING CHARGE-SEPARATED-STATE LIFETIME IN NANOCRYSTAL–MOLECULE HYBRIDS VIA RATIONAL MOLECULAR DESIGN

[EFRC - EPN] Olivia F. Bird[1], Faith A. Flinkingshelt[2], Sophia M. Click[1], Hyuna Kwon[3], Della Hagemann[4], Kenneth M. Drbohlav[4], Evan K. Gowdy[4], Yisrael M. L. Lamb[4], Tadashi Ogitsu[3], Jenny Y. Yang[2], Kenneth A. Miller[4], Gordana Dukovic[1]

[1]University of Colorado Boulder; [2]University of California, Irvine; [3]Lawrence Livermore National Laboratory; [4]Fort Lewis College

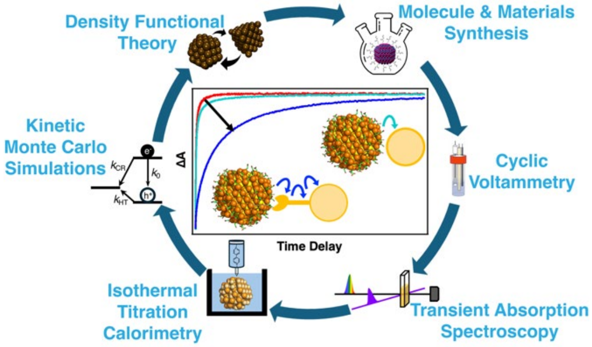


Figure 1: Illustration of lifetime lengthening through design of specific binding groups to molecular charge acceptors, with outer cycle illustrating the techniques used in this work.

Most reactions of practical importance — including those that constitute water splitting — require that multiple charges be accumulated at a single reaction site. Nanocrystal–molecule hybrids are attractive systems for driving such reactions with light. They benefit from the remarkable light-harvesting properties of semiconductor nanocrystals and the synthetic tunability of molecular catalysts. Such systems have previously been demonstrated to achieve near-unity quantum yields for charge separation, but subsequent catalytic yields remain low due to the short lifetimes (~10s of nanoseconds) of charge-separated states. Here, we report the synthesis of a suite of rationally designed molecular charge acceptors, including electron acceptors[1], hole acceptors[2], and hydrogen evolution electrocatalysts[3], for binding to nanocrystals with different anionic donor linker groups to tune rates of charge transfer and recombination. The energetics and thermodynamics of nanocrystal–molecule binding were rigorously evaluated using isothermal titration calorimetry[1] and density functional theory calculations.[3] Transient absorption spectroscopy revealed that our molecular acceptors extend the charge-separated-state lifetime by multiple orders of magnitude, from nanoseconds to microseconds, while maintaining high yields for charge separation.[1,2] We demonstrated hydrogen evolution activity from our catalysts, both electrocatalytically and photocatalytically.[3] We also conducted kinetic Monte Carlo simulations to predict the effects that the charge-transfer dynamics observed in these new systems will have on reactivity.[1] Simulations identified conditions where significant lifetime extension could improve overall photocatalytic yield, providing guidance on new molecular targets. This work represents a step forward in using rational molecular design, and particularly tunable binding, to control charge-separation dynamics.

Contributions: Molecular and materials syntheses were conducted by F.A.F, D.H., K.M.D., E.K.G., K.A.M., and S.M.C. Electrochemical experiments were conducted by F.A.F. Spectroelectrochemical experiments were conducted by F.A.F and Y.M.L.L. Transient absorption spectroscopy experiments were conducted by S.M.C. and O.F.B. Isothermal titration calorimetry experiments and kinetic Monte Carlo simulations were conducted by O.F.B. Density functional theory calculations were performed by H.K. All authors contributed to experimental design and conception.

References: (1) Bird, *et al.*, *The Journal of Physical Chemistry C*, **2025**, *129*, 5556, DOI: 10.1021/acs.jpcc.5c00740. **(2)** Click, *et al.*, **2025**, *under review*. **(3)** Flinkingshelt, *et al.*, *Energy & Fuels*, **2025**, *39*, 2196, DOI: 10.1021/acs.energyfuels.4c05559.

Session III: Tuesday, August 12, 2025, 9:00 – 10:20 AM, Forest Glen

9:00 AM

B-III-1: Functionalization of Post-Consumer Plastics into Novel Products

[EFRC - iCOUP] Anne LaPointe[1], Megan Fieser[2], Geoffrey Coates[1], Moritz Kränzlein[1], Shilin Cui[1], Jaqueline Lopez[2], Zachary Wood[2], Tyeshia Sapp[2], Bailey Eberle[3], Xuchun Wang[4], Samuel Hunt[4], Sarah Barber[3], Mary Dana Czarinah Cheng-Tan[2], Tommy Yunpu Zhao[5], Frédéric Perras[5,6], Massimiliano Delferro[4], Byeongdu Lee[4], Mark Dadmun[3]

[1]Cornell University; [2]University of Southern California; [3]University of Tennessee; [4]Argonne National Laboratory; [5]Ames National Laboratory; [6]Iowa State University

The development of selective methods for converting post-consumer plastics into valuable products is critical to addressing the global plastics waste challenge. Although catalytic upcycling into small-molecule products such as lubricants and surfactants has shown promise, a complementary approach is to selectively functionalize polymers without substantial depolymerization. In one application of this method, high-density polyethylene (HDPE) was reacted with organic peroxides to generate secondary macroradicals which could be trapped to introduce functionality or grafting. This metal-free route is compatible with post-consumer plastics and utilizes commercial peroxides. This strategy was used for the synthesis of polyethylene-graft-polypropylene copolymers (PE-graft-iPP) for use as compatibilizers for mixed polyolefin waste. Reaction of a 30:70 HDPE:iPP blend with organic peroxides at 160–180 °C produced PE-graft-iPP copolymers that effectively compatibilized HDPE/iPP blends at loadings as low as 2.5 wt. %. Another application uses silylium catalysis to dechlorinate poly(vinyl chloride) (PVC) to form the first examples of block copolymers of PVC and polyethylene (PE). Using this method, products can be isolated across the full range of dechlorination, while maintaining the PVC repeating unit in chlorinated blocks. Interfacial adhesion studies identify approximately 60% dechlorination to show the greatest promise for compatibilization of PVC/PE mixed waste.

9:20 AM

B-III-2: Bridging the Gap: Experiments and Simulations of Polyethylene Transport in Catalytic Deconstruction

[EFRC - CPI] Alex H. Balzer[1], Heyi Liang[2], Jessie A. Sun[1], Dionisios G. Vlachos[1], Juan de Pablo[3], Thomas H. Epps, III[1], LaShanda T.J. Korley[1]

[1]University of Delaware; [2]University of Chicago; [3]New York University

Catalytic deconstruction has emerged as a promising approach to convert polyethylene (PE) waste into valuable products such as oils, fuels, surfactants, and lubricants. Most catalytic reactions operate in viscous polymer melts, which leads to mass transfer limitations. A previously developed analysis in CPI of molecular weight (MW) distributions and thermal characterization was applied to PE deconstruction solids, which enabled more thorough identification of polymer chains. Critical distinctions among solids obtained from various hydroconversion reactions were captured, emphasizing how mass transfer limitations, driven by high melt viscosities, hinder chain diffusion to the catalyst surface. A successive pyrolysis-catalysis reaction approach developed herein is shown to efficiently reduce melt viscosity through random chain scission without mass diffusion constraints, thereby enhancing mixing and reaction kinetics for catalytic hydroconversion. Additionally, rheological experiments and bottom-up multiscale modeling provided further insight into the diffusion of entangled polymer chains. Predictive models were established to optimize pre-treatment parameters for any PE feedstock, ideal for ultra-high MW PE. These results will enable the incorporation of changes in intrinsic polymer properties (e.g., MW distributions, branching) into process-specific catalyst, reaction, and reactor-design calculations to enhance the economic potential of PE deconstruction.

9:40 AM

B-III-3: Programming the Architecture of Self-Assembling Protein Nanomaterials

[EFRC - CCBC] Timothy K. Chiang[1], Alexander Jussupow[2], Antonino Caliò[1], Kyleigh L. Range[1,2], Arinita Pramanik[1], Aimee Chi Soe[1], Greg L. Hura[1,3], Michael Feig[2], Markus Sutter[1,2], Cheryl A. Kerfeld[1,2]
[1]Lawrence Berkeley National Laboratory; [2]Michigan State University; [3]University of California, Santa Cruz

Bacterial Microcompartments (BMCs) are self-assembling protein nanocages involved in metabolic compartmentalization and biocatalysts in bacteria. BMC proteins have been observed to assemble into a variety of morphologies, making them attractive platforms for applications ranging from engineering synthetic biomaterials to confining catalysts. However, predicting and controlling the assembly behavior of such systems remains challenging. In this talk, I will describe efforts to develop methods for controlling and understanding the in vitro self-assembly of synthetic BMC-based materials, with particular focus on the controllable formation of mesoscale polymorphic crystalline structures by a single BMC shell protein. These systems serve as models for engineering synthetic nanoreactors and provide a framework for investigating the emergent physical, mechanical, and chemical properties of protein-based materials.

10:00 AM – Team Science Finalist

B-III-4: ENGINEERING SOLUTIONS FOR COMPLEX PLASTICS WASTE USING POLYMER SCIENCE AND CATALYSIS

[EFRC - CPI] Zoé O. G. Schyns, Pedro A. R. Moura, Christine M. Oberhausen, Alex W. Hawkins, Dionisios G. Vlachos, LaShanda T. J. Korley
University of Delaware

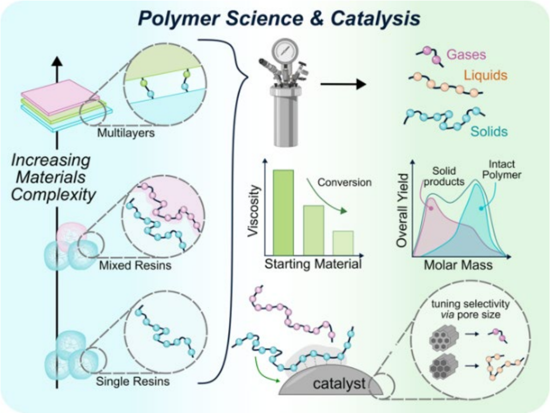


Figure 2 – Schematic representation of polymer science and catalysis concepts used to develop deconstruction strategies for increasingly complex plastic materials.

Most plastics valorization research has focused on single-component systems,[2,3] with limited attention to multicomponent, real-world waste. Overlooking the complexities associated with real-life waste streams (additives, contaminants, multiple resin codes, etc.) can reduce the efficacy of a valorization strategy and hinder sustainable process development.[1-4] By leveraging the multidisciplinary environment within CPI, we integrated catalysis and polymer science to develop robust processes for valorizing structurally complex multilayer plastics. Initially, we explored the deconstruction of key polymer components in multilayer plastic wastes, including heat-sealing and moisture-barrier layers, such as ethylene vinyl acetate (EVA)[5] and ethylene vinyl alcohol (EVOH)[6], and structural outer layers, such as low-density polyethylene (LDPE), and linear-LDPE (LLDPE). We focused on hydrogenolysis over ruthenium-supported catalysts (*e.g.*, Ru/ZrO_2) and hydrocracking over platinum-supported acid zeolite catalysts (*e.g.*, Pt/HY) to produce valuable lubricants and precursors for specialty chemicals, respectively, from the pure resins. We then examined the catalytic activity in physical mixtures of these polymers relevant to multilayer films (LDPE/EVOH or LDPE/EVA). Results showed that pure EVOH and EVA resins and physical mixtures with LDPE (LDPE/EVA and LDPE/EVOH) are slower to deconstruct *via* hydrogenolysis than pure LDPE, resulting in lower conversion and higher methane selectivity. Hydrocracking showed no such limitations, achieving full conversion and yielding valuable (naphtha-range) products. Further investigation of these catalytic findings using polymer characterization (rheology) revealed thermal degradation, which led to cross-linking (EVA) or conjugated aromatic molecule formation (EVOH), both of which favor hydrogenolysis deactivation mechanisms and support hydrocracking as a promising valorization strategy. Finally, our team utilized these deconstruction strategies to investigate real-world, industrial multilayer films. Initial experiments showed that tie-layer bonds within 5-layer films (LLDPE/LLDPE-gMAH/EVOH/LLDPE-gMAH/LLDPE) inhibited deconstruction. To further explore the effects of tie-layer content, we synthesized maleic-anhydride-based tie layers (LLDPE-gMAH) *via* reactive extrusion to quantitatively assess tie-layer chemistry on deconstruction. Through this sequential work, we aimed to uncover how the complexities of waste-representative materials impacted emerging hydrogenolysis/hydrocracking techniques with the overarching aim of developing plastics valorization strategies more tolerant of difficult-to-recycle materials, as an alternative to landfilling.

References:

[1] Nixon, K. D., *et al.*, *Nat. Chem. Eng.*, 2024, 1, 615–626; **[2]** Nakaji, Y., *et al., Appl. Catal., B*, 2021, 285, 119805; **[3]** Tennakoon, A., *et al.*, *Nature,* 2020, 3; **[4]** Hinton, Z. R., *et al., Green Chem.*, 2022, 24, 7332–7339; **[5]** Moura, P., *et al. ACS Sustain. Chem. Eng.*, 2024, 12, 8717–8728; **[6]** Oberhausen, C. M., *et al.*, *ChemSusChem*, 2024, 17, e202400238.

Contributions: P.R.M. and C.M.O. performed catalytic deconstruction experiments. Z.O.G.S. and A.W.H. performed polymer characterizations and generated polymeric materials. Z.O.G.S. and P.R.M. wrote the abstract.

Session IV: Tuesday, August 12, 2025, 1:30 – 3:10 PM, Forest Glen

1:30 PM

B-IV-1: Exploring the basic science of durability and performance of CO_2 reduction solar fuels devices under diurnal operating conditions

[Hub - LiSA] Adam Nielander[1,2], Harry A. Atwater[1,3], Chengxiang Xiang[1,3], Walter Drisdell[1,4], Thomas F. Jaramillo[1,2], Kyra M. K. Yap[1,2], Sol A. Lee[1,3]

[1]Liquid Sunlight Alliance; [2]SLAC National Accelerator Laboratory; [3]California Institute of Technology; [4]Lawrence Berkeley National Laboratory

The outdoor operation (photo)electrochemical solar fuels devices driving CO_2 reduction (CO_2R) must contend with challenges presented by dynamic changes in operating condition (e.g., solar irradiance, temperature) under day/night (i.e., diurnal) cycles. These dynamics drive changes in performance and can strain the durability of CO_2R solar fuels device over a diurnal cycle. Herein, we highlight recent efforts within LiSA to understand the basic electrochemical and durability science of CO_2R solar fuels devices. We discuss the effects of diurnal cycling on 'ideally' durable operation, including changes in CO_2R selectivity as a function of irradiation and temperature. Using models that incorporate both experimental insight and daily meteorological conditions from the National Solar Radiation Database (NSRD), we interrogate how diurnal variations impact performance as a function of geography, suggesting co-design strategies. We also discuss our efforts using advanced operando methods to understand how varying operating conditions affect the structure of electrochemical microenvironments and translate to changes in observed CO_2R performance. Using synchrotron-enabled operando x-ray tomography methods, we observed changes at a catalyst/ionomer interface as a function of electrochemical conditions (e.g. applied voltage, current) in a 'zero-gap' membrane electrode assembly driving CO_2R. Correlation between changes in the interfacial microenvironment and the observed CO_2R performance suggests that fast flooding at the ionomer interface is a primary driver of performance degradation. These studies serve as a platform for continued study within LiSA of the basic science that underpins durable performance of (photo)electrochemical solar fuels devices and inform design of a broad range of energy-conversion technologies.

1:50 PM

B-IV-2: Metal-Organic Frameworks for the (de)Hydrogenation of Liquid Organic Hydrogen Carriers Enabled by Polarizable Metal Active Sites

[EFRC - CD4DC] Haomiao Xie[1], Milad Ahmadi Khoshooei[1], Mukunda Mandal[2], Simon M. Vornholt[3], Jan Hofmann[3], Luke M. Tufaro[3], Kent O. Kirlikovali[1], Dawson Grimes[1], Seryeong Lee[1], Shengyi Su[1], Susanne Reischauer[1], Debabrata Sengupta[1], Kira Fahy[1], KaiKai Ma[1], Xiaoliang Wang[1], Fanrui Sha[1], Wei Gong[1], Yongwei Che[1], Jenny G. Vitillo[4], Massimiliano Delferro[5], John S. Anderson[2], Justin M. Notestein[1], Karena W. Chapman[3], Laura Gagliardi[2], Omar K. Farha[1]

[1]Northwestern University; [2]University of Chicago; [3]Stony Brook University; [4]Università degli Studi dell'Insubria; [5]Argonne National Laboratory

Metal-organic frameworks (MOFs) are advanced materials known for their high internal surface areas and structural versatility, making them ideal candidates for catalysis. This study explores a novel approach to enhance the catalytic performance of MOFs by introducing sulfur-containing active sites through post-synthetic modification. Sulfur is highly polarizable and plays a critical role in improving chemical reactivity, as seen in natural enzymes. However, incorporating sulfur into MOFs has been challenging due to stability and synthetic limitations. Here, we demonstrate a two-step process to convert metal-chloride-based MOFs into their sulfur-containing counterparts. Using cobalt (Co) and nickel (Ni)-based MOFs as examples, we successfully replaced chloride and hydroxide groups with sulfhydryl (-SH) groups. Advanced characterization techniques, including in situ powder X-ray diffraction and pair distribution function analysis were used to evaluate the structural mechanism for the post-synthetic modification, while electron microscopy and spectroscopy confirmed the structural integrity and successful modification of the MOFs. The modified MOFs were tested in hydrogenation reactions, specifically the reduction of 4-nitrophenol to 4-aminophenol, a model reaction relevant to industrial applications. The sulfur-modified MOFs showed significantly improved catalytic activity compared to their chloride and hydroxide-based precursors. Computational studies revealed that the sulfur groups enhance the lability of metal-sulfur bonds, facilitating efficient hydrogen activation. This research highlights the potential of post-synthetic modification to create high-performance MOF-based catalysts. By integrating sulfur components, we unlock new possibilities for designing materials that mimic the reactivity of natural enzymes while offering greater stability and scalability for industrial applications.

2:10 PM

B-IV-3: Co-designing Sorbents and Catalysts for Integrated CO_2 Capture and Conversion

[EFRC - 4C] Jounghwan Choi[1], Shawn Chiu[1], Avishek Banerjee[1], Dominic Ross[2], Zisheng Zhang[1], Manu Gautam[3], Ciara Gillis[1], Ab Mir[1], Robert L. Sacci[4], Gabriel M. Veith[4], Joshua Spurgeon[3], Chantal Stieber[5], Christopher Hahn[2], Anastassia N. Alexandrova[1], Carlos G. Morales-Guio[1], Aaron Appel[6], Jenny Yang[1]

[1]University of California, Irvine; [2]Lawrence Livermore National Laboratory; [3]University of Louisville; [4]Oak Ridge National Laboratory; [5]California State Polytechnic Institute, Pomona; [6]Pacific Northwest National Laboratory

Integrated CO_2 capture and conversion can significantly reduce the cost and energy requirement of CO_2 valorization from dilute sources to product. While there has been substantial research in the two separate processes – CO_2 Capture and Concentration (CCC) and catalysts for electrolytic CO_2 Reduction Reactions (CO_2RR), there is minimal overlap between these two communities, resulting in critical knowledge gaps in integration. While the CCC community has focused on selectivity, stability, and efficiency at scale, efforts in CO_2RR have primarily used pure CO_2 streams to improve rate, selectivity, and durability. The unique metrics defined for successful CCC and CO_2RR do not seamlessly translate to integrated processes. The introduction of a sorbent into a catalytic system introduces new challenges. Because CO_2 is an electrophile, sorbents are typically nucleophilic, which can competitively bind to electron-rich catalytic active sites, resulting in catalyst poisoning or corrosion. Amines have been the most commonly studied sorbent in integrated capture and electrocatalytic conversion systems, as they are currently used in point source CO_2 capture and concentration. However, amines form an equivalent of ammonium upon capture, which can promote hydrogen evolution and loss of Faradaic efficiency for carbon-based products. Additionally, most sorbed-CO_2 species result in anionic species, such as carbamates or carbonates from amines and alkoxides, respectively, that are inhibited in their approach to negatively charged or polarized catalyst sites. General guidelines for sorbent and catalyst co-design will be outlined, as well a theory and experimental workflow for integrative discovery.

2:30 PM

B-IV-4: Impact of Organic Films on Electrocatalytic CO_2 Reduction with Metal Electrodes

[Hub - LiSA] Theodor Agapie[1,2], Jonas C. Peters[1,2], Weixuan Nie[1,2], Matthew Salazar[1,2], Madeline H. Hicks[1,2], Yungchieh Lai[1,2], Nicholas B. Watkins[1,2], Gavin P. Heim[1,2], Meaghan A. Bruening[1,2], Alonso Rosas-Hernández[1,2], Arnaud Thevenon[1,2], Joel A. Haber[1,2], William A. Goddard III[1,2], John M. Gregoire[1,2], Harry A. Atwater[1,2]
[1]Liquid Sunlight Alliance; [2]California Institute of Technology

Targeting the utilization of CO_2 as a carbon source for the generation of liquid fuels and other value-added chemicals using renewable energy has prompted the development of chemical transformations and multistep processes for the preparation of reduced C_1 and multicarbon products. Electrochemical CO_2 reduction (CO_2R) on Cu electrodes generates a mixture of products, including CO, methane, ethylene, ethanol, and propanol, and it competes with hydrogen evolution. To improve the selectivity of CO_2R, hybrid electrodes based on Cu coated with an organic layer were prepared targeting microenvironments that facilitate the formation of C_2+ products. Addition of certain organic films results in almost complete suppression of methane formation and decrease in hydrogen generation in CO_2R with Cu, for a combined selectivity for C_2 and C_3 products of ~80%. The electrochemical reduction selectivity is also impacted on copper alloys and silver electrodes. Organic coatings enable CO_2R with Cu at low pH. A variety of molecular organic precursors and ionomers have been explored to optimize the organic film generation and its impact on CO_2R performance. Mechanistic implications will be discussed.

2:50 PM

B-IV-5: Alkali Cation Inhibition of Imidazolium-Mediated Electrochemical CO_2 Reduction on Silver

[EFRC - 4C] Francois Nkurunziza[1], Saudagar Dongare[2], Soumya Chatterjee[3], Bhavi Shah[1], Manu Gautam[1], Baleeswaraiah Muchharla[4], Bijandra Kumar[4], Michael J. Janik[3], Burcu Gurkan[2], Robert L. Sacci[5], and Joshua M. Spurgeon[1]

[1]University of Louisville; [2]Case Western Reserve University; [3]The Pennsylvania State University; [4]Elizabeth City State University; [5]Oak Ridge National Laboratory

Imidazolium-based ionic liquids (ILs) have led to enhanced CO_2 electroreduction activity by stabilizing reaction intermediates through cation reorientation at the electrode-electrolyte interface, which enhances the interfacial electric fields, thereby decreasing the activation energy. In aqueous media, alkali cations are also known to improve CO_2 reduction on metals like Ag, with the enhancement attributed to electrical double layer effects and trending with the size of the alkali cation. However, the effect of a mixed catholyte solution of alkali cations in the presence of an imidazolium-based IL has not been well-explored. Herein, 1-ethyl-3-methylimidazolium tetrafluoroborate, [EMIM][BF_4], in water was investigated with alkali salts to unravel the interaction effects for CO_2 reduction on Ag. Although both $[EMIM]^+$ and alkali cations have individually improved CO_2 to CO conversion on Ag in water, results showed that alkali cations hindered [EMIM]-mediated CO_2 reduction at most conditions. Li^+, in particular, was sharply inhibitory compared to other alkali cations and strongly redirected the selectivity to hydrogen evolution. The nature of the alkali cation inhibition was investigated via advanced spectroscopy techniques along with computational insights. The data suggest that alkali cations inhibit [EMIM]-mediated CO_2 reduction by competing for adsorption sites, preventing the potential-dependent structural reorientation of imidazolium, and promoting hydrogen evolution by bringing solvated water to the cathode surface.

C. Catalysis II

Session II: Monday, August 11, 2025, 1:40 – 3:20 PM, Glen Echo

1:40 PM

C-II-1: Pushing the Frontiers of Exchange-Correlation

[CCS - WFT2XC] Paul Zimmerman, Vikram Gavini

University of Michigan

The Zimmerman and Gavini research groups have brought wave function theory and density functional theory closer and closer together over the last few years. Our strategies for computing high-accuracy wavefunctions and converting them into the Kohn-Sham (KS) framework allow modeling of exchange-correlation (XC) functionals with unprecedented precision. Combined with state-of-the-art, massively parallel GPU-accelerated DFT code in the DFT-FE program, this CCS project is leading to the practical realization of systematically improvable DFT simulations at scale.

This presentation will introduce our synergistic WFT/DFT strategy for scaling up correlated electronic structure simulations. Central to this endeavor is the derivation of high-accuracy, spatially resolved XC information using WFT at the full configuration interaction level, and then training of machine-learning-based DFT models with this precise data. Previously, XC data in the form of XC potentials was not available due to serious deficiencies in the inversion process (which in turn stemmed from use of incomplete basis sets). Having overcome this challenge we can now make use of XC profiles in training, leading to models that are more accurate than conventional functions within each rung of the DFT ladder. Prospects for treatment of strong correlation at the DFT level will also be discussed.

2:00 PM

C-II-2: Isolating intermediates of the photo-excited oxygen evolution reaction on titanium oxides

[EFRC - CEDARS] Tanja Cuk[1], Shay McBride[2], Cassius Boyd[1], Sheilah Cherono[3], Moritz Lang[1], Jennifer Sormberger[1], David Jonas[1], Luca Mitrovic[4], Darrell Schlom[4], Junko Yano[5], Ethan Crumlin[5], Dhananjay Kumar[3], Geoffroy Hautier[2,6]

[1]University of Colorado Boulder; [2]Dartmouth College; [3]North Carolina A&T State University; [4]Cornell University; [5]Lawrence Berkeley National Laboratory; [6]Rice University

One of CEDARS's goals is monitoring the photo-excited oxygen evolution reaction (OER) through the lens of electron and proton transfer intermediates. Titanium oxides have been a platform for this investigation, owing to the efficiency with which light drives OER on their surfaces. CEDARS applies pulsed light excitation to initiate the photo-catalytic cycle and separate intermediate steps along the time axis. However, assigning the electron and proton transfer intermediates (e.g., OH*, O*) to the experimental spectra is challenging. A spectral signature that exists upon photoexcitation is a broad, visible excited state absorption (ESA) below the wide-band gap of these semiconductors. Hole-polarons, for which the atomic structure distorts around the oxygen site and traps holes, are predicted to occur as mid-gap states. Within CEDARS, we have been able to explain a larger ~1 eV shift in the broad ESA observed experimentally between rutile TiO_2 and perovskite $SrTiO_3$ with optical dipoles for terminal $O^{\bullet-}$ and lateral $Ti_2O^{\bullet-}$ calculated by time-dependent density functional theory. We have also focused on understanding the polarization dependence of the optical spectra seen for uniaxial rutile TiO_2. Since the optical dipole is a sensitive function of their electronic and phononic structure, epitaxial thin film deposition was harnessed, affording a forthcoming test of our understanding across a range of materials, including anatase, rutile, and perovskite crystal symmetries on lattice matched and mis-matched substrates. Future work consists of studying doped (Ir-TiO_2) and alloyed titanium oxides (TiON), for which CEDARS has already characterized the dark electrochemistry and ground state optical spectra.

2:20 PM

C-II-3: Advance Accuracy and Efficiency in Self-interaction-free Density Functional Theory

[CCS - FLOSIC] Kushantha Withanage[1], Koblar Jackson[2], Mark Pederson[1]
[1]University of Texas at El Paso; [2]Central Michigan University

Approximated exchange-correlation (XC) functionals in density functional theory (DFT) calculations lead to a residual self-interaction of the electrons. This is responsible for major drawbacks of the method. A remedy for this is the Perdew-Zunger self-interaction correction (PZ-SIC). The traditional implementation of PZ-SIC relies on the localization equations to find optimal orbitals, which makes the method computationally demanding. In the novel implementation of PZ-SIC with Fermi-Loewdin orbitals (FLOs), the appearance of orbitals in the energy functional remains, but each of the orbitals is explicitly dependent on the density matrix. For large-scale calculations, the orbital dependency in FLO-SIC becomes the bottleneck of the method. Using group theory and the sparsity that naturally arises within the method, one can perform meaningful large-scale FLO-SIC calculations. We show this by applying the FLO-SIC method to a trianionic Cr complex surrounded by more than 100 water molecules, where DFT calculations predict unphysical charge transfer between the solute and solvent. In addition, we developed a way to create complex FLOs that have the potential to solve the overcorrection of self-XC energies in real FLOs due to their nodality. We also have developed post-processing tools required for analyzing results from these calculations. One example is the adaptation of the vibrational configuration interaction (VCI) method for improved vibrational spectroscopic analysis.

2:40 PM – Team Science Finalist

C-II-4: PHOTO-ELECTROCHEMISTRY OF TITANIUM OXIDES: A PLATFORM FOR ASSIGNING VISIBLE SPECTRA TO OXYGEN EVOLUTION INTERMEDIATES

[EFRC - CEDARS] C. Boyd[1], S. McBride[2], S. Cherono[3], M. Lang[1], L. Mitrovic[4], J. Sormberger[1], D. Schlom[4], D. Jonas[1], D. Kumar[3], G. Hautier[2], T. Cuk[1]
[1]University of Colorado Boulder; [2]Dartmouth College; [3]North Carolina A&T State University; [4]Cornell University

Oxygen evolution intermediates that arise from the electron and proton transfer from water on heterogeneous surfaces inform catalytic mechanism, but their experimental validation by spectroscopy has been challenging. In addition to their efficiency in driving the oxygen evolution reaction (OER), titanium oxides have been a focus of (photo)-electrochemical mechanisms due to an electronic structure that allows for the separation of states associated with electron deficient oxygen configurations (*e.g.* terminal $TiO^{\bullet-}$, lateral $Ti_2O^{\bullet-}$).

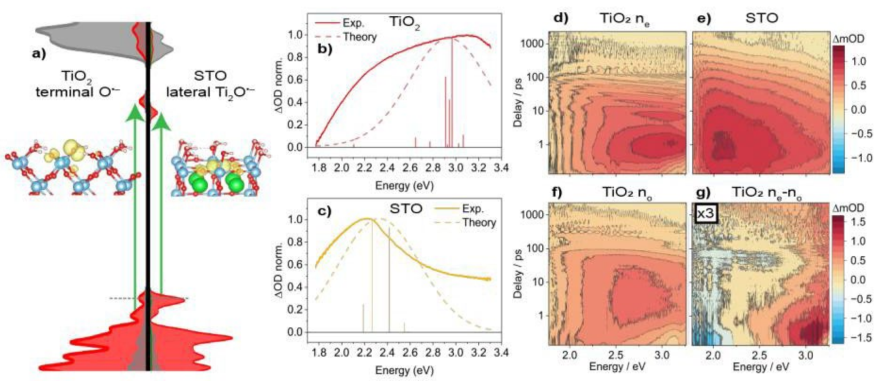


Figure 1 Excited state absorption in titanium oxides a) ESA: transition of valence band electron to unoccupied hole-polaron mid-gap state (yellow orbitals), b) and c) theoretical and experimental spectra compared for rutile TiO_2 100 and perovskite $SrTiO_3$ 100 (STO) respectively, d) and e), corresponding time-spectral contour plots of the transient optical data, f) rutile TiO_2 contour plots for the probe orientated along the ordinary axis, g) the difference between the extraordinary (n_e, d) and ordinary contour plots (n_0, f).

However, while these local electronic states have long been predicted theoretically, matching them to experimental spectra has been challenging. Here, we use an excited state absorption (ESA) that arises in the visible regime (Fig. 1a-1c) ultrafast time scales to connect experiment to theory. The data are taken by a broad-band white light probe in reflectance after above bandgap excitation in a pump-probe setup. To obtain the optical dipoles, the calculations use a hybrid functional (PBE0) and time-dependent density functional theory (TD-DFT). The essential challenge is that the optical transitions are broad both intrinsically (due to vibronic transitions and multiple sites hosting the intermediate configurations) and extrinsically (due to sample structural and chemical heterogeneity). It is therefore imperative to use multiple crystal structures of titanium oxide (rutile, perovskite, and anatase) and several material forms (bulk crystals, epitaxial thin films) to correlate calculated and measured spectra with fidelity. A recently published highlight[1] is rationalizing the ~1 eV change in the ESA between rutile TiO_2 (Fig. 1d) and perovskite $SrTiO_3$ (Fig. 1e). We also analyze the polarization dependence of the ESA in uniaxial rutile TiO_2 (Fig. 1d, 1f, 1g) and the coherent acoustic waves that result from an ultrafast strain associated with the ESA formation. Here we present our progress to date, which involves four CEDARS institutions across single crystalline thin film growth (pulsed laser deposition, molecular beam epitaxy), theory, and optical spectroscopy.

Contributions: C. Boyd, M. Lang took the transient optical data and analyzed the results, guided by T. Cuk. S. McBride performed the DFT calculations, guided by G. Hautier. S. Cherono grew epitaxial films of doped rutile TiO_2, guided by D. Kumar. L. Mitrovic grew epitaxial films of anatase TiO_2, guided by D. Schlom. J. Sormberger orientated the rutile polarization axis at the suggestion of D. Jonas.

1. Boyd, C.; McBride, S.; Paolino, M.; Lang, M.; Hautier, G.; Cuk, T., Assigning Surface Hole Polaron Configurations of Titanium Oxide Materials to Excited-State Optical Absorptions. *Journal of the American Chemical Society* **2025,** *147* (13), 10981-10991.

3:00 PM

C-II-5: Molecular Dynamics using highly correlated electronic structure methods driven by the Many-Body Expansion (MBE-MD)

[CCS - SPEC] Joseph P. Heindel[1], Kristina M. Herman[1], Sotiris S. Xantheas[1,2]
[1]University of Washington; [2]Pacific Northwest National Laboratory

Classical and nuclear statistical molecular dynamics simulations based on energies and gradients obtained from ab-initio suffer from the steep scaling of highly correlated electronic structure methods. These simulations are typically performed at the Density Functional Theory (DFT) with current extensions to the second order perturbation theory level (MP2) of theory. An alternative approach to solving the Schrödinger equation for the whole system (usually under periodic boundary conditions) is to partition it in the individual “bodies” (monomers, dimers, trimers, etc.). This approach becomes competitive when the energies and gradients are obtained from an electronic structure method that scales as N^(k+1) when terms up to the k-body are computed. We will demonstrate this protocol for classical potentials and electronic structure methods, its extension to include periodic boundary conditions and its application to aqueous clusters and molecular crystals.

Session III: Tuesday, August 12, 2025, 9:00 – 10:20 AM, Glen Echo

9:00 AM – Team Science Finalist

C-III-1: ACCURATE ELECTROCHEMICAL PREDICTIONS WITH MANY-BODY AND MACHINE-LEARNING METHODS

[CCS - BEAST] Sophie Gerits[1], Daniel Weinberg[2], Nima Karimitari[3], Cooper Tezak[1], Jacob Clary[4], Taylor Aubry[4], Charles Musgrave[1], Mauro Del Ben[2], Christopher Sutton[3], Derek Vigil-Fowler[4], Ravishankar Sundararaman[5]
[1]University of Colorado Boulder; [2]Lawrence Berkeley National Laboratory; [3]University of South Carolina; [4]National Renewable Energy Laboratory; [5]Rensselaer Polytechnic Institute

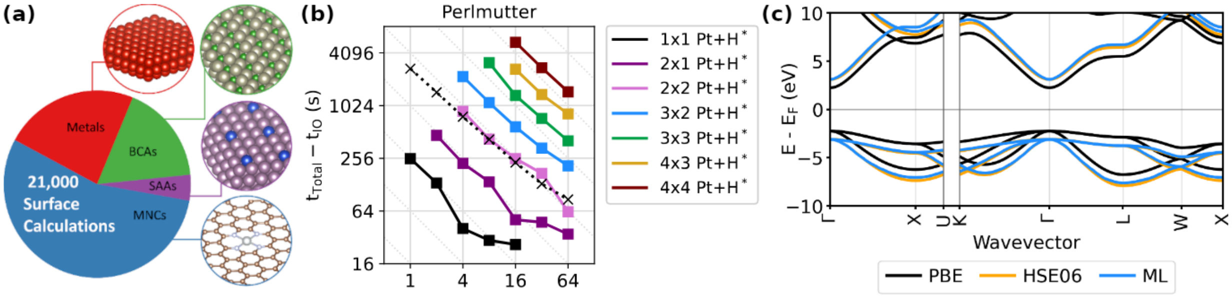


Figure 1. To enable accurate, rapid first-principles predictions for electrochemical reactions, we have (a) established a database (BEAST DB) with >20,000 grand-canonical density functional theory (GC-DFT) calculations, (b) scaled beyond-DFT electrochemical calculations based on the random phase approximation (RPA) to GPU-based supercomputers, and (c) demonstrated machine learning methods to predict higher-level electronic structure from DFT inputs, targeting RPA-quality electrochemical predictions at DFT cost using BEAST DB.

Manipulating chemical dynamics at complex heterogeneous interfaces requires accurate *ab initio* methods beyond density functional theory (DFT) to design materials such as electrocatalysts. We have developed scalable and efficient algorithms for performing many-body calculations for electrocatalysts using the random-phase approximation (RPA), formulated machine learning (ML) techniques to rapidly predict beyond-DFT outputs from DFT inputs, and created an electrocatalytic database with grand-canonical DFT simulations of electrochemical systems to facilitate combined application of the RPA and ML techniques for rapid, accurate electrochemical predictions. This open-source database, BEAST DB, contains over 20,000 surface calculations at fixed electrode potential, covering a broad set of heterogeneous catalyst materials and electrochemical reactions (Figure 1(a)), with continued expansion leveraging automated high-throughput workflows for grand-canonical DFT.

To facilitate accurate simulation of these electrochemical systems beyond the limitations of DFT, we implemented highly scalable and efficient RPA calculations using the static subspace approximation and a compressed representation of the frequency-dependent polarizability. This technique enables RPA calculations of typical surface slabs within a few hundred GPU-hours (Figure 1(b)), thereby facilitating RPA calculations for hundreds to thousands of prototypical electrochemical systems. Finally, we have developed ML techniques based on graph neural networks that can predict higher-level electronic structure using energies and atomic orbital projections from DFT (Figure 1(c)), including for the highly inhomogeneous electrochemical interface calculations. Training such ML techniques to RPA calculations on a subset of BEAST DB will enable rapid RPA-quality predictions for the entire DB as well as for any additional electrochemical systems with just DFT-level calculations and computational cost.

Contributions: Sophie Gerits developed the high-throughput workflow for grand-canonical calculations enabling BEAST DB. Daniel Weinberg implemented the static subspace approximation to optimize RPA calculations on GPU supercomputers. Nima Karimitari developed machine learning methods to predict higher-level electronic structure.

9:20 AM

C-III-2: Chemistry Beyond the Sabatier Limit: Programmable Photons for Accelerated Catalysis for Energy

[EFRC - CPEC] Ali Mohammed[1], Silvia Marino[2], Ryan Berry[2], Kenneth Kusima[1], Paul Dauenhauer[3], Michael Gordon[2], Lars Grabow[1], Phillip Christopher[2], Omar Abdelrahman[1]
[1]University of Houston; [2]University of California, Santa Barbara; [3]University of Minnesota

The dehydrogenation of liquid organic energy carriers on catalytic surfaces is hindered by significant kinetic barriers and the buildup of spectator species, limiting their effectiveness for on-demand energy delivery. While thermal, electrochemical, and photochemical strategies have been explored independently, the cooperative use of multiple energy inputs remains underutilized. In this work, we investigated the role of visible light (440–650 nm) in enhancing the thermal dehydrogenation of formic acid over precious metal catalysts. Using Pt nanoparticles supported on insulating oxides (e.g., silica, alumina), we show that continuous-wave illumination at 440 nm significantly accelerates the decomposition rate of formic acid. The observed rate enhancement was insensitive to temperature, yielding an apparent activation energy near zero—

indicative of a non-thermal, photo-driven process. Furthermore, programmable light waves whose photon incidence frequencies are matched to the characteristic timescales of surface chemistry, enabled significant quantum yield enhancement and catalytic turnover acceleration. Photon incidence frequency coordination yielded rate enhancements exceeding four orders of magnitude relative to thermal catalysis alone, enabling efficient formic acid dehydrogenation at near-ambient conditions and circumventing limitations imposed by conventional scaling relations such as the Sabatier principle.

9:40 AM

C-III-3: Photolysis of Nickel-Halide Bonds as a General Mechanism of Ni/Sensitizer Photocatalyst Activation

[EFRC - BioLEC] Max Kudisch[1], Reagan X. Hooper[4], Lakshmy K. Valloli[3], Justin D. Earley[1], Anna Zieleniewska[1], Jin Yu[5], Stephen DiLuzio[6], Rebecca W. Smaha[1], Hannah Sayre[6], Xiaoyi Zhang[5], Matthew J. Bird[3], Amy A. Cordones[4], Garry Rumbles[1,2], Obadiah G. Reid[1,2]
[1]National Renewable Energy Laboratory; [2]University of Colorado Boulder; [3]Brookhaven National Laboratory; [4]SLAC National Accelerator Laboratory; [5]Argonne National Laboratory; [6]Northeastern University

We report a general mechanism of how Ni(II)X_2 (X=Cl or Br) starting materials become activated to Ni(I)X carbon-carbon cross-coupling catalysts, revealed by a sequence of unique spectroscopy and photochemistry experiments that spanned 3 National Laboratories and two universities. Photolysis of a Ni(II)-X bond via either direct excitation or energy transfer produces bond homolysis. The product radicals rapidly react with the most readily available hydrogen-atom source, which is often the solvent. This process produces HX and a ubiquitous family of new organonickel compounds Ni(II)RX, where R is derived from solvent radical addition at Ni(I)X, which have red-shifted absorption and can be photolyzed back to Ni(I)X with another visible photon. NI(II)RX thus acts as a reservoir species that both protects Ni(I)X from unproductive dimerization and allows its repeated re-formation via subsequent photoexcitation. These results explain how Ni(II)X_2 activation happens, why specific solvents work particularly well in cross electrophile coupling, and present a new strategy to control the Ni(I)X concentration during catalysis.

10:00 AM

C-III-4: Diverting Polyolefin Hydrogenolysis to Olefins with Low Gas Formation via Reactor and Catalyst Design

[EFRC - iCOUP] Wenyu Huang[1,2], Aaron D. Sadow[1,2], Baron Peters[3], Andreas Heyden[4], Yi-Yu Wang[1,2], Ruoyu Cui[1,2], Changhae Andrew Kim[3], Mubarak Bello[4]
[1]Iowa State University; [2]Ames National Laboratory; [3]University of Illinois Urbana-Champaign; [4]University of South Carolina

The plastic waste crisis has spurred an influx of research within the catalysis community. To effectively address this issue, catalytic conversion of used polymers must be conducted through continuous flow processes that can manage the scale of plastic waste. However, most existing

studies on catalytic polyolefin deconstruction are carried out in sealed and pressurized autoclaves at small scales, which present a significant gap for their application in commercial-scale catalytic approaches for plastic deconstruction. In this talk, we discuss the catalytic hydrogenolysis of polyolefins using a unique semi-flow reactor system. Our semi-flow experiments establish pseudo-steady state conditions and create a reactive separation that allows for an in-depth analysis of the catalytic hydrogenolysis mechanism, particularly targeting the elementary processes following the turnover-limiting C–C cleavage step. The concept of reactive separation works in synergy with processive catalyst design principles to achieve a high selectivity for products with fewer than 20 carbon atoms, while significantly minimizing the "over-hydrogenolysis" of liquid products into low-value gases, even at near-quantitative conversion of the polymer reactant. Notably, the yields of terminal alkenes increase as hydrogen pressure decreases. This research paves the way for more in-depth mechanistic studies of polymer deconstruction reactions and demonstrates new methods to catalytically convert waste plastics into more valuable chemicals, such as terminal alkenes, an area that remains underexplored.

Session IV: Tuesday, August 12, 2025, 1:30 – 3:10 PM, Glen Echo

1:30 PM

C-IV-1: Implications and Methods of Programmable Catalysis for Energy

[EFRC - CPEC] Paul Dauenhauer
University of Minnesota

An emerging research frontier of catalysts that change with time on the timescale of a catalytic turnover is revealing new strategies to control surface reaction pathways and drive reactions beyond the limits of static catalysts. The Center for Programmable Energy Catalysis (CPEC) pursues the temporal perturbation of catalyst active sites using pulsed illumination and charge modulation to understand the fundamental mechanisms and characteristic dynamics of catalytic reactions. Through simulation and first principles calculations, variation of the repeating pattern of active site perturbation (i.e., program) has led to the discovery of the underlying mechanics and characteristic descriptors defining programmable catalysts. In parallel, collaborative efforts to synthesize and characterize programmable catalytic materials along with experimental expertise in kinetics and spectroscopy have discovered new fundamental capability to drive catalysis beyond the Sabatier limit and achieve unprecedented selectivity to targeted chemical products. These joint efforts across multiple institutions have developed state-of-the-art tools to understand chemistry at the millisecond timescale on surfaces with only fractional electron transfer from reacting adsorbates. Parallel novel calculation and simulation methods have been developed to understand the physics of active site perturbation and its implications to accelerate and control dynamic chemistry. Collective efforts across the center are establishing the foundational concepts and mathematical principles that will drive programmable catalysis to solve the biggest energy problems.

1:50 PM

C-IV-2: Tuning Functional Properties of Oxide Coatings and their Influence on Nanoreactor Photosynthetic Redox Selectivity that is Crucial to Ensemble Performance

[EFRC - EPN] Daniel V. Esposito[1], Rohini Bala Chandran[2]
[1]Columbia University; [2]University of Michigan

EPN EFRC aims to understand, predict, and control the ensemble activity, selectivity, and stability of inorganic nano-to-micro-particles driving photosynthetic reactions. Control over redox reaction selectivity is being achieved through the codesign of multicomponent interphases that impart species-specific permeabilities and stabilities at spatially distinct active sites. Atomic layer deposition (ALD) was used to encapsulate metallic and molecular electrocatalysts in ultrathin nanoporous oxide coatings. Mechanistic details that support observed species selectivities were obtained through a theory/experiment workflow that included electroanalytical, spectroscopic, and microscopic characterization, and computational modeling. A major advancement was the ability to use surface chemistry to control the location of TiO_2 growth, which enabled the discovery of area-selective ALD process parameters that strike an optimal balance between surface protection and targeted redox activity. The same ALD chemistry was shown to impart immobilization of Co(TCPP) molecular catalysts, where TCPP is 5,10,15,20-*tetrakis*(4-carboxyphenyl)porphyrin, protecting them without compromising electrocatalytic activity. Mechanistic insight into the effects of physical confinement, surface charge, and pH on proton and water transport through coatings were provided by molecular dynamics simulations using first-principles deep-neural-network machine-learned interatomic potentials coupled with complementary experimental measurements of surface charge. Numerical simulations revealed an additional layer of complexity due to the interparticle effects of photon recycling, via emission and reabsorption of light, and nearby generation of reaction products. Together, these insights inform spatially distinct oxide interphase codesign properties that result in necessary levels of redox reaction selectivity and stability of relevance to meeting EPN aims.

2:10 PM

C-IV-3: Resolving the Coverage Dependence of Surface Reaction Kinetics with Machine Learning and Automated Quantum Chemistry Workflows

[CCS - ECC] Matthew S. Johnson[1], David H. Bross[2], Judit Zádor[1]
[1]Sandia National Laboratories, Livermore; [2]Argonne National Laboratory

A large body of theoretical investigations of heterogeneous catalysis relies on detailed microkinetic models. These models consist of elementary surface reactions and their rate coefficients, whose calculation typically require DFT-level exploration and characterization of key stationary points along low-energy pathways. We recently introduced the Pynta workflow code (https://github.com/zadorlab/pynta) that transforms the way these quantum chemical calculations are conducted, taking advantage of supercomputers running and analyzing a large number of DFT calculations automatically, leveraged by our algorithmic advances in saddle guess generation and searches.

The presence of nearby co-adsorbates on the surface can dramatically alter the kinetics via lateral interactions. However, there are combinatorially many co-adsorbed configurations on the surface, and thus computing the coverage dependence of these parameters requires and algorithm that dramatically cuts down on the number of configurations to be investigated. To this end, we extended our Pynta framework to directly generate, run, and analyze co-adsorbed configurations for stable species and for saddle points, and ultimately predict coverage-dependent parameters for microkinetic models.
To combat the large configuration space, we train subgraph isomorphic decision trees (SIDTs), which can predict chemical properties based on information encoded in the connectivity of the structures, and possess error cancellation properties that are particularly favorable for predicting kinetics. We demonstrate the SIDT-Pynta workflow on a series of examples along with an active learning strategy for further efficiency gains.

2:30 PM

C-IV-4: Feeding the furnace: molecular-scale permeability and catalysis within bacterial microcompartments

[EFRC - CCBC] Saad Raza[1], Neetu Yadav[1], Alexander Jussupow[1], Nicholas D. Tefft[1], Xiaobing Zuo[2], Markus Sutter[1,3], Michela A. TerAvest[1], David M. Tiede[2], Cheryl A. Kerfeld[1,3], Michael Feig[1], Josh V. Vermaas[1]
[1]Michigan State University; [2]Argonne National Laboratory; [3]Lawrence Berkeley National Laboratory

Bacterial microcompartments (BMCs) are protein shells that encapsulate enzymes to accelerate multi-step catalysis, creating nanoscale reactors within living organisms. The enzyme cargos within these BMCs can be specifically tailored to carry out a wide range of metabolic functions within the organism, including designer pathways that are not native to BMCs. Efficient catalysis along these pathways demands that reactants and products can transit across these BMC shells quickly through nanoscale pores, a process that is difficult to measure on the benchtop. However, atomic-scale computational models based on experimental proteomics, cryo-EM, and small angle x-ray scattering data offer a window into the nanoscale motions responsible for molecular transit. Through advanced molecular simulation techniques, we quantify permeability at the nanoscale for multiple metabolites both at high and low concentrations. The permeability coefficients for typical small molecule metabolites are measured to be in the range of 10^{-2} to 10 cm/s, comparable to permeabilities for highly permeable molecules in other contexts, such as lipophilic molecules across the cell membrane. These insights suggest that the main benefit to catalysis is the confinement itself, where intermediates along the pathway remain inside the shell by a kinetic trap that offers more opportunities for productive interactions between enzymes and small molecules. These insights are valuable for engineering designer BMCs and keeping the nanofoundries fueled up to make tailored bioproducts.

D. Energy Storage I

Session I: Monday, August 11, 2025, 9:10 – 10:30 AM, Salon F

9:10 AM

D-I-1: New Perspectives on Ion-Matter Interactions

[Hub - ESRA] Y. Shirley Meng[1,2], Bryan McCloskey[3,4], Wei Wang[5], James Burrow[1,2], Yang Shao-Horn[6], Dan Steingart[7], Brett Helms[3], Yan Yao[8], Paul Fenter[1], Vijay Murugesan[5], Gerbrand Ceder[3,4], Maria Chan[1], Kamila Wiaderek[1], Ethan Crumlin[3], Kelsey Hatzell[9]
[1]Argonne National Laboratory; [2]University of Chicago; [3]Lawrence Berkeley National Laboratory; [4]University of California, Berkeley; [5]Pacific Northwest National Laboratory; [6]Massachusetts Institute of Technology; [7]Columbia University; [8]University of Houston; [9]Princeton University

With the newly established ESRA, an Energy Innovation Hub funded by the U.S. Department of Energy (DOE), we focus on energy storage materials beyond lithium-ion. ESRA aims to enable transformative discoveries in sodium and zinc electrochemistry as abundant and sustainable energy solutions. We hope to lay the scientific foundations for breakthroughs in energy storage technologies enabled by sodium and zinc chemistry and train the next-generation battery workforce to ensure U.S. scientific and economic leadership. In this talk, I will discuss a few new perspectives for energy storage materials including new solvation architecture design for liquid electrolytes, new superionic conductors in soft or hard materials, and their interfacial engineering. With recent advances in photon and electron characterization tools and computational methods, we can explore ionic mobility, charge transfer, and ion-matter interactions in electrochemical system in operando. I will also give our new perspective on how we can leverage modern machine learning and artificial intelligence, powered by our materials acceleration platform and correlative characterization to enable the discovery of new phenomena in ion-matter interactions.

9:30 AM

D-I-2: Aqueous Battery Consortium

[Hub - ABC] Yi Cui[1,2]
[1]Stanford University; [2]SLAC National Accelerator Laboratory

In order to have major impacts on integrating clean electricity from solar and wind into electricity systems, global battery energy storage needs to be scaled up to multiple 100 TWhs. Battery chemistries need to be based on earth abundant materials and solvents. Water stands out as the most attractive solvent for scaling, low cost and safety. Here this presentation will also introduce the newly awarded DoE Energy Innovation Hub: Aqueous Battery Consortium (ABC). The ABC Hub will generate fundamental breakthroughs to enable aqueous batteries for energy storage with a potential of 10x reduction in the cost floor compared with lithium-ion batteries, while ensuring excellent safety and scalability for global impacts. The Hub is organized in six aims + three crosscuts to study low-cost redox chemistries such as Zn, Mn and Fe.

9:50 AM

D-I-3: Hybrid Photoelectrode Architectures for Liquid Solar Fuels

[Hub - CHASE] Gerald Meyer, Jillian Dempsey
University of North Carolina at Chapel Hill

The overarching goal of the Center for Hybrid Approaches in Solar Energy to Liquid Fuels (CHASE) is to develop the fundamental science necessary for the realization of hybrid photoelectrodes that generate liquid fuels from the small molecules in air and sunlight. CHASE has developed hybrid photoelectrodes using semiconducting Si light absorbers with integrated molecular catalysts that mediate cascade reduction of CO_2 to CH_3OH. Si is chosen as the primary light absorber in CHASE due to its favorable bandgap for solar light harvesting and well-known optoelectronic and surface modification properties. Molecular catalysts are used in CHASE due to their highly selectivity for CO_2 reduction and for the ability to optimize catalysis through structure–property relationships. CHASE's cross-disciplinary research team have worked towards two distinct "Architectures" for solar fuel production: a Wired Architecture, where catalysis at the semiconductor-electrolyte interface is driven by conduction band electrons and electrolyte protons feed a catalyst cascade, and a Decoupled Architecture utilizing recyclable proton–electron mediators to drive thermal catalytic reactions away from the semiconductor. This talk will discuss CHASE research highlights towards the pursuit of high-performing hybrid photoelectrodes for the production of liquid solar fuels, and the factors that limit the performance of these systems.

10:10 AM

D-I-4: Mechano-chemical Understanding of Solid Ion Conductors

[EFRC - MUSIC] Jeff Sakamoto[1,2], Neil Dasgupta[1], Matt McDowell[3], Partha Mukherjee[4], David Kwabi[5], Kelsey Hatzell[6], Miaofang Chi[7], Donald Siegel[8], David Mitlin[8], Bart Bartlett[1], Yet-Ming Chiang[9], Sossina Haile[10], Nicola Perry[11], Katsuyo Thornton[1], Michael Thouless[1], Bilge Yildiz[9], Raphaele Clement[2]
[1]University of Michigan; [2]University of California, Santa Barbara; [3]Georgia Institute of Technology; [4]Purdue University; [5]Yale University; [6]Princeton University; [7]Oak Ridge National Laboratory; [8]University of Texas at Austin; [9]Massachusetts Institute of Technology; [10]Northwestern University; [11]University of Illinois Urban-Champaign

MUSIC was created to meet the growing need for a concerted effort to integrate the fields of mechanics, chemistry, and electrochemistry to understand electro-chemo-mechanical phenomena underlying the synthesis and use of ceramic ion conductors for energy storage. MUSIC will advance the frontier of energy storage R&D by understanding and controlling emergent mechano-chemical phenomena. Integral to its scientific aspirations, MUSIC will mentor, train, and educate the next-generation energy science workforce, providing opportunities for knowledge generation and professional development. Connecting experiments to theory, leaders in the fields of multi-scale modeling with experience in mechano-electro-chemistry are integral to MUSIC. Augmenting the ability to better understand complex phenomena under dynamic conditions and at buried interfaces, MUSIC also includes key researchers that are advancing the state-of-the-art of in situ/operando and multi-scale modeling over all relevant length and time scales. To bolster efforts to create a viable and independent energy industry, processing and manufacturing science pervades across all themes within MUSIC. Most importantly, MUSIC acknowledges the role that postdocs and students will play in enabling science within the center and in future decades.

Session III: Tuesday, August 12, 2025, 9:00 – 10:20 AM, Salon F

9:00 AM

D-III-1: Probing reactive fracture dynamics with experiments and modeling

[EFRC - GMCS] Chelsea Neil[1], Hoang Nguyen[1], Wenfeng Li[1], Uwaila Iyare[1], Yun Yang[1], Lawrence Boampong[1], Prakash Purswani[1], Jeffrey Hyman[1], Peter Kang[2], Hari Viswanathan[1], Emmanuel Detourney[2]
[1]Los Alamos National Laboratory; [2]University of Minnesota

Understanding the potential for reaction-driven cracking in fractured geomedia is critical for optimizing injectivity, reaction, and storage applicable to many subsurface engineering operations. Through our center, we combine advanced experiments and modeling to investigate the conditions under which chemical reactions influence fracture propagation and permeability evolution. Using triaxial direct shear (TDS) tests with real-time X-ray tomography, batch reactor experiments, microfluidics, and neutron reflectometry, we explore the interplay between reactive transport, mechanical deformation, and fracture interface chemistry during the mineralization of olivine-rich rocks. Results demonstrate that, while reaction-induced cracking was not observed under our experimental conditions, mechanical stimulation can significantly enhance fracture complexity and permeability under low confining stresses. Flow rate further governed precipitation extent and distribution, with higher flow promoting more reaction and deeper penetration of the reaction front into fractures. Experimental observations are incorporated into field-scale models to explore reactivity in a realistic fracture network using LANL-developed dfnWorks. Our findings highlight the critical roles of fracture geometry, flow dynamics, and mineralogy in controlling the extent and nature of reaction in fractured systems. While direct evidence for reaction-driven cracking remains elusive, we identify key mechanisms, including stimulation, reactive surface passivation, and fracture aperture effects, that will strongly influence mineralization. Ongoing work aims to refine predictive models and explore longer-duration reactions to better constrain conditions under which chemically-driven fracture propagation may occur.

9:20 AM

D-III-2: Mechano-chemical Understanding of Solid Ion Conductors (MUSIC) Selected topics

[EFRC - MUSIC] Jeff Sakamoto[1,2], Neil Dasgupta[1], Matt McDowell[3], Partha Mukherjee[4], David Kwabi[5], Kelsey Hatzell[6], Miaofang Chi[7], Donald Siegel[8]
[1]University of Michigan; [2]University of California, Santa Barbara; [3]Georgia Institute of Technology; [4]Purdue University; [5]Yale University; [6] Princeton University; [7]Oak Ridge National Laboratory; [8]University of Texas at Austin

The rapidly-evolving field of mechano-chemistry creates the impetus to adapt MUSIC's scientific priorities to bridge emergent knowledge gaps. Responding to these needs, MUSIC is emphasizing the following topical areas: 1) Reaction Processes at Metal/CIC Interfaces, 2) Advanced Cathodes, 3) Fluid Interfaces, and 4) Electrochemically Driven Fracture Processes. Integral to these areas are MUSIC's cross-cutting themes: Manufacturing, in situ/operando characterization, and multiscale modeling. This presentation will highlight recent progress in MUSIC's topical areas and cross-cutting themes and will showcase the synergy and impact to the field of mechano-chemistry and the related fields of materials science, electrochemistry, ceramic electrolytes, and manufacturing.

9:40 AM

D-III-3: Elucidating Productive Electrochemically Induced Dissolution/Deposition Systems

[EFRC - m2M#s] Kenneth Takeuchi[1,2], Alan West[3], Shan Yan[2], Yimei Zhu[2], Ping Liu[2], Amy Marschilok[1,2], Esther Takeuchi[1,2]
[1]Stony Brook University; [2]Brookhaven National Laboratory; [3]Columbia University

For intercalation materials, the kinetics and uniformity of mass transport across the nanocrystalline domains dictate the structural reversibility and transport capability at the macroscopic level. Conversion materials which undergo more significant changes of state and/or phase upon electrochemical redox bring added challenges for phase identification and prediction of resultant electrochemical behavior at the systems level. For batteries with solid electrodes and liquid electrolyte one of the most dramatic changes of phase is dissolution of active transition metal species as a result of electrochemical redox. In lithium ion systems dissolution of transition metal species from the positive electrode into the electrolyte is a life limiting phenomenon, however for aqueous zinc systems, dissolution/deposition of manganese can be a productive process for energy storage. This presentation highlights progress in mechanistic elucidation and predictive modeling of battery behavior by coupling ex-situ, in-situ, and operando electrochemistry, spectroscopy, microscopy, and diffraction data with physics-based continuum modeling.

10:00 AM

D-III-4: Geo-processes in mineral carbon storage - fundamental challenges

[EFRC - GMCS] Haiying Huang[1], Emmanuel Detournay[2], Zdeněk Bažant[3], Giuseppe Buscarnera[3], Bojan Guzina[2], Lars Hansen[2], Jeffrey Hyman[4], Peter Kang[2], Qinjun Kang[4], Joseph Labuz[2], Jialiang Le[2], Juerg Matter[5], Sofia Mogilevskaya[1], Chelsea Wren Neil[4], John Rudnicki[3], Gowri Srinivasan[4], Hari Viswanathan[4], Vaughan Voller[2]
[1]Georgia Institute of Technology; [2]University of Minnesota; [3]Northwestern University; [4]Los Alamos National Laboratory; [5]University of Southampton

Mineral carbon storage presents a promising solution to mitigate anthropogenic CO_2 emissions. By taking advantage of mineralization reactions that occur when CO_2 gets in contact with Mg, Fe, and Ca-rich minerals present in mafic and ultramafic rocks such as basalt and peridotite, we can transform CO_2 into solid carbonates, thus making permanent subsurface storage feasible. Mafic and ultramafic rock masses are abundant in the Earth's crust. Over the past decade, the concept of mineral carbon storage has been successfully pilot-tested in basalt formations, where reservoir permeability is relatively high and the presence of natural fractures expected. CarbFix and CarbFix2 in Iceland and the Wallula project in Washington state have both demonstrated carbon mineralization could occur on a time scale of months to years. However, the feasibility in low permeability ultramafic rocks such as peridotite is yet to be shown. Efficient mineralization of these rock masses requires the existence or development of a penetrating fracture network that accommodates the flow and reaction of CO_2 bearing fluids. For both types of rocks, there are significant knowledge gaps in our current understanding of the relevant geochemistry, flow and transport processes, and the coupling between geomechanics and reactive transport for realistic engineering of large-scale mineralization operations. In this talk, our latest efforts to address the fundamental questions on reaction induced cracking will be presented. Through hydro-chemo-mechanically coupled modeling, we show that an ultramafic rock reservoir could be highly fractured due to volume expansion types of hydration and carbonation reactions over geological time.

Session IV: Tuesday, August 12, 2025, 1:30 – 3:10 PM, Salon F

1:30 PM – Team Science Finalist

D-IV-1: UNLOCKING HIGH CONDUCTIVITY IN COMPOSITE ELECTROLYTES FOR NEXT GENERATION ENERGY STORAGE

[EFRC - FaCT] Ji-young Ock[1], Amit Bhattacharya[2], Lauren B. Shepard[3], Tao Wang[1], Miaofang Chi[1], Sheng Dai[1,4], Susan B. Sinnott[3], Alexei P. Sokolov[1,4], Raphaële J. Clément[2], Xi Chelsea Chen[1]
[1]Oak Ridge National Laboratory; [2]University of California, Santa Barbara; [3]The Pennsylvania State University; [4]University of Tennessee-Knoxville

To accelerate advancements in energy storage and conversion technologies, the FACT-EFRC integrates advanced characterization and computation, bridging atomic and mesoscale processes. Our goal is to uncover ion transport mechanisms in polymer-ceramic composites, which combine robust mechanical strength with high ionic conductivity. A key focus is understanding how ions move along and across polymer–ceramic interfaces and how this

influences transport properties, ultimately enabling the rational design of next-generation, high-performance energy storage devices.

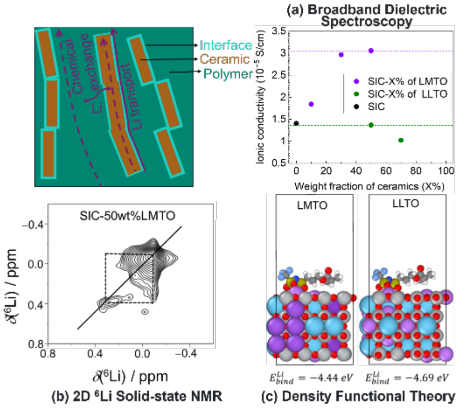


Fig 1. (top-left) Schematic of Li-ion transport in polymer–ceramic composite. (a) Conductivity enhancement with LMTO nanorods. (b) No observable Li-ion exchange between SIC and LMTO (NMR). (c) DFT confirms reduced Li–anion binding at the LMTO interface.

We have developed a flux strategy to synthesize 1D $Li_{0.11}Na_{0.24}K_{0.02}La_{0.43}TiO_{2.82}$ (LMTO) single-crystal nanorods with an A-site disordered cubic perovskite phase, overcoming the challenge of achieving cubic symmetry in LMTO. These LMTO nanorods were incorporated into a vinyl ethylene carbonate (VEC)-based single-ion conducting (SIC) polymer electrolyte. Notably, the composite containing 50 wt. % LMTO exhibited a two-fold increase in ionic conductivity, while micron-sized commercial $Li_{0.33}La_{0.55}TiO_3$ (LLTO) showed no enhancement. To elucidate the underlying conduction mechanism, we employed a combination of experimental techniques, including solid-state nuclear magnetic resonance (NMR), in conjunction with density functional theory (DFT) calculations. We hypothesized that the conductivity enhancement originates from the formation of a thin interfacial polymer layer around the LMTO nanorods with enhanced Li^+ mobility. We tracked ion transport pathways in the composite electrolyte using tracer exchange NMR and probed Li exchange at the polymer-ceramic interface using 2D ^6Li exchange spectroscopy measurements and a new $^6Li/^7Li$ isotope exchange method to probe ‘ultra-slow’ chemical exchange processes occurring on timescales of hours to days. Our experiments confirm that LMTO nanorods function as passive fillers and likely enhance conductivity by reducing electrostatic interactions between Li^+ and the polyanion matrix. Complementary DFT calculations quantify the Li-ion binding energy at the polymer–ceramic interface and show that the Li-ion is less strongly bound to the anion at the LMTO interface compared to the LLTO interface, suggesting that the LMTO composition can also enhance interfacial Li^+ transport. Our experiments suggest that the formation of a percolation pathway and fast ion exchange at the polymer–ceramic interface are key to achieving ultra-high conductivity, as further supported by Li binding energies from DFT calculations. Overall, this work illustrates the interdisciplinary capabilities of FaCT for unveiling interfacial ion transport in polymer-ceramic composite electrolytes for next generation energy storage materials.

References: [1]Ock, J., et al. *Macromolecules* **2024**, *57*, 7489.; [2]T. Wang, et al., *Adv. Sci.* **2025**, 12, 2408805.; [3]Ock, J., et al. *(under review)* **2025**.; [4]Bhattacharya, A.; et al. *(under revision)* **2025**.

Contributions: A.B. performed the NMR spectroscopy characterizations, J.O. synthesized the composite electrolytes and performed electrochemical measurements, L.B.S. conducted the DFT calculations, T.W. synthesized the LMTO ceramic, M.C. performed the TEM. S.D, S.B.S, A.P.S, R.J.C, X.C.C supervised.

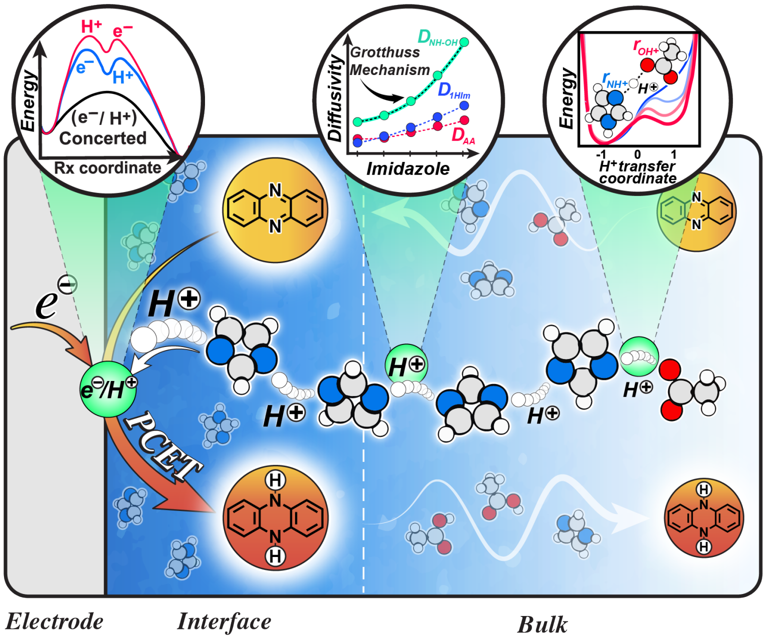
1:50 PM – Team Science Finalist

D-IV-2: QUANTUM-TUNED CONCENTRATED HYDROGEN-BONDED ELECTROLYTES FOR ENHANCED PROTON TRANSFER

[EFRC - BEES2] Miguel Muñoz[1], Giselle de Araujo Lima e Souza[2], Michael S. Chen[3], Kaylie Glynn[4], Benworth B. Hansen[4], Peisen Qian[5], Thomas Simunovic[6], Mrinlini Kolaprath[6], Mark Dadmun[6], Thomas Zawodzinski[6], Joaquín Rodríguez-López[5], Steve G. Greenbaum[2], Mark Tuckerman[3], Joshua R. Sangoro[4], and Burcu Gurkan[1]

[1]Case Western Reserve University; [2]Hunter College-CUNY; [3]New York University; [4]The Ohio State University; [5]University of Illinois Urbana-Champaign; [6]University of Tennessee-Knoxville

Concentrated hydrogen-bonded electrolytes (CoHBEs) are electrochemically stable and less-volatile alternatives to conventional electrolytes that present heterogeneous liquid structure. While the species diffusivity via vehicular transport, where species move with their solvation shell is hindered in viscous structured electrolytes like CoHBEs, Grotthuss transport where hopping occurs through the dynamic reorganization of the solvating species, is fast and hypothesized to enhance electrokinetics. This work presents a fundamental understanding of the proton conduction mechanism in CoHBEs where the dynamic hydrogen-bond networks in mixtures of acids and amphoteric azoles were leveraged to probe the hypothesis for proton coupled electron transfer (PCET) reactions that are relevant to energy storage and conversion processes. In particular, the analysis of proton transfer energy barriers calculated by path integral molecular dynamics (PIMD) simulations showed a reduction at specific compositions with a shift in proton localization toward azole driven tunneling when nuclear quantum effects were incorporated. Broadband Dielectric Spectroscopy (BDS) and Pulsed Field Gradient (PFG) NMR studies, in complement to FTIR and small-angle neutron scattering (SANS) further provided evidence to the decoupling of viscosity and conductivity in protic CoHBEs as the acid dimers are disrupted by the azole and as the extended azole chains enable virtually barrierless proton hopping. For example, despite its high viscosity (55 cP at room temperature), 1H-imidazole (1HIm) and acetic acid (AA) at 70:30 (1HIm:AA) molar mixture exhibit unexpectedly fast PCET kinetics for phenazines (rate constant of 10^{-4} cm/s) that is comparable to conventional electrolytes, as confirmed by rotating disk electrode (RDE) and scanning electrochemical microscopy (SECM) measurements. This is particularly unexpected when compared to the analogous mixture of 1-methyl-imidazole (1MIm) and AA that present lower viscosity (15 cP), however slower PCET reaction rates.



Therefore, promoting hydrogen-bonded chain formation among amphoteric species in protic CoHBEs without steric hindrances for proton conduction is shown to enhance PCET kinetics.

Contributions: M. Muñoz - development of CoHBEs, physical property and RDE kinetic measurements; G. de Araujo Lima e Souza - PFG NMR; M. Chen - PIMD simulations; K Glynn and B. B. Hansen - BDS and dynamic measurements; P. Qian - SECM capability development for kinetics; T. Simunovic - relaxation NMR; M. Kolaprath - SANS

2:10 PM

D-IV-3: Atomic Insights into Proton Conduction in Phosphosilicate Glass

[EFRC - HEISs] Bright Ogbolu[1], Jordan Meyer[2], Rongfu Zhang[1], Erica Truong[1], Zihan Lin[2], Sossina M. Haile[4], Ju Li[2], Bilge Yildiz[2], Yan-Yan Hu[1,4]
[1]Florida State University; [2]Massachusetts Institute of Technology; [3]Northwestern University; [4]Center of Interdisciplinary Magnetic Resonance, National High Magnetic Field Laboratory

Electrochemical ionic synaptic devices developed by our MIT team members function as programmable resistors for energy-efficient AI hardware. In our synaptic devices, working ion is the proton. A gate voltage drives protons from a reservoir through a solid electrolyte into a semiconducting channel, modulating its conductance. While nanosecond switching with very low energy has been demonstrated, high gate voltages are currently needed. To achieve low-voltage operation, inorganic, scalable fast proton conductors are needed-a gap for the field broadly. Here we explore nanometer-thin proton conductors based on phosphosilicate glass (PSG), a material with proton conductivity well below mS/cm at room temperature. Thin PSG films were fabricated via plasma-enhanced chemical vapor deposition (PECVD) with deposition parameters tuned to vary composition, structure, and morphology. Atomic force microscopy and gas physisorption reveal porous, granular structures with 2–4 nm pore sizes, and increasing pore surface area at higher power and phosphorus content. High-resolution multinuclear NMR of the most conductive films shows phosphorus-rich pore surfaces with hydroxyl groups hydrogen-bonded to absorbed water. P–OH species chemically exchanging with surface water exhibit the fastest proton dynamics, while Si–OH groups show moderate mobility. Electrochemical ^{1}H–^{2}H tracer-exchange NMR confirms that P–OH and Si–OH groups exchanging with adsorbed water mediate conduction. Pulsed-field gradient NMR reveals restricted proton diffusion. Ongoing molecular dynamics simulations aim to further elucidate conduction mechanisms informed by experimentally derived structures. These mechanistic insights will guide the optimization of PSG thin films to enable low-voltage, high-speed operation of next-generation synaptic devices.

2:30 PM

D-IV-4: Challenges and Opportunities for Aqueous Batteries

[Hub - ABC] Linda Nazar
University of Waterloo

Advancing the electric grid requires long-duration energy storage capacity of at least several hundred TWh, while lithium-ion batteries present issues due to resource availability, safety, and cost. Aqueous batteries – driven by electrodeposition reactions for both metal anodes and metal oxide cathodes and based on abundant electrode chemistries such as zinc, iron and manganese – offer wide opportunities. The multiple valence states of Fe and Mn even enable them to be used as both anodes and cathodes. In the case of $Zn^{2+}/Zn||MnO_2/Mn^{2+}$, an initially dual-electrode-free (anode/cathode) configuration can provide energy densities of over 200 Wh kg^{-1}, but with limited cycle life. While promising, the electrodeposition/stripping mechanism presents multiple fundamental knowledge gaps and significant technical hurdles to viable aqueous battery technologies. This talk will give an overview of some approaches we are taking in the Aqueous Battery Consortium to overcome such challenges. For example, these include soft templating that utilizes an in situ formed liquid crystal interphase; and strategies to disrupt water's hydrogen bonding network. Such tactics regulate the morphology of the Zn anode, and the phase of the deposited MnO_2, promoting layered structures with enhanced ion transport pathways that significantly improve stripping efficiency. Such dual-electrode-free batteries can achieve high Coulombic efficiency for extended cycling (>5000 cycles), opening exciting research directions for next-generation high-energy-density and long-duration energy storage based on aqueous chemistries.

2:50 PM

D-IV-5: Understanding Hydroxide Transport in Anion Exchange Membranes using Molecular Simulations

[EFRC - UNCAGE-ME] Mohammed Al Otmi[1], Ping Lin[1], William Schertzer[2], Coray M. Colina[1], Rampi Ramprasad[2], Janani Sampath[1]
[1]University of Florida; [2]Georgia Institute of Technology

Anion exchange membranes (AEMs) used in alkaline fuel cells rely on the selective transport of hydroxide ions through the membrane to produce electricity. The low conductivity of hydroxide ions in AEMs has prevented their widespread use and improving AEM conductivity is of significant fundamental and industrial relevance. The target for conductivity in AEMs set by the Department of Energy is typically ≥ 70 mS/cm at operating conditions. An understanding of the hydroxide transport mechanisms through the polymer can help in the design of membranes with improved performance. In prior work, we leveraged atomistic molecular dynamics (MD) simulations to capture correlations in hydroxide transport across four polyethylene AEMs with different functional groups. While the trends in conductivity were consistent with experiments, there was a significant difference in the magnitude between experiments and simulations. We ascribed this to the inability of our model to capture the reactive Grotthuss transport (proton hopping) mechanism which is dominant in these systems. In our current work, to account for Grotthuss transport, we use the heuristic reaction protocol REACTER that allows us to model reactions within the framework of classical simulations. We find that the simulated hydroxide conductivity is in better agreement with experimental values after the inclusion of Grotthuss transport. We extend our analysis across different AEM chemistries, including polyethylene and polynorbornene, and find that the balance between vehicular and Grotthuss transport strongly depends on the polymer's microstructure and water uptake.

E. Energy Storage II

Session I: Monday, August 11, 2025, 9:10 – 10:30 AM, Salon H

9:10 AM

E-I-1: Operando Characterization of Energy Materials and Devices

[EFRC - CABES] Andrej Singer, David Muller
Cornell University

We will discuss the use of operando methods for the characterization of energy materials and devices. Emphasis will be placed on the use operando electron microscopy, including 4D-STEM and ptychography and synchrotron-based X-ray studies including X-ray absorption spectroscopy and X-ray diffraction. Studies of materials including catalysts, supports and membranes as well as fuel cells and electrolyzers will be presented.

9:30 AM

E-I-2: High Entropy Oxides from the Molecular to the Mesoscale

[EFRC - m2M#s] Kenneth Takeuchi[1,2], Shan Yan[2], Yimei Zhu[2], Marca Doeff[3], Stanislaus Wong[1], Amy Marschilok[1,2], Esther Takeuchi[1,2]
[1]Stony Brook University; [2]Brookhaven National Laboratory; [3]Lawrence Berkeley National Laboratory

The high entropy materials concept is appealing because it opens additional possibilities for the materials designer to incorporate more of the periodic table, including abundant and sustainable elements. In the case of high entropy oxides (HEO), entropy is quantified based on configurational entropy of mixing, where multiple metal (ions) occupy the same crystallographic site. However, it is important to recognize that there is further opportunity to tune entropy from the atomic to the mesoscale in such materials. At the molecular or atomic level, the oxygen anion can be very important, where HEOs can be stabilized by the entropic contribution of oxygen vacancies, impacting both synthesis and electrochemical behavior. At the nanoscale to the micron scale, stacking faults and short-range order can be deterministic factors. This presentation will describe how adjusting the elemental ratios, as well as the elemental selection, can tune the structural and functional properties of the materials to create a family of related HEOs. Through deliberate synthesis and detailed characterization, correlations among HEO properties and resulting electrochemical behavior, including structure-function dependencies can be revealed. The complementary benefits of tunable synthesis, spectroscopy, microscopy, diffraction, electrochemically based characterization toward mechanistic understanding will be discussed.

9:50 AM

E-I-3: Ion Transport Enhancement and Interfacial Resistance in Polymer-Li-Garnet Composite Electrolytes

[EFRC - FaCT] Ji-young Ock[1], Michelle L. Lehmann[1], Chang Li[2], Kana Onoue[3], Yangyang Wang[1], Harry M. Meyer III[1], Raphaële J. Clément[3], Jeffrey Sakamoto[3], Zhezhen Fu[2], Alexei P. Sokolov[1], Xi Chelsea Chen[1]

[1]Oak Ridge National Laboratory; [2]Pennsylvania State University-Harrisburg; [3]University of California, Santa Barbara

Composite electrolytes that combine the high ionic conductivity of inorganic materials with the processability and conformal interfacial contact of polymers are promising candidates to meet the growing energy storage demands for national energy security. In such systems, the mechanism of ion transport enhancement is critically influenced by polymer–ceramic interfacial interactions. In this study, we demonstrate that incorporating high-entropy (HE) Li-garnet ceramics ($Li_7La_3Zr_{0.5}Nb_{0.5}Ta_{0.5}Hf_{0.5}O_{12}$) into a vinyl ethylene carbonate–based single-ion-conducting (SIC) polymer electrolyte results in a seven-fold increase in ionic conductivity (8.6×10^{-5} S/cm at 30 °C) compared to the neat polymer, while maintaining a high Li-ion transference number of 0.73.[1] In contrast, conventional Al-doped Li-garnet causes nearly an order-of-magnitude decrease in the composite's ionic conductivity. This difference is attributed to the HE Li-garnet's reduced susceptibility to surface passivation and Li_2CO_3 formation relative to the Al-doped counterpart. To mitigate carbonate buildup on the Li-garnet surface, we show that acid treatment effectively reduces the interfacial resistance between the model SIC polymer and a Ta-doped Li garnet. Finally, we present an estimate of the polymer-ceramic interfacial layer thickness[2] and a guideline for the maximum tolerable interfacial resistance that still enables conductivity enhancement in polymer–ceramic composite electrolytes.

1. J. Mater. Chem. A (2025), 10.1039/D5TA02665B. 2. Macromolecules (2024), 57, 7489.

10:10 AM

E-I-4: Beating the Viscosity-Conductivity Inverse Relation Barrier to Create a Breakthrough Electrolyte for Emerging Battery Applications: Does Quantum Mechanics Hold the Key?

[EFRC - BEES2] Mark Tuckerman[1], Joshua Sangoro[2], Steve Greenbaum[3], Burcu Gurkan[4]

[1]New York University; [2]The Ohio State University; [2]New York University; [3]Hunter College; [4]Case Western Reserve University

Candidate systems for next-generation battery electrolytes, such as deep eutectic solvents and ionic liquids, often suffer from the limitation of an empirical inverse relation between viscosity and conductivity, govern by the Walden's rule, which suppresses rates of charge transport and limits their electrochemical performance. Within the broader context of these ionic systems, the BEES2 team has been focusing on concentrated hydrogen-bonded electrolytes (CoHBEs), which are structured, electrochemically stable, and less-volatile. In addition, CoHBEs can be designed such that charge transport kinetics and solvent dynamics are largely decoupled, thus breaking the viscosity-conductivity tradeoff. The basic strategy for achieving this breakthrough performance is to leverage the Grotthuss transport mechanism by choosing organic molecular solvent species, such as imidazole, capable of supporting proton hops through a dynamic, amphoteric hydrogen-bond network along with redox-active molecules capable of reversibly exchanging protons with the solvent species and undergoing proton-coupled electron transfer (PCET) reactions with each other. Through a synergistic combination of experimental techniques and AI-drive quantum simulations, we have achieved a proof of concept of this strategy and uncovered the key solvent structures, namely hydrogen-bonded chains, and their reorientation dynamics, leading to a fundamental understanding of how these systems attain their unusual performance. Additionally, we have revealed the significant role played by cooperative nuclear quantum effects in these systems, thus suggesting a new paradigm in the design of structured electrolytes exhibiting breakthrough, quantum-dominated charge transport dynamics.

Session III: Tuesday, August 12, 2025, 9:00 – 10:20 AM, Salon H

9:00 AM

E-III-1: Tracking Behavior in Microemulsions from Bulk Structure and Transport to Interfacial Processes

[EFRC - BEES2] Thomas Zawodzinski[1], Eliandreina Cruz-Barrios[2], Adam Imel[1], Brian Barth[1], Damilola Ojedeji[1], Ashraful Haque[1], Mark Dadmun[1], Emmanouil Doxastakis[1], Emily Pentzer[2]
[1]University of Tennessee-Knoxville; [2]Texas A&M University

In microemulsion-based electrolytes, redox activity does not just depend on nanophase organization; it depends on location. Where do the redox-active species go in a multiphase environment during the charge and discharge of an electrochemical system? How does the interface between oil, water, and surfactant domains dictate accessibility, mobility, and electron transfer? This talk explores the interfacial structure of microemulsions and their central role in governing electrochemical behavior. Using model systems, including ferrocene derivatives and rubrene, we trace the partitioning of redox-active molecules and how their local environment, such as bicontinuous phases or surfactant-rich interfaces, affects the electrochemical response. We will connect molecular-scale insights, including coarse-grained and atomistic simulations and neutron reflectivity in an electric field.

9:20 AM

E-III-2: Controlling the Energy Barriers for Ion Transport in Polymers

[EFRC - FaCT] Catalin Gainaru[1], Harmandeep Singh[2], Ivan Popov[3], Michelle L. Lehmann[1], Md Anisur Rahman[1], Valentino R. Cooper[1], Kenneth S. Schweizer[4], Rajeev Kumar[1], Tomonori Saito[1,2], Alexei P. Sokolov[1,2]
[1]Oak Ridge National Laboratory; [2]University of Tennessee-Knoxville; [3]University of Tennessee-Oak Ridge Innovation Institute; [4]University of Illinois Urbana-Champaign

The development of novel polymer electrolytes for energy storage and conversion requires a fundamental understanding of the parameters controlling their energy barriers E for ion

transport. These are usually extracted using apparent Arrhenius laws. We demonstrated that this procedure strongly overestimates E values and developed a novel approach with more accurate estimates[1]. Employing this new approach to single-ion conducting polymers, we show that E decreases continuously with mobile cation size and is sensitive to the dielectric permittivity of the matrix[2]. Using this knowledge, we demonstrated that the conductivity of dual-ion conducting polymers can be significantly enhanced through an increase in the polarity of side chains and their self-organization into specific morphologies acting as ionic channels. To this end, we functionalized a Li salt-doped polymer matrix by tailored amounts of zwitterionic (ZI) groups[3]. Our results reveal the emergence of a percolation conductivity regime above a specific ZI concentration, with ion hopping decoupled from segmental dynamics by up to ten orders of magnitude. Consequently, in the highly concentrated ZI regime, our polymers exhibit in their glassy state energy barriers for ion hopping similar to superionic ceramics. Our investigation also revealed that at room temperature ion dynamics in the glassy poly(zwitterion) is significantly faster than that in the liquid monomeric ZI compound. These results call for revisions of earlier Arrhenius analyses and highlight the crucial role played by local morphology for the design of solid-state superionic polymers for energy applications.

1. Macromolecules (2023), 56, 6051; 2. ACS Appl. Polym. Mater. (accepted); 3. Mater. Today (accepted).

9:40 AM – Team Science Finalist

E-III-3: STRUCTURE–PROPERTY RELATIONSHIPS FOR MULTI-ELECTRON ORGANIC POSITIVE ELECTRODE MATERIALS

[EFRC – ESRA] Alae Eddine Lakraychi[1], Harshan Reddy Gopidi[1], Jiaqi Wang[2], Zeqian Zhang[3], Yu Chen[4], Ying Chen[3], Kamila Magdalena Wiaderek[2], Mary C. Scott[4], Pieremanuele Canepa[1], Yan Yao[1]
[1]University of Houston; [2]Argonne National Laboratory; [3]Pacific Northwest National Laboratory; [4]Lawrence Berkeley National Laboratory

Soft organic materials offer a promising platform for solid-state batteries due to their design flexibility and ability to create conformal interfaces with solid electrolyte. However, their design has traditionally focused on molecular-level attributes while neglecting structure, limiting their implementation in energy storage. *Here, we aim to bridge this knowledge gap by understanding structure–property relationships underlying the performance of soft organic electrode materials.* Our research strategy combines expertise in materials design, synthesis, operando characterization, and theoretical modeling through collaboration among various institutions. This integrated approach enables a comprehensive understanding of redox events, structural evolution, and coupled ion–electron transport dynamics as a function of the state of charge.

We have selected *bis*-tetraaminobenzoquinone (TAQ) as a model compound, due to its layered crystal structure and high intrinsic room-temperature electrical conductivity ~10^{-4} S cm^{-1}. To date, we have synthesized all relevant Li_xTAQ (x = 0, 2, and 4) intermediates and independently characterized their physicochemical and electrochemical properties to elucidate the complete reaction pathway. *Ex-situ* and *operando* X-ray diffraction analysis revealed that TAQ undergoes a reversible expansion of the interlayer spacing upon Li intercalation within TAQ layers. The preferred Li-ion insertion sites were accurately predicted using two distinct computational algorithms developed within ESRA.

We investigated the mixed ionic–electronic conduction (MIEC) properties using electrochemical and spectroscopic characterizations. The electrical conductivity was found to be proportional to the concentration of radical species within the material, peaking at ~10^{-2} S cm^{-1} for Li_2TAQ. In contrast, the ionic conductivity increased with lithium content in Li_xTAQ, reaching ~10^{-6} S cm^{-1} for Li_4TAQ. By exploiting the inherent MIEC properties of LixTAQ, we demonstrated solid-state cells operating with a high cathode fraction (~70 wt%) and at low stack pressures (~1 MPa).
These initial exciting findings from ESRA offer fundamental insights into the structure–property relationships of TAQ system, providing a foundational framework for designing novel multi-electron conformal organic electrode materials for durable energy storage systems.

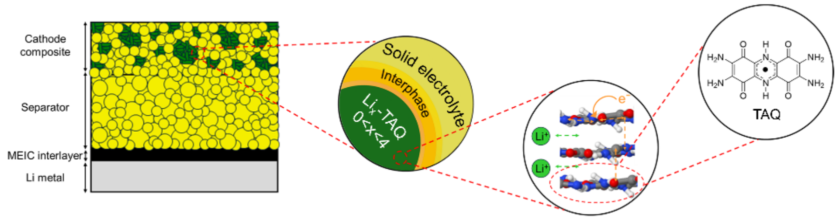


Figure 1: Interdisciplinary research strategy to investigate structure-property relationships in soft organic materials.

Contributions: A.E.L performed material synthesis and characterization, H.R.G carried out theoretical modeling, Y.C micro-electronic diffraction, Z.Z. operando electron paramagnetic resonance, and J.W. X-ray diffraction and pair distribution function.

10:00 AM

E-III-4: Designing Silicon Coatings and Interfaces to Enable Efficient Charge Transfer to Molecule Catalysts, Impart Long-Term Stability, and Control Product Distributions

[Hub - CHASE] Oluwaseun Oyetade[1], Shi He[1], Ryan Gentile[1], Hannah Margavio[2], Conor Rooney[3], Marisé Garcia-Batlle[1], Pablo Fernandez[1], John Dickenson[1], Samuel Bottom[1], Stephen Tereniak[1], Carrie Donley[1], Renato Sampaio[1], Matthew Lockett[1], Gerald Meyer[1], Rene Lopez[1], Hailiang Wang[3], Gregory Parsons[2], James Cahoon[1]
[1]University of North Carolina at Chapel Hill; [2]North Carolina State University; [3]Yale University

The Center for Hybrid Approaches in Solar Energy to Liquid Fuels (CHASE) integrates Si photoelectrodes with molecular catalysts to produce liquid fuel products from sunlight, CO_2, and water. These hybrid systems must satisfy a myriad of requirements, including efficient charge transfer and aqueous stability, where success is determined by both the solid-state engineering and molecular design of the interface. Here, we briefly review key design elements and hybrid platforms in active development within CHASE and highlight two major platforms. First, CHASE developed a 2–3 nm thermal oxide layer on Si that exhibits stability in aqueous solution, high photovoltage, and a photocurrent density of ∼10 mA/cm^2 for solar-driven photoelectrochemical reduction with a cobalt bis(terpyridine) molecular catalyst. An electron inversion layer with metal-like electron density facilitates electron transfer via tunneling even if a catalyst's reduction potential is beyond the semiconductor's conduction band edge. Second, CHASE developed a process to grow out-of-plane 'fuzzy' graphene covalently anchored to the Si surface via a silicon oxycarbide interfacial layer. This interface exhibits excellent durability under aqueous conditions. Integrated with cobalt phthalocyanine molecular catalyst microcrystals, the system can exhibit a unity Faradaic efficiency for CO_2 reduction to CO. With the addition of an ionomer overlayer that modulates the surface microenvironment, CO_2 reduction to methanol is observed with a Faradaic efficiency approaching 20%. Because both Si thermal oxide and fuzzy graphene exhibit excellent stability and charge transfer characteristics, they represent robust platforms on which to continue to design more complex CHASE hybrid photoelectrodes for liquid fuel production.

F. Energy-Water

Session I: Monday, August 11, 2025, 9:10 – 10:30 AM, Brookside B

9:10 AM

F-I-1: Impacts of Acid Gases on Microporous Materials for Use in Polar/Non-Polar Gas Separations

[EFRC - UNCAGE-ME] Ryan Lively
Georgia Institute of Technology

Many industrial gas separation challenges focus on refining polar from non-polar species, often in the presence of acidic compounds. For instance, biogas (a mixture of CO_2, H_2S, CH_4, and other compounds) is a renewable energy source that can be utilized by municipalities around the country; however, creating pipeline-grade natural gas from biogas using compact separations equipment is a challenge. In particular, the removal of H_2S and CO_2 is critical prior to further transportation and processing as both are acid gases that cause equipment and pipeline corrosion. A long-standing objective of the UNCAGE-ME (Understanding and Controlling Accelerated and Gradual Evolution of Materials for Energy) EFRC has been to develop fundamental structure-property relations describing how acid gases interact with adsorbents and catalysts. This has been achieved via an interdisciplinary effort that combined machine learning techniques, molecular modeling, novel synthesis, and advanced in situ/operando characterization techniques. Several examples of this approach will be provided in this talk with a focus on adsorptive gas separations.

9:30 AM

F-I-2: Center for Materials for Water and Energy Systems (M-WET)

[EFRC - M-WET] Christopher Bates[2], Raphaële Clément[2], Phillip Christopher[2], Ethan Crumlin[3], Berkin Dortdivanlioglu[1], Glenn Fredrickson[2], Benny Freeman[1] (director), Venkat Ganesan[1], Craig Hawker[2], Graeme Henkelman[1], Lynn Katz[1] (associate director), Manish Kumar[1], Gabriel Sanoja Lopez[1], Nathaniel Lynd[1], Dylan McReynolds[1], Zachariah Page[1], Rachel Segalman[2] (associate director), Scott Shell[2], Todd Squires[2], Gregory Su[3]
[1]University of Texas at Austin; [2]University of California, Santa Barbara; [3]Lawrence Berkeley National Laboratory

M-WET's mission is to discover and understand the fundamental science necessary to design new membrane materials and develop tools and knowledge to predict new materials' interactions with targeted solutes. We are inspired by the need to provide fit for purpose water from low quality water sources and recover valuable solutes with less energy. Specific interactions (and non-interactions) facilitate solute selectivity and fouling resistance, yet they cannot currently be "designed" a priori into membranes. This critical advance requires fundamental insights into the impact of functional groups on water dynamics near interfaces, an understanding of the impact of hydration on solute transport and membrane properties, and new routes to manufacture robust porous and nonporous membranes at scale. Motivated by the Basic Research Needs Report on Energy and Water, our specific goals are to: (1) design new interfaces with controlled topology and functionalities to achieve, for example, fouling-resistant surfaces and highly selective membranes; (2) precisely control mesoscopic material architecture to build novel, highly permeable, and selective membranes with rapid, component-resolved transport at multiple scales for resource recovery and producing fit-for-purpose water, while introducing design principles from (1); (3) develop novel imaging characterization tools for these systems; and (4) model multicomponent materials, fluid mixtures, and mesoporous architectures from atomistic to macroscale to radically transform membrane/materials systems' energy demands, resiliency, and efficiency. This presentation will highlight M-WET's scientific advances in support of these goals, including highlighting M-WET's advances on the relevant disciplinary fields and our training of next generation interdisciplinary researchers addressing the water/energy nexus.

9:50 AM

F-I-3: Unifying Structure–Property Relationships in 2D Laminar Membranes: Insights from Phyllosilicates, TMDs, and MXenes

[EFRC - AMEWS] Seth B. Darling[1,2], Kelsey B. Hatzell[3], Chong Liu[2]
[1]Argonne National Laboratory; [2]University of Chicago; [3]Princeton University

Understanding and controlling structure–property relationships in laminar membranes assembled from two-dimensional (2D) materials is critical to advancing selective transport. In this collaborative presentation, we bring together complementary insights from three classes of 2D materials—phyllosilicates, transition metal dichalcogenides (TMDs), and MXenes—to construct a unified framework for the design and deployment of next-generation membranes.

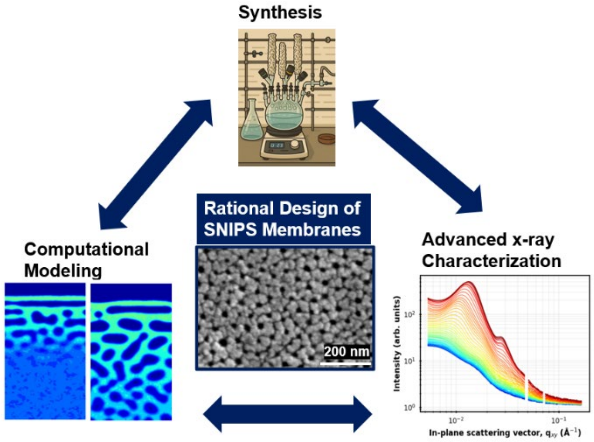
Despite differences in composition, charge, and dimensionality, these materials share key structural motifs: tunable interlayer spacings, anisotropic transport pathways, and surface chemistries that strongly influence ion and molecular selectivity. By systematically probing how hydration, layer stacking disorder, and defect landscapes govern transport properties, we uncover cross-cutting principles that transcend individual material classes. For example, we show how the interplay of interlayer electrostatics and dynamic swelling modulates selectivity in phyllosilicates and MXenes, while pore-edge chemistry in TMDs provides a contrasting but complementary route to control flux and rejection.

Our integrated approach combines advanced synthesis, high-throughput characterization, and modeling to identify how local atomic environments translate into emergent membrane behavior. By comparing transport regimes across these systems—from ultrathin ion sieves to thick, hierarchical assemblies—we aim to distill broadly applicable design rules. This convergence of material-specific expertise enables a richer understanding of the mechanisms underpinning selective transport, offering new pathways for membrane innovation in water treatment, energy technologies, and separations.

10:10 AM – Team Science Finalist

F-I-4: TOWARDS RATIONAL DESIGN OF TOUGHER SNIPS MEMBRANES FOR WATER AND ENERGY SYSTEMS

[EFRC - M-WET] Noah P. Wamble[1], Chuqiao Chen[2], José Carlos Díaz[1,3], Benjamin J. Pedretti[1], Adam N. Mann[1], Matthew R. Landsman[1,3], Louise Kuehster[1], Mostafa Nassr[1], Lynn E. Katz[1], Nathaniel A. Lynd[1], Glenn H. Fredrickson[2], Gregory M. Su[3], Gabriel E. Sanoja[1], Benny D. Freeman[1]
[1]University of Texas at Austin; [2]University of California, Santa Barbara; [3]Lawrence Berkeley National Laboratory



Ultrafiltration membranes with high selectivity and permeability are essential for reducing the pernicious coupling between water and energy, enabling low-energy routes to clean water. SNIPS (i.e., self-assembly plus nonsolvent-induced phase separation) membranes, which combines block copolymer self-assembly with nonequilibrium membrane manufacturing methods, yields asymmetric, isoporous membranes with a narrow surface pore size distribution and high permeances and selectivities. In this process, a block copolymer is cast into a film from a solution where the polymer has formed micelles. The cast film is evaporated (i.e., the dry step) to preferentially concentrate polymer at the polymer solution/air interface, then placed in a non-solvent (usually water) to bring about nonsolvent-induced phase separation to form a well-ordered membrane having pores of nearly the same size, rather than a broad pore size distribution as is found in conventional membranes. However, the design space for these membranes is vast, and control over membrane morphology (and hence membrane performance) during this nonequilibrium process requires laborious optimization. Additionally, polystyrene-b-poly(4-vinylpyridine) (SV), which works well with SNIPS, has a brittle, polystyrene membrane matrix with poor mechanical properties that limits the utility of these high-performance membranes. In this project, tough, isoporous membranes were cast using an ABAC tetrablock polymer, polystyrene-*b*-polyisoprene-*b*-polystyrene-*b*-poly(4-vinylpyridine) (SISV), synthesized by anionic polymerization. This unique architecture gave membranes with an order of magnitude higher toughness than SV membranes due to rubber toughening. Resonant soft x-ray scattering experiments were used to probe the length scales of these rubbery and glassy domain sizes to understand the impact of nanoscale morphology on membrane performance. Additionally, micelle morphology and evolution during the dry step were investigated via NMR experiments and in situ grazing incidence small angle x-ray scattering experiments to elucidate the connection between casting conditions and membrane performance (i.e., rejection and permeance). To study the impact of solvent blend choice on membrane performance, self-consistent field theory (SCFT) simulations were conducted and revealed that solvent-nonsolvent interactions influence how well-connected the membrane substructure is during diffusion-induced phase separation, which could rationalize membrane performance. Together, these efforts lay the groundwork for rational codesign of SNIPS membranes with high permeability, selectivity and enhanced mechanical toughness.

Contributions: B.J.P. and L.K. synthesized the polymers. N.P.W. cast membranes, performed scattering, NMR, and membrane characterization studies. N.P.W. conducted data analysis, led the project, and wrote the first draft of the manuscript. C.C. performed SCFT simulations. M.R.L., J.C.D., and M.N. helped design and conduct x-ray scattering experiments. A.N.M performed mechanical tests. L.E.K., N.A.L., G.H.F., G.M.S., G.E.S., and B.D.F. secured the resources to conduct this study and provided guidance for the project.

Session II: Monday, August 11, 2025, 1:40 – 3:20 PM, Brookside B

1:40 PM

F-II-1: A New, Unified Theory of Confined Fluid Thermodynamics

[EFRC - CENT2] Michael S. Strano[1], Sanjay S. Garimella[1], Yu-Ming Tu[1], Rahul P. Misra[1], Cody L. Ritt[1], Daniel Blankschtein[1], Xintong Xu[2], Arun Majumdar[2], Jordan Hachtel[3], Narayana Aluru[4], John Cumings[5], YuHuang Wang[5]
[1]Massachusetts Institute of Technology; [2]Stanford University; [3]Oak Ridge National Laboratory; [4]University of Texas at Austin; [5]University of Maryland

Numerous technologies at the Water–Energy Nexus rely upon fluidic transport and phase behavior at the nanoscale, from membrane separations for desalination to energy production and storage via reverse electrodialysis and water electrolysis. A fundamental understanding of fluid behavior when confined to the narrowest of pores—termed single-digit nanopores (SDNs)—is thus paramount to advance water and energy security efforts. In SDNs, fluids commonly deviate from our classical understanding of physics, giving rise to extraordinary enhancements in transport and selective separations beyond theoretical predictions. This talk will highlight developments by the Center for Enhanced Nanofluidic Transport (CENT) toward a unified theory of confined fluid thermodynamics. Using precision SDN platforms of isolated carbon nanotubes (CNTs) with diameters from 0.72 to 1.64 nm, CENT validated the first confined fluid equation of state (EOS) based on the Peng-Robinson formulation. Reformulating the EOS for a 2D geometry was found to predict the well-known maximum capillary pressure at 1.3 nm spacing for a rectilinear graphene pore. The newfound unified theory of confined fluid dynamics is further supported by experimental photoluminescence and vibrational electron energy loss spectroscopy (vEELS) measurements of strongly confined water in CNTs at CENT. This new EOS serves as an important engineering tool for modeling the thermodynamics of any nanoconfined fluid, thereby informing the rational design of critical nanofluidic technologies.

2:00 PM

F-II-2: Structure and Dynamics of Water and Solutes Near Interfaces and in Solution

[EFRC - M-WET] Lynn E. Katz[1], M. Scott Shell[2], Graeme Henkelman[1], Benny Freeman[1], Gregory Su[3], Ethan Crumlin[3], Raphaële Clément[2], Rachel Segalman[2], Nathaniel Lynd[1], Craig Hawker[2]
[1]University of Texas at Austin; [2]University of California, Santa Barbara; [3]Lawrence Berkeley National Laboratory

The Center for Materials and Water and Energy Systems (M-WET) seeks to advance the utilization of alternative water sources and enhance resource recovery in energy-related water cycles by discovering the key science drivers that link polymer structure and interfacial interactions to hydration, solute interactions, and fouling. M-WET's goals include: (1) elucidating the structure and dynamics of hydration water and solutes near and within membranes; (2) quantifying thermodynamic and kinetic properties of solutes in aqueous mixtures, near and within membranes; and (3) developing rational design strategies for selectivity-enhancing interactions among water, solutes, and membranes. This talk highlights research that has combined novel experimental and molecular simulation approaches to reveal the role of zwitterionic functionalities on hydration dynamics and the role of ion pairing on salt sorption and permeability in ion exchange membranes. For example, we used Overhauser dynamic nuclear polarization (ODNP) to demonstrate that local hydration dynamics near zwitterionic and polyelectrolyte surfaces mimic the behavior seen in bulk water, suggesting that water moves swiftly near these groups to help resist foulant adsorption. Advanced molecular dynamics simulations then sampled the conformations and free energy landscape in these polymers and captured relationships between hydration water structure, dynamics, and solute adsorption. We enhanced our understanding of ion pairing by coupling dielectric relaxation and Raman spectroscopy with DFT and molecular dynamics simulations. We found that ion speciation is dependent on properties such as ion size, polarizability, and valence, as well as the dielectric constant of the medium.

2:20 PM – Team Science Finalist

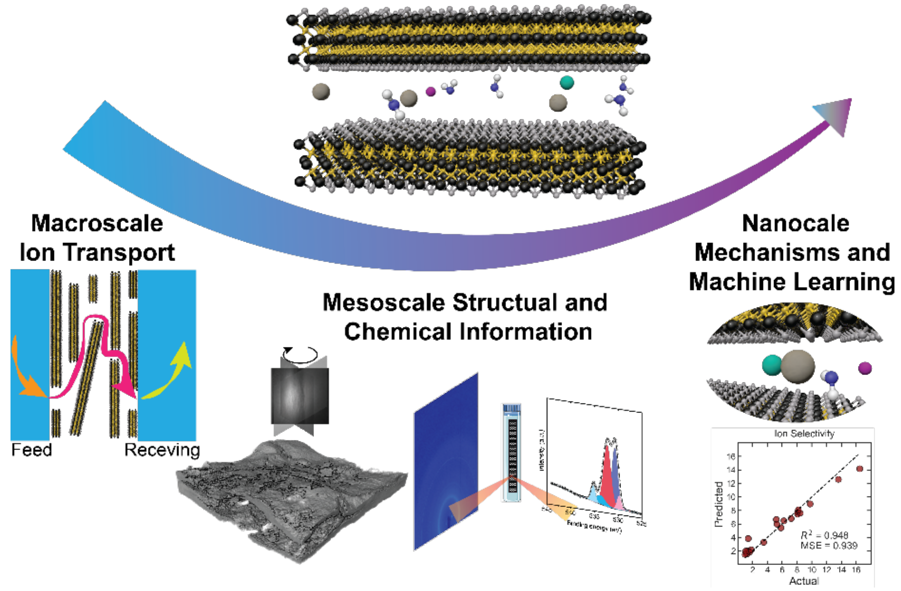
F-II-3: MORE THAN A SPECTATOR: CRITICAL ROLE OF WATER IN ION TRANSPORT THROUGH 2D MEMBRANES

[EFRC - AMEWS] Yaguang Zhu[1], Qinsi Xiong[2], George C. Schatz[2], Kelsey B. Hatzell[1]
[1]Princeton University; [2]Northwestern University

The accelerating depletion of freshwater resources coupled with increasing interest in recovering resources from water underscores an urgent scientific imperative to develop technologies for efficient ion separations in aqueous systems. Understanding solute–interface interactions in membrane systems is a core focus of the Advanced Materials for Energy-Water Systems (AMEWS) Center. Among the most challenging impurities to remove are small, tightly hydrated solutes, which exhibit strong interactions with water. Two-dimensional (2D) membranes, such as those based on transition metal carbides (MXene), show great promise for ion sieving and separation in such contexts. This presentation highlights a close collaboration by the Hatzell and Schatz groups to elucidate the key role of water in ion transport through 2D MXene membranes. First, at the **macroscale**, we discovered that intercalation of chaotropic cesium ions (Cs^+) into the 2D MXene membranes significantly inhibits ion permeation, resulting in enhanced ion sieving performance. Second, **mesoscale** three-dimensional imaging and synchrotron-based characterization revealed that Cs^+–intercalation uniquely reduces water content within the membrane both at the surface and within the membrane, thereby **mitigating membrane swelling**. Third, at the **nanoscale**, all-atom molecular dynamic simulations revealed critical roles of ion hydration and confinement in tuning selectivity. Guided by machine learning, we identified physicochemical descriptors and developed a predictive model of ion transport under nanoconfinement, which was experimentally validated. This framework enables effective separation of critical resource ions, including Ni^{2+}, Co^{2+}, and Cu^{2+}. By integrating experiments and simulations across scales, this work advances the understanding of solute–interface interactions in 2D membranes and supports the rational design of next-generation ion-selective materials, in alignment with the AMEWS mission.

References: Zhu, Y., Xiong, Q.,et al., (2025). Water content modulation enables selective ion transport in 2D MXene membranes. PNAS, under review

Contributions: Y.Z. designed and conducted the experiments. Q.X. developed the computational model and performed the simulations. G.S. and K.H. conceived the presented idea and supervised this work.



2:40 PM

F-II-4: Gating Nanofluidic Transport with Ions, Solvent, and Local Electric Potential

[EFRC - CENT2] Zuzanna S. Siwy[1], Jake Polster[1], Savannah Silva[1], Mohammad H. Motevaselian[2], Juan Pablo Martinez Cordeiro[3], Narayana R. Aluru[3], Fikret Aydin[4], Tuan Anh Pham[4], J. Pedro de Souza[5], Martin Z. Bazant[5], Cody L. Ritt[6], Menachem Elimelech[6], Amanda J. Souna[7], Ovuokenye Omadoko[7], Siddharth Singh[7], John Fourkas[7]
[1]University of California, Irvine; [2]University of Illinois Urbana-Champaign; [3]University of Texas at Austin; [4]Lawrence Livermore National Laboratory; [5]Massachusetts Institute of Technology; [6]Yale University; [7]University of Maryland

Single digit nanopores (SDNs) exhibit tunable transport properties due to their unique sensitivity to changes of the electrochemical properties of the pore walls/solution interface. SDNs are thus responsive to adsorption of ions, local hydrophobicity, changes in the local potential and even organization of solvent molecules. This sensitivity of nanofluidic transport to the properties of the solid/liquid interface is the basis of gating. The talk will provide examples of design guidelines for nanofluidic gating developed in the Center for Enhanced Nanofluidic Transport (CENT). A nanopore system with a broken electrochemical symmetry containing a junction between hydrophobic and hydrophilic zones was shown to switch ionic and water transport in response to voltage as well as presence of large polarizable anions. Experiments paired with multiscale modeling provide a molecular understanding of how voltage-controlled ionic concentrations in the pore facilitate wetting-dewetting transition by adsorption/desorption of ions in the hydrophobic zone. Ion adsorption can also gate ionic transport by modulating the surface charge through "charge regulation," which synergistic experimental and theoretical efforts in CENT found to be ion specific. CENT has also pioneered methods to probe the effects of spatial organization of solvent molecules at the pore walls to help drive the nascent field of chiral electrochemistry. An ionic field effect transistor composed of van der Waals materials and graphene as the gate will also be presented. The transistor whose structure is controlled with sub-nanometer precision provides a model system to understand how local and temporal changes of electric potential modulate transmembrane transport.

3:00 PM

F-II-5: Probing the Electrochemical Interface and Local Electrostatic Fields with Ultrafast IR Spectroscopy

[EFRC - AMEWS] Jeffrey W. Elam[1], Nicholas H. C. Lewis[2], George C. Schatz[3], Andrei Tokmakoff[2]
[1]Argonne National Laboratory; [2]University of Chicago; [3]Northwestern University

In this talk, we will discuss an ongoing effort to understand the structural and dynamical properties of aqueous electrolytes and the electrified interface through a combined experimental and theoretical approach. We have developed new approaches for performing ultrafast IR spectroscopic measurements of molecules at the active electrochemical interface. This has required the development of a layered electrode suited for the varied needs of both electrochemistry and ultrafast IR spectroscopy. The interpretation of the spectra is facilitated by

molecular dynamics simulations, which, comparing polarizable and fixed-charge simulations, allow us to connect frequency shifts to molecular configurations via the local electrostatic fields. Using this platform, we have demonstrated the ability to probe electrochromism with 2DIR spectroscopy, which has revealed the details of the vibrational lineshape and the coupling between the vibration and the plasmon that facilitates monolayer sensitivity. We have continued to apply this technique to a variety of molecular monolayers designed to probe different aspects of the electrochemical double layer via carbonyl groups, nitriles, and redox-active moieties. By using different functional groups as probes we can modify the sensitivity to the solution, while changes in the linker allow us to tune the conjugation of the probe to the electrode, and the region of the double layer being probed.

G. Hydrogen

Session III: Tuesday, August 12, 2025, 9:00 – 10:20 AM, Brookside B

9:00 AM

G-III-1: Tethering and Crosslinking Approaches to Build Resilient Multilayer Polymer Catalyst Architectures

[EFRC - SPECS] Eui Hyun Suh[1], Yadong Zhang[2], Abhisek Mohapatra[2,3], Debasmita Pariari[2], Zhiting Chen[4], Qing Zhang[2], Ann Greenaway[3], Elisa Miller[3], Stephen Barlow[2,3], Melissa Gish[2], Andrew Ferguson[2], Natalie Stingelin[1], Erin Ratcliff[1], Seth Marder[2,3], Neal Armstrong[4]
[1]Georgia Institute of Technology; [2]University of Colorado; [3]National Renewable Energy Laboratory; [4]University of Arizona

Organic semiconducting polymers present a versatile platform for developing photocathodes in hydrogen evolution due to their tunable optical and transport gaps, compatibility with electrolytes, and scalability via solution processing. Within SPECS, we aim to establish design rules for robust photocathode systems that elucidate key structure–property relationships related to charge transport, charge transfer, and operational durability. Our initial device employs a bulk heterojunction (BHJ) strategy, combining PTB7-Th (hole transport) and N2200 (electron transport) polymers, deposited on passivated ITO and capped with a hydrogen evolution reaction (HER) catalyst (e.g., Pt or RuO_2), all immersed in an acidic electrolyte. Insights from optoelectronic analogs guided our focus toward enhancing chemical and mechanical interfacial stability and enabling selective charge extraction.

To this end, we utilize bifunctional molecules bearing phosphonic acid groups for anchoring and azide or diazirine moieties for covalent crosslinking. This allows post-synthetic and post-film interface engineering, improving adhesion and stability at polymer–ITO and polymer–catalyst interfaces. Additionally, crosslinking enables multilayer device architectures with enhanced control over charge separation, transport, and electrolyte ingress.

Ongoing work explores: local pH modulation near the catalyst; surface modification of polymers post-deposition to tune hydrophobicity; attachment of redox-active probes to monitor electron transfer kinetics; and ligand development to affix molecular catalysts to polymer surfaces. Together, these advances support the creation of efficient, durable HER photocathodes, offering new design guidelines for polymer-based solar hydrogen platforms.

9:20 AM

G-III-2: Triple Play: Disentangling Protons, Oxygen Vacancies, and Holes and Their Role in the Electrocatalytic Activity of the $BaCo_xFe_{0.8-x}Zr_{0.1}Y_{0.1}O_3$-d (BCFZY, 0.1≤x≤0.7) Triple-Conducting Oxide System

[EFRC - HEISs] Ryan O'Hayre[1], Yewon Shin[1], Michael Sanders[1], Zhen Jiang[2], Christopher Wolverton[2], Sossina M. Haile[2], Kennedy Agyekum[3], Bernadette Cladek[3], Katharine Page[3,4], Jue Liu[4], Erica Truong[5], Bright Ogbolu[5], Yan-Yan Hu[5,6]

[1]Colorado School of Mines; [2]Northwestern University; [3]University of Tennessee; [4]Oak Ridge National Laboratory; [5]Florida State University; [6]Center of Interdisciplinary Magnetic Resonance, National High Magnetic Field Laboratory

Triple-conducting oxides (TCOs) are emerging mixed ionic and electronically conducting materials that show great promise for oxygen reduction/evolution reactions (ORR/OER)—primarily in high-temperature ceramic electrochemical cells. Their high activity stems, in part, from their ability to incorporate and transport three charge carriers: protons, oxygen vacancies, and electron-holes. Despite their promise, fundamental studies of TCOs are challenging, as transport dynamics from three charge carriers cannot be fully disentangled via traditional electrical techniques. Characterizing proton dynamics in TCOs is particularly difficult as protons are generally the minority carrier, and their conduction response is obscured by the major carriers. Here, we leverage the unique capabilities of our interdisciplinary team, including high-precision thermogravimetric analysis, H/D isotope exchange, high-resolution nuclear magnetic resonance spectroscopy, neutron diffraction, and atomistic simulations, to successfully isolate the proton behavior in an archetypal TCO system, $BaCo_xFe_{0.8-x}Zr_{0.1}Y_{0.1}O_3$-d (BCFZY).

Despite their primary application in protonic electrochemical devices, we find the concentration of oxygen vacancies to greatly exceed the concentration of protons in the BCFZY system. Conversely, we find that the proton mobility far exceeds that of oxygen vacancies, particularly at moderate to low temperatures. These factors result in proton kinetics exceeding the oxygen vacancy kinetics at temperatures of interest (≤ 500°C), despite their exceptionally low concentration (~0.001 H per formula unit). The result surprisingly implies that electrocatalytic performance enhancement in BCFZY and related TCO systems requires accelerating the oxygen (rather than proton) surface reaction kinetics, but without sacrificing the exceptionally high bulk diffusivities of both species.

9:40 AM

G-III-3: Large Polarons and Exciton Polarons in Titanium Dioxide

[CMS - EPW] Feliciano Giustino
The University of Texas at Austin

Titanium dioxide (TiO_2) is a wide-gap semiconductor with numerous applications in photocatalysis, photovoltaics, and neuromorphic computing. The functional properties of this material critically depend on its ability to transport charge in the form of polarons, namely electrons and holes dressed by the quanta of lattice vibrations. It is currently well established that the most important polymorphs of TiO_2, the rutile and anatase phases, host small electron polarons and small hole polarons, respectively. However, whether additional polaronic species exist in TiO_2, and under which conditions, remain open questions. Furthermore, it is unclear why rutile exhibits thermally activated transport while anatase exhibits phonon-limited transport. Here, I will describe recent work aimed at answering these questions. We explored the rich landscape of polaron quasiparticles in TiO_2 via our recently developed ab initio theory of polarons and exciton polarons and recent advances in the EPW code including GPU refactoring. We identified three new polaron species in addition to the previously known small polarons: a large hole polaron in rutile, a large quasi-two-dimensional electron polaron in anatase, and a large exciton polaron in anatase. In addition, we are able to explain the difference in the carrier transport properties of rutile and anatase in terms of the sizes and hopping barriers of their respective electron polarons. These findings complete the puzzle on the polaron physics of TiO_2 and pave the way for systematically probing and manipulating polarons in a broad class of complex oxides and quantum materials [Z. Dai and F. Giustino, PNAS 121, e2414203121 (2024)].

10:00 AM – Team Science Finalist

G-III-4: UNDERSTANDING AND MANIPULATING THE NANOENVIRONMENT OF RIBBON-LIKE (SOFT) POLYMER SEMICONDUCTORS TO ENABLE PHOTOELECTROCHEMISTRY

[EFRC - SPECS] Henry J. Kantrow[1], Yael Tsarfati[2,3], Spencer Yeager[4], Megan Brown[5], Arianna Magni[2], Eui Hyun Suh[1], Jude Kpare[1], Chad Risko[5], Alberto Salleo[2], Erin Ratcliff[1], Natalie Stingelin[1]
[1]Georgia Institute of Technology; [2]Stanford University; [3]Lawrence Berkeley National Laboratory; [4]University of Arizona; [5]University of Kentucky

Ribbon-like polymer semiconductors, comprised of rigid electron donating/withdrawing groups, have exceptional promise as next-generation energy conversion and storage materials, providing exquisite control over redox properties, high efficiencies in radiation-to-electrical energy conversion, long-lived charge carriers, and ease of large-scale processing.[1,2] In contrast to traditional flexible-chain macromolecules, ribbon-like polymers feature a rich structural landscape that cannot be described solely by the classical picture of amorphous and semicrystalline domains.[3] To enable rational materials design, a holistic understanding of the distribution in local nanoenvironments is needed to control charge transport and transfer across length and time scales. For example, there are contributions from both static and dynamic

energetic disorder that vary across 100s of nanometers and femtosecond timescales, which contribute to significant differences in charge transport (Figure 1).

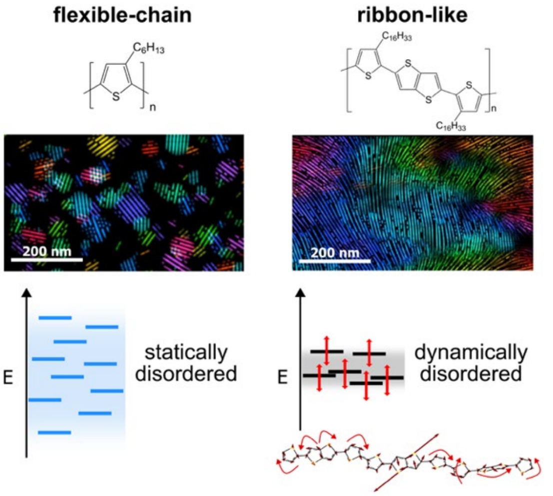


Figure 1: *Top: Chemical structures and corresponding 4D-scanning transmission electron microscopy of flexible-chain and ribbon-like polymers. Bottom: Schematic energy level distributions for the two polymers, with a vector schematic of a torsional mode that contributes to dynamic disorder in the ribbon-like polymer.*

We demonstrate state-of-the-art characterization tool suites developed within the SPECS EFRC to investigate processes at multiple length scales in soft materials. Using prototype polymers, we demonstrate for the first time that ribbon-like polymers feature distinct, dynamically disordered energy landscapes. Combinations of multimodal characterization using spectroelectrochemistry, *operando* X-ray scattering, electron microscopy, and coherent electronic spectroscopy reveal that flexible-chain polymers are often structurally heterogeneous and statically disordered. Ribbon-like polymers, however, display a homogenous structure, leading to narrower distributions in energy levels that are highly dynamic, driven by coupling to torsional vibrational modes. Concurrent modeling across scales reveals that charge carrier (polaron) transport and densities of states (DOS) depend on the local and dynamic nanoenvironments of these complex systems, with polymer morphologies and electrolyte compositions (solvent/ions) impacting polaron signatures and transport. These differences in electronic disorder translate to control of rates of charge transfer in polymer–electrolyte interphase regions. This work paves the way for elucidating the complex multiscale polymer structure across the broad temporal scales (fs to ms) relevant to ion and polaron transport. This dynamic structure ultimately controls charge-transfer reactivity to promote specific redox chemistries, such as H_2 evolution, and is a critical step toward design guidelines for creation of future transducers of light to chemical energy.

Contributions: H.J.K. conducted coherent electronic spectroscopy experiments. Y.T. performed electron microscopy. S.Y. and E.H.S. executed electrochemical measurements and the photoelectrochemistry. M.B. performed DFT and MD simulations. C.R., A.S., E.R., and N.S. helped design the experiments and supervised the project.

References: [1] F. Machui et al. *Energy Environ. Sci* **7** (9), 2014. [2] J. Kosko et al. *Nat Energy* **7** (4), 2022. [3] E. Ratcliff & N. Stingelin *Nat Mater* **24** (1), 2025.

H. Microelectronics

Session I: Monday, August 11, 2025, 9:10 – 10:30 AM, Brookside A

9:10 AM

H-I-1: Exploring New Materials for Magnonics

[EFRC - CEEMag] Junwei Tong[1], Xiangcheng Liu[1], Katya Mikhailova[2,3], Lerato Takana[3], Orion Smedley[4], Thow Min Cham[4], Kelly Luo[4], Srishti Pal[4], Gregory Fuchs[4], Dan Ralph[4], Durga Paudyal[5], Yuri Suzuki[2,3], Xiaoqin (Elaine) Li[1]
[1]University of Texas at Austin; [2]SLAC National Accelerator Laboratory; [3]Stanford University; [4]Cornell University; [5]University of Iowa

Magnonics is a promising new technology for low loss information and energy transfer. Among candidate magnon materials, low damping insulating ferrimagnetic and antiferromagnetic thin films are most promising as they minimize charge current dissipation. One class of materials that we have identified is epitaxially grown lithium aluminum ferrite (LAFO) thin films. Our electronic structure calculations indicate that LAFO has a bandgap of 2.8 eV with weak spin-phonon coupling correlating with low magnetic damping. In order for these materials to support magnon propagation in interconnects, it is critical that we understand propagating magnons through Raman and Brillouin light scattering experiments. Spectroscopic studies of magnons in LAFO thin films with a range of thicknesses reveal multiple surface magnon modes. The lowest frequency modes exhibit frequencies similar to those observed in ferromagnetic resonance experiments. With increasing thickness, more magnon modes are observed in the film thickness direction. We tune magnon frequency by film thickness and magnetic field. The magnetic field-dependence of magnon frequencies allows us to extract the exchange constant and magnetic anisotropy and compare with ab initio calculated values. We have also demonstrated effective interfacing of magnons in LAFO with charge in the form of high spin-orbit torque (SOT) efficiency. SOT efficiencies for LAFO determined by different types of electrical measurements give conflicting results because artifacts can overwhelm the desired signals in samples with small magnetoresistance. Instead, we have developed reliable optical measurements of SOT efficiencies using Sagnac interferometry. Together we find LAFO to be a promising material for magnon interconnects.

9:30 AM

H-I-2: Switching in Wurtzite Ferroelectrics for Non-volatile Ferroelectric Memories

[EFRC - 3DFeM2] Leonard Jacques[1], Betul Akkopru Akgun[1], Sebastian Calderon[2], Erdem Ozdemir[1], Clive Randall[1], Elizabeth Dickey[2], Jon-Paul Maria[1], Susan Trolier-McKinstry[1]
[1]The Pennsylvania State University; [2]Carnegie Mellon University

Ferroelectric materials offer the possibility of a low-power non-volatile memory that can be close-coupled with the processor to reduce both system latency and power. The 3DFeM2 center is investigating development of new materials, new device instantiations, and autonomous

processes for new generations of ferroelectric material for this application. This talk will concentrate on the physics underlying polarization switching in the new family of wurtzite ferroelectrics. Full switching of the polarization in wurtzite ferroelectrics was demonstrated for the first time in $Al_{1-x}Sc_xN$ in 2019. Since that time, ferroelectricity has been demonstrated in $Al_{1-x}B_xN$, $Al_{1-x}Y_xN$, AlN, $Ga_{1-x}Sc_xN$, and $Zn_{1-x}Mg_xO$. Most of these films are unipolar as grown, such that they need to be woken up. Typical activation energies for the wake-up process in nitride wurtzites in ~0.15±0.05 eV. Once woken up, the pseudo-activation energies that describe switching between room temperature and 300°C are ~ 20 – 40 meV. In $Al_{1-x}B_xN$, switching occurs through a non-polar intermediate that bears strong structural similarity to the inversion domain boundaries known in the wurtzites. An independent column switching mechanism drives polarization inversion in some of these materials, which may explain the observation of proximity ferroelectricity. This talk will discuss the kinetics of switching, and the failure mechanisms on bipolar cycling. It is found that many of these films show history-dependent switching kinetics, such that films can be switched faster after several cycles. Prolonged cycling, however, tends to produce slow tails on the switching curves that cannot be fit with any single switching model.

9:50 AM

H-I-3: Stability and Dynamic Responses of Ferroelectric Polar Structures Under Light

[CMS - COMMS] Fei Yang, Aiden Ross, Tiannan Yang, Maohua Zhang, Akash Saha, Xiaojiang Li, Venkat Gopalan, Long-Qing Chen
The Pennsylvania State University

This presentation highlights recent advances from CMS-COMMS in developing novel thermodynamic theories and dynamic phase-field models to understand ferroelectric phase transitions and the formation and evolution of light-induced transient phases and mesoscale polar structures. We formulate a quantum statistical theory of displacive ferroelectricity that can be employed to predict finite-temperature properties and the criticality of phase transitions using only the ground-state properties. Applied to the quantum paraelectrics, $SrTiO_3$ and $KTaO_3$, and the classical ferroelectric $PbTiO_3$, the theory accurately predicts the transition temperatures, dielectric responses, and strain dependence of critical temperatures, all in excellent agreement with experiments, without fitting parameters. We explore the non-equilibrium dynamics under ultrafast THz excitations by integrating this quantum statistical theory into a dynamic phase-field model to simulate the soft-mode behaviors of quantum paraelectric $KTaO_3$ under ultrafast terahertz excitation, uncovering a new mechanism for the experimentally observed behaviors of SHG amplitude oscillations. We simulated the light-induced formation and evolution dynamics of polar structures in $PbTiO_3/SrTiO_3$ ferroelectric/paraelectric superlattices by simultaneously incorporating the coupled dynamics of charge carriers, strains, and polarization. We discover that these polar structures exhibit emergent mesoscale dynamics and undergo phase transformations between different mesoscale polar structures. These results guided the interpretation and understanding of temporal polar structural evolution dynamics observed in optical-pump and X-ray-probe measurements. Overall, these advances contribute to one of the objectives of CMS-COMMS towards building a computational framework that can reveal complex light-matter interactions in materials, providing a bridge from fundamental materials science to device relevant behaviors.

10:10 AM

H-I-4: High Fidelity Green's function theory for low dimensional systems

[CCS - QuestC] Mark van Schilfgaaarde[1], Swagata Acharya[1], Dimitar Pashov[2], Peyton Cline[1], Mushir Thodika[1]
[1]National Renewable Energy Laboratory; [2]King's College London

Our CCS is aimed at development of diagrammatic Green's function methods in low dimensional systems, doing so both efficiently and with high fidelity Green's function theory generates both response functions and the effective time-dependent potential that yields the electronic structure from the one-particle Green's function. However, much depends on the fidelity of the theory employed. In traditional ab initio formulations, the potential is calculated at the lowest order (GW) as a perturbative correction to density functional theory. However, uncontrolled approximations in the starting point propagate to the solution, which obscures and also limits the range of validity. We show how a special kind of self-consistency -- Quasiparticle self-consistent GW and makes it more uniformly accurate for a given level of theory and removes starting point bias. Errors that appear are systematic and can be traced to missing diagrams. The most important of these can be traced to missing electron-hole interactions that can be captured by ladder diagrams. With their addition to the polarizability in the self-consistency cycle, both one-particle and two-particle features are already very well described in many systems. The fidelity in both the charge susceptibility, and the potential, is very high for a wide range of systems. We demonstrate the theory's versatility and fidelity with a number of illustrations, and also point to systems where other diagrams are still needed. If time permits I will present progress towards large systems and the total energy with high fidelity.

Session II: Monday, August 11, 2025, 1:40 – 3:20 PM, Brookside A

1:40 PM

H-II-1: Resonant Inelastic X-ray Scattering on programmable van der Waals materials

[EFRC - Pro-QM] Connor Occhialini[1,2], Vivek Bhartiya[2], Benjamin Zager[2], Taehun Kim[2], Yifeng Cao[2], Jonathan Pelliciari[2], Xavier Roy[1], Xiaoyang Zhu[1], Xiadong Xu[3], Dmitri N. Basov[1], Valentina Bisogni[2]
[1]Columbia University; [2]Brookhaven National Laboratory; [3]University of Washington

The scientific vision of the Energy Frontiers Research Center on Programmable Quantum Materials (Pro-QM) is the discovery, characterization, and deployment of new forms of quantum matter controllable by light, gating, magnetic proximity, electromagnetic environment, and nano-mechanical manipulation, effectively programming their quantum properties. The Pro-QM team investigates two-dimensional (2D) van der Waals QMs in view of their outstanding diversity of

ultra-manipulatable properties, and focuses on programmable topology (Thrust 1) and programmable quantum interfaces (Thrust 2).

The progress of these research activities harnesses and relies on cross-cutting research themes, such as material design. To guide and gain full control of the QMs functionalities, it is indeed vital to achieve a complete understanding of the electronic properties and the microscopic mechanisms at play in the QMs switching processes. Using high-energy resolution Resonant Inelastic X-ray Scattering (RIXS) at the SIX Beamline of National Synchrotron Light Source II (Brookhaven National Laboratory), we focus on the electronic investigation of novel van der Waals (vdW) materials and two-dimensional (2D) Moiré materials, in full synergy with the Pro-QM team. Unique information on the electronic and magnetic excitations, and on the exciton dynamics can be extracted, contributing to the advancement of novel material design.

2:00 PM

H-II-2: Magnon detection and function for next-generation energy efficient interconnects

[EFRC - CEEMag] T.M.J. Cham[1], J. Kang[2], A. D'Addario[1], R. Jain[1], K. Hu[3], D.G. Chica[4], X. Huang[1], K. Watanabe[5], T. Taniguchi[6], X. Roy[4], S.K. Cheung[2], M. Hamdi[2], S. Shim[1], L. Yuan[2], W. Rogers[2], M. Tey[2], G. Lim[2], G. Finocchio[7], M. Hersam[2], J. Rondinelli[2], Y. Luo[1], K. Nowack[1], M. E. Flatté[3], D.C. Ralph[1], P. Khalili[2], G.D. Fuchs[1]

[1]Cornell University; [2]Northwestern University; [3]University of Iowa; [4]Columbia University; [5]Research Center for Electronic and Optical Materials; [6]Research Center for Materials Nanoarchitectonics; [7]University of Messina, Italy

CEEMag aims to harness magnons for energy efficient interconnects for microelectronics. The shift from copper interconnects to magnon wave-based interconnects requires efficient excitation and detection of magnons at extremely high frequencies, and it offers new opportunities to add function to interconnects.

First, we focus on efficient detection of antiferromagnetic magnons using tunnel junctions. Antiferromagnetic order or dynamics can be electrically read out in tunnel junctions in either two ways – either the tunnel barrier is magnetic and acts as a spin filter depending on magnetic configuration, or the electrodes are magnetic and tunneling is most efficient when spin configurations of both electrodes align. We explore both ideas. We discuss the detection of antiferromagnetic spin dynamics in CrSBr tunnel barriers. Here tunnel magnetoresistance arises from spin filtering, resulting in the ability to efficiently detect antiferromagnetic precession modes. Next, we consider the case where the electrodes are antiferromagnets in $Mn_3Pt/MgO/Mn_3Pt$ tunnel structures. We study the switching and magnetoresistance of these devices and analyze the results considering scanning nitrogen-vacancy (NV) center microscope images of Mn_3Pt to better understand the detailed antiferromagnetic domains. Finally, we explore added functionality that is possible with magnon interconnects. We investigate harmonic conversion in NiFe/Pt channels driven by microwave current using NV center magnetic imaging and micromagnetic simulations. We find efficient and high harmonic generation at low magnetic field, discover chiral nonlinear responses, and localize the spatial positions of efficient conversion to the imaged magnetic sample texture.

2:20 PM

H-II-3: Ultra Materials for a Resilient, Smart Electricity Grid (ULTRA)

[EFRC - ULTRA] Robert Nemanich[1], Stephen Goodnick[1], Houqiang Fu[1], Nidhin Kurian Kalarickal[1], Fernando Ponce[1], Marco Saraniti[1], Arunima Singh[1], David Smith[1], Mary Ellen Zvanut[2], Alexander Balandin[3], Richard Wilson[4], Debdeep Jena[5], and H. Grace Xing[5], Timothy Grotjohn[6], Michael Spencer[7], Hongping Zhao[8], Yuji Zhao[9], Jack Flicker[10], and Robert Kaplar[10], Srabanti Chowdhury[11], Martin Kuball[12]

[1]Arizona State University; [2]University of Alabama-Birmingham; [3]University of California, Los Angeles; [4]University of California, Riverside; [5]Cornell University; [6]Michigan State University; [7]Morgan State University; [8]The Ohio State University; [9]Rice University; [10]Sandia National Laboratories; [11]Stanford University; [12]University of Bristol

ULTRA EFRC explores the nature and synthesis of diamond, c-BN, AlN and BAlN (which includes non-polar cubic to polar hexagonal semiconductors). Epitaxial layer synthesis has now been demonstrated, and efforts focus on high purity, low defect density growth and heterostructure formation.

For power-semiconductor technologies, interfaces or heterostructures determine specific functionalities. New efforts include MOCVD nitrides and oxides to enable UWBG transistor action. New approaches to doping in UWBG semiconductors including distributed polarization doping of AlN and BAlN structures, charge transfer doping using multi-layer dielectrics (diamond), and photo-induced doping (diamond). Moreover, space charge limited transport with undoped semiconductors has shown record current density in diamond diodes.
Carrier dynamics and breakdown of UWBG semiconductors are expected to differ substantially from other semiconductors based on the wide bandgap, high mobilities, high field strength, and deep donors/acceptors. Approaches to characterize breakdown at fields >10 MV/cm will measure single event properties from photon or alpha particle excitation to understand impact ionization and breakdown.

While the thermal properties of pure bulk UWBG semiconductors have been carefully determined, the thermal conductivities of epitaxial layers will be dependent on defects, doping and the interface boundary resistance, which often dominates heat flow, and needs to be established and understood for realistic heterostructure configurations.
The knowledge gained in ULTRA EFRC is incorporated into simulations that enable device designers to explore new configurations for specific applications. Leading researchers, serving as members of the ULTRA Future Grid Co-Design Ecosystem, will incorporate UWBG components and subsystems to enable a smart and resilient grid.

2:40 PM

H-II-4: Floating Zone Crystal Growth and Characterization of Metallic Ceramics for Future Microelectronics

[EFRC - APEX] Evan N. Crites[1], Ahamed Rahan[2], Astrid Dzotcha Kengne[2], Daniel Harrison[2], Shipra Rai[2], MVS Chandrashekhar[2], Sharad Mahatara[3], Michelle Smeaton[3], Steven Spurgeon[3], Shivashree Shivamade Gowda[4], Scott A. Ethan[4], Patrick E. Hopkins[4], Brooks Tellekamp[3], Kirstin Alberi[3], Satya K. Kushwaha[1]: Tyrel M. McQueen[1], Jessica L. McChesney[5], Michael Spencer[2], Nancy M. Haegel[3]

[1]Johns Hopkins University; [2]Morgan State University; [3] National Renewable Energy Laboratory; [4]University of Virginia; [5]Argonne National Laboratory

For fifty years, many advances in electronic and optoelectronic device technologies have been driven by the properties and quality of III-V semiconductors. The next fifty years can leverage approaches fusing III-Vs with ultra-wide band gap (UWBG) materials and heterogeneous integration. The mission of APEX is to expand UWBG semiconductor and substrate choices and advance the science of heterogeneous integration to allow materials for power electronics functionality to be selected and combined based on fundamental properties, interface control, and transformative manufacturing, rather than existing material and growth constraints. We will present the development and characterization of novel (semi-)metallic diborides (MB_2) and carbides (MC) refractory crystals. These refractory crystals provide potential lattice matching well within the range of $Al_xGa_{1-x}N$, offering a platform for engineering the band structure and heat transport characteristics of a key power electronic III-V material. The high electrical and thermal conduction of these novel substrates allows for minimization/removal of thermal loads with improved thermal figure of merit. The MB_2 and MC materials are also candidates to host various topological states, and these protected electronic states could lead to exotic electronic and thermal properties. However the extreme melting points and volatility of these materials make them difficult to grow. Leveraging the high power densities of state-of-the-art laser diode floating zone furnaces, APEX has succeeded in synthesizing ScB_2 and $Ta_{0.8}Hf_{0.2}C$ crystals. Their initial crystalline quality and structural, electronic, and thermal materials properties will be discussed, with progress towards heterogeneous integration with AlxGa1-xN films described.

3:00 PM

H-II-5: Harnessing Atomic Ordering in Semiconductor Alloys Through Theory-Experiment Synergy

[EFRC - μ-ATOMS] Shunda Chen[1], Shang Liu[2], Lilian Vogl[3], Anis Attiaoui[4], Xiaochen Jin[1], Yunfan Liang[5], Nirosh Eldose[6], Haochen Zhao[7], Yicheng Wang[2], Adelaide Maria Bradicich[8], Sophia Lafia Arvin[3], Xiaoxin Wang[2], Yuping Zeng[7], Ezra Bussmann[8], Tzu-Ming Lu[8], Paul McIntyre[4], Damien West[5], Shengbai Zhang[5], Greg Salamo[6], Shu-Qing Yu[6], Andrew Minor[3], Tianshu Li[1], Jifeng Liu[2]

[1]George Washington University; [2]Dartmouth College; [3]University of California, Berkeley; [4]Stanford University; [5]Rensselaer Polytechnic Institute; [6]University of Arkansas; [7]University of Delaware; [8]Sandia National Laboratories

Harnessing atomic ordering in semiconductor alloys has recently emerged as a new degree of freedom for band-engineering to potentially leap beyond CMOS. Here we present a synergistic theory-experimental study to understand and engineer atomic ordering in Group-IV SiGeSn alloys towards novel electronic and photonic properties. Leveraging a side-by-side experiment-theory comparison at the same spatial scale enabled by machine-learning neuroevolution potentials of first-principles accuracy, we successfully quantified and spatially mapped the chemical short-range order (SRO) of (Si)GeSn semiconductor alloys in both real space via atom probe tomography (APT) and reciprocal space via energy-filtered four-dimensional scanning transmission electron microscopy (EF 4D-STEM). The excellent agreement between theory and experiment, as well as real and reciprocal space characterization, develops a new set of tools for SRO characterization that has long been challenging for medium and high entropy alloys and they can be extended to other advanced alloy systems such as nitride semiconductors alloys. Furthermore, supported by molecular dynamics and first-principles band-structure modeling, we also identified engineering surface termination via precursors or surfactants as an effective approach for in situ SRO control, while ion beam processing and annealing offers further ex situ SRO control. These in situ and ex situ methods potentially enable SRO-based phase change materials for reconfigurable electronics/photonics beyond CMOS. Last but not least, first-principles modeling also guides the discovery of semiconductor-compatible topological digital alloys by engineering atomic ordering in the growth direction, opening the door towards scalable semiconductor-topological material integration to greatly extend the functionality beyond conventional CMOS electronics.

Session III: Tuesday, August 12, 2025, 9:00 – 10:20 AM, Brookside A

9:00 AM

H-III-1: Shining Light on Short-Range Ordering in Group-IV Semiconductor Alloys

[EFRC - μ-ATOMS] Anis Attiaoui[1, 2], Soham Joshi[1], Shunda Chen[3], Joseph C. Woicik[4], J. Zach Lentz[1], Lilian Vogl[5], Jarod Meyer[1], Kunal Mukherjee[1], Tianshu Li[3], Andrew Minor[5], Paul C. McIntyre[1,2]
[1]Stanford University; [2]SLAC National Accelerator Laboratory; [3]George Washington University; [4]National Institute of Standards and Technology; [5]Lawrence Berkeley National Laboratory

The direct band gap of CMOS-compatible (Si)GeSn semiconductor alloy has sparked significant research interest in these alloys and their potential for silicon-compatible optoelectronics. The low solid solubility of α-Sn in Ge (1 at. %) and the large lattice mismatch between α-Sn and Ge of approximately 14%, make it difficult to prepare dislocation-free GeSn, and to maintain its thermal stability during post-deposition fabrication processes. We present a method to counteract annealing-induced surface segregation in Ge core/$Ge_{0.9}Sn_{0.1}$ shell nanowires (NWs) grown by reduced-pressure chemical vapor deposition. Surface passivation via atomic layer deposition of a thin Al_2O_3 layer (<3 nm) significantly enhances the thermal stability of these GeSn alloys. We systematically investigate the effects of annealing these ALD-coated NWs at temperatures ranging from 300°C to 450°C, greatly exceeding the Ge-Sn binary eutectic growth temperature (~275°C). Structural characterization through X-ray diffraction and scanning transmission electron microscopy confirmed that strain state, composition (9±1 at. % Sn), and morphology of the GeSn shells remained unchanged after annealing. Low-temperature infrared photoluminescence spectroscopy revealed two key findings: up to a 5-fold increase in PL integrated intensity post-annealing and a pronounced blueshift of the band-to-band optical transition. The absence of detectable strain variation, Sn composition reduction, or dislocation formation suggests that increased short-range ordering in GeSn during annealing contributes to this blueshift. This possibility was further explored through extended X-ray absorption fine structure (EXAFS) spectroscopy, employing a novel theoretical approach to fit the local atomic environment and to systematically evaluate the short-range order in these nanowire structures.

9:20 AM

H-III-2: Design of Dynamical Response in Electro-Thermal Neurons

[EFRC - reMIND] Patrick J. Shamberger[1], Fatme Jardali[1], Timothy D. Brown[2], Jenny L. Chong[1], Yeonju Yu[1], George Agbeworvi[1], Sarbajit Banerjee[1], Suhas Kumar[2], R. Stanley Williams[1]
[1]Texas A&M University–Texas A&M Engineering Experiment Station; [2]Sandia National Laboratories, Livermore

Artificial neurons exhibiting volatile threshold switching and action potential-like oscillations are critical for brain-inspired computing. Despite improved understanding of the electro-thermal coupling that explains the origin of negative differential resistance, quantitative connections between neuronal performance (spike frequency, amplitude, etc.) and intrinsic material properties remain under-explored, preventing predictive neuron design and rational materials selection. Here, we describe a physics-aware compact model and a higher fidelity finite element multiphysics simulation to advance the design of dynamical response in electro-thermal neurons. First, we develop the compact model and apply it to interrogate a palette of materials with electrical and thermal properties varying by orders of magnitude. The space of viable materials is identified to be much larger than previously recognized, with candidates from a range of materials classes. Combinations of material properties yielding desired neuronal performance are reported. Finally, we demonstrate application of this approach to single crystals of $(Pb,Cu)_xV_2O_5$, illustrating the ability to couple the predictive capabilities of this model with atomic-level control of intercalated layered oxides.

Next, we introduce coupled circuit-multiphysics simulations which describe the spontaneous collapse of current into narrow channels of high density current. We map time-dependent voltage output to specific steps in this electro-thermal localization process, as validated by experimental observations in alloyed $LaCO_3$, and map the impact of compositionally driven changes in properties to changing device response. Together, this work solidifies forward design principles for electro-thermal neuron devices, a necessary pre-condition for inverse design from desired neuronal performance to required materials properties.

9:40 AM

H-III-3: Engineering Nanoelectronic Devices for Energy Efficient Neuromorphic Computing

[EFRC - Q-MEEN-C] Duygu Kuzum[1], Ivan K. Schuller[1], Alex Frano[1], Robert Dynes[1], Shriram Ramanathan[2], Catherine Schuman[3]
[1]University of California, San Diego; [2]Rutgers University; [3]University of Tennessee

As conventional computing architectures face limitations in efficiency and scalability, nanoelectronic devices have emerged as key enablers for neuromorphic computing, offering brain-inspired functionality with enhanced energy efficiency, density, and adaptability. Quantum materials offer unique electronic properties that can be harnessed to emulate neural dynamics and enable new non-von Neumann, adaptive computing paradigms. In this presentation, I will discuss our collaborative work on nanoelectronic neuromorphic devices based on highly correlated oxides, trilayer metal oxides, and perovskite nickelates for large-scale energy efficient neuromorphic computing. I will share our results for each technology and then present our hardware/software co-design approach to optimize devices and achieve high computational efficiency. I will conclude my talk with future directions towards developing scalable, energy efficient nanoelectronic devices based on quantum materials with improved reliability and adaptability to support real-time, brain-inspired learning in complex neuromorphic systems.

10:00 AM

H-III-4: Hierarchical Materials for High Precision EUV Patterning: Directed Self-Assembly, Area-Selective Deposition and their Advanced Characterization

[EFRC - CHiPPS] Ricardo Ruiz[1], Paul Nealey[2], Stacey Bent[3], Weilun Chao[1], Oleg Kostko[1], Cheng Wang[1], Kyunghyeon Lee[2], Ki Hyun Kim[2], Christopher Eom[2], Emma Vargo[1], Beihang Yu[1], Maggy Harake[3], Yujin Lee[3], Qi Zhang[1], Kas Andrle[1], Honggu Im[1]
[1]Lawrence Berkeley National Laboratory; [2]Argonne National Laboratory; [3]Stanford University

Controlling stochastic variations in pattern formation is a critical challenge in extreme ultraviolet (EUV) lithography, where random fluctuations can compromise the accuracy and yield of nanoscale devices. Researchers at the Center for High Precision Patterning Science (CHiPPS) have been addressing this challenge through the design and synthesis of hierarchical materials for EUV patterning, including directed self-assembly (DSA) of high-χ, low-N block copolymers, which are essential for achieving EUV-relevant dimensions below 10 nm. This research has included the development of guiding patterns for DSA that work with both positive and negative tone resists, enabling greater flexibility in patterning. Advanced characterization techniques, including resonant soft X-ray reflectivity (RSoXR) and 3D metrology workflows, have been applied to understand the interfacial width and thermodynamic properties of these block copolymers, revealing a need for new physics to describe their behavior. The development of these characterization techniques is crucial for understanding and controlling the self-assembly of high-χ, low-N block copolymers, which exhibit unique properties that deviate from traditional strong segregation theory. Additionally, materials have been designed for area-selective deposition, including polypeptoids as "growth promoters" that efficiently capture metal organic precursors during vapor phase infiltration, enabling an efficient Al_2O_3 hard mask for pattern transfer during

RIE with high selectivity over Si. These advances aim to enable patterning and pattern transfer methods with atomic or molecular precision, mitigating the impact of stochastic variations on device performance and yield.

Session IV: Tuesday, August 12, 2025, 1:30 – 3:10 PM, Brookside A

1:30 PM

H-IV-1: Discovery of Dynamical Electro-Thermal Transistors with High Signal Gain

[EFRC - reMIND] Frederick U. Nitta[1,2], Sanjana Goyal[1,3], Timothy D. Brown[1], Elena Salagre Rubio[1], Kyung Seok Woo[1,4], Elliot J. Fuller[1], A. Alec Talin[1], Suhas Kumar[1], R. Stanley Williams[4]
[1]Sandia National Laboratories, Livermore; [2]Stanford University; [3]University of California, Berkeley; [4]Texas A&M University–Texas A&M Engineering Experiment Station

While attempting to optimize the properties of our $LaCoO_3$ active transmission line (ATL), some young interns and their postdoctoral mentors kept observing anomalous results. They would periodically see signal gains up to 80 when testing their circuits. This made no sense, because the Edge of Chaos theory that provided the basis for the ATL was based on small signals and should not yield a gain more than 2. More senior researchers would send them back into the lab to check for shorts in their wiring and the calibrations of their instruments, but the large gains kept reappearing.

We redesigned the test circuit in order to isolate one particular phenomenon that is not included within the theory of nonlinear dynamics, which is the collapse of the current density in an isotropic material when current biased in negative differential resistance, as predicted by B. K. Ridley in 1963. We then saw the consistent appearance of high signal gains whenever this hot current channel formed, as imaged using thermal cameras. We developed a simple model for the gain based on Kirchoff's Current Law, and found remarkable agreement with our experimental results. After considerable debate, we concluded that we had discovered a completely new type of transistor, defined as a solid-state triode transimpedance amplifier. There are no chemical dopants or p-n junctions in our material. Regions of majority and minority carriers are induced by the current density collapse. We will present a detailed description of this dynamical electro-thermal transistor and its operation.

1:50 PM

H-IV-2: Toward Efficient Neuromorphic Computing with Ion-Modified Quantum Materials

[EFRC - Q-MEEN-C] Alex Frano[1], Ivan K. Schuller[1], Shriram Ramanathan[2], Robert Dynes[1], Marcelo Rozenberg[1], Oleg Shpyrko[1]
[1]University of California, San Diego; [2]Rutgers University

Artificial intelligence, despite its remarkable progress, remains fundamentally constrained by thermal issues with conventional CMOS hardware. To sustain the demand for exponential growth of computation, new, radically different computing paradigms are needed. Neuromorphic computing, inspired by the brain, offers a promising path—particularly when built upon the rich multiphase behavior and tunability of quantum materials.

In this talk, we will present our efforts to harness ion modification as a tool to program and control the energy landscape of correlated oxides, thereby enabling emergent neuromorphic functionalities. This approach echoes the spin glasses based neuromorphic model where information is stored in metastable energy minima. But unlike in spin glasses, quantum materials allow us to directly "navigate" these landscapes with precision.

We focus on rare-earth nickelates as a versatile platform. Hydrogenation transforms these materials into functional analogs of synapses, displaying adaptive, plastic behavior. Helium ion implantation, on the other hand, expands the out-of-plane lattice, suppresses correlations, and promotes metallicity. This could facilitate the lateral diffusion of hydrogen and the reconfigurability of synaptic networks. Gallium ions-based modification offers yet another degree of control, enabling the selective seeding of conductive filament pathways through localized structural modification in vanadate-based devices.

Together, these results show that ion-induced modifications provide a powerful method to modify the behavior of complex oxides and realize programmable, efficient neuromorphic architectures. This work points toward a future where computing hardware is co-designed using quantum materials to provide a materials-first solution to the thermal challenges of AI.

2:10 PM – Team Science Finalist

H-IV-3: FORGING THE FUTURE OF FERROELECTRIC MEMORY

[EFRC - 3DFEM2] Ece Gunay[1], Drew Behrendt[2], Albert Suceava[3], Ian Mercer[3], Quyen Tran[3], Elizabeth C. Dickey[1], Thomas Jackson[3], Jon-Paul Maria[3], Venkatraman Gopalan[3], Andrew M. Rappe[2], Susan Trolier-McKinstry[3]
[1]Carnegie Mellon University; [2]University of Pennsylvania; [3]The Pennsylvania State University

Breakthroughs in computation technologies are deeply tied to growing demands for energy consumption and large data volumes. To meet these needs and power the future of artificial intelligence and large language models, stepwise advancement of current technology is not enough; a new paradigm of accessible memory capable of performing in-situ computation at the atomic level is required. For low-power compute- in-memory architectures, The Center for Three-Dimensional Ferroelectric Microelectronics Manufacturing (3DFeM2) believes that next generation ferroelectrics, materials with a spontaneous polarization that is reversible with application of external electric field, is the answer. The realization of this revolutionary idea however faces challenges in both the implementation of devices and in the understanding of the underlying behavior of such materials. Here, we present significant advances by our team in (1) the theoretical modeling and experimental characterization of the most interesting candidate materials aimed at improving underlying material properties (2) how these materials can be used in real functional memory devices and (3) how our quest can be augmented by automated machine learning experiments. Through collaborative efforts from across universities and

scientific backgrounds, we have managed to discover new ferroelectric materials tailored to our application, unravel how they work at the atomic level, and ultimately leverage these insights to implement them into electronics that can eventually become the backbone of the next generation of computer memory.

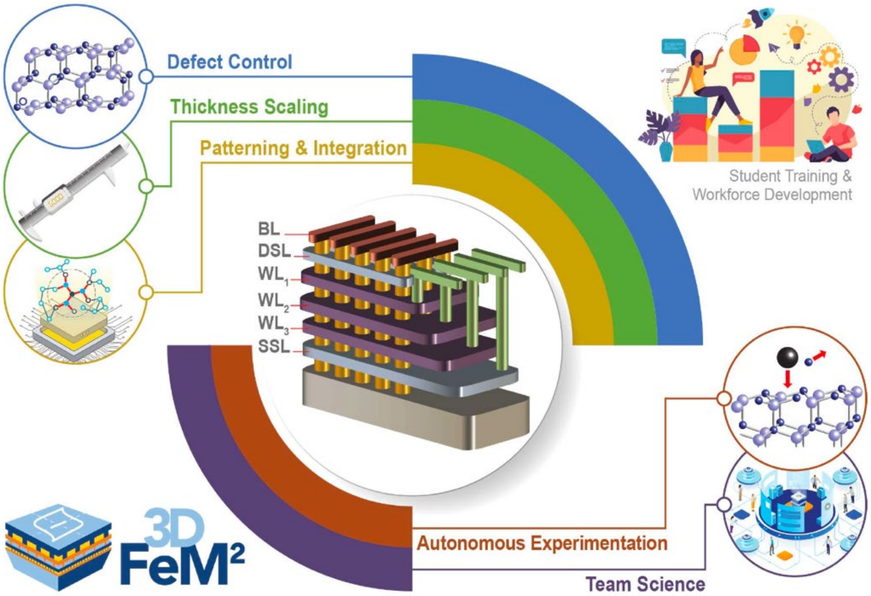


Fig. 1: Vision for 3DFeM2 in which fundamental materials science and processing science enable 3D ferroelectric memory for low power computing.

Contributions: E.G., D.B., A.S., I.M., and Q.T. organized and prepared the presentation based on their original research. S.T.M., T.J., J.P.M., V.G., A.M.R., and E.C.D., planned and guided the research as well as supervised and edited the presentation.

2:30 PM – Team Science Finalist

H-IV-4: MAPPING ATOMISTIC STRUCTURE TO NEUROMORPHIC FUNCTION THROUGH SINGLE-CRYSTAL NEURONAL OSCILLATORS

[EFRC - reMIND] John Ponis[1], Kenna Ashen[1], Michelle Smeaton[2], Jialu Li[3], Fatme Jardali[1], George Agbeworvi[1], Jinghua Guo[3], Xiaofeng Qian[1], Katherine Jungjohann[2], Lance Wheeler[2], Patrick Shamberger[1], Sarbajit Banerjee[1]
[1]*Texas A&M University;* [2]*National Renewable Energy Laboratory;* [3]*Lawrence Berkeley National Laboratory*

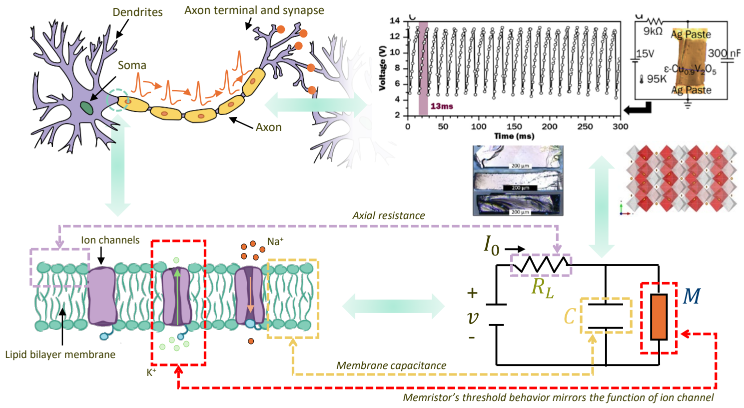


Figure 1. A memristive neuromorphic element is fabricated from an entire single crystal and X-ray crystallography is used as a powerful lens to image structural rearrangements underpinning memristive behavior with sub-Å resolution.

The superexponential increase in demand for computing power accompanying the rise of artificial intelligence, combined with the end of Moore's Law and Dennard's scaling, has spurred intense interest in alternative computing architectures. Neuromorphic computing aims to mimic the human brain by leveraging materials with non-linear conductance to emulate neuron function. However, mechanisms to describe such conductance nonlinearities remain obscure, and have rarely ever been framed in terms of atoms and electrons. As such, strategies for atomistic materials design remain exceedingly empirical. Our collaborative team has addressed critical gap in the field. We have achieved the long-cherished goal of fabricating a memristive neuromorphic element out of an entire single crystal and have used X-ray crystallography as a powerful lens to image structural rearrangements underpinning memristive behavior with sub-Å resolution.[1] We discover interstitial copper-ion migration and reordering in **ε**-$Cu_{0.9}V_2O_5$ and β'-$Cu_xV_2O_5$, mapping ion trajectories with atomic resolution, as the defining structural rearrangement underpinning the structural transformation.[1,2] We further map the nature of charge and spin ordering in the insulating phase. Based on mechanistic understanding, we have devised co-intercalation and topochemical modification as atom-precise methods for broadening the first-order electronic transition, which maps directly to an expanded range of stable and persistent self-sustaining oscillations. The results demonstrate mapping of complex circuit properties to specific features of atomistic and electronic structure in strongly electron correlated materials and are an exemplar for bridging across decades of length and time scales using multimodal characterization, scale-bridging simulations, and iterative materials design and discovery. The results further demonstrate the promise of reMIND's distinctive library of single crystals.

1. J. Ponis, et. al. Atomistic Origins of Conductance Switching in an **ε**-$Cu_{0.9}V_2O_5$ Neuromorphic Single Crystal Oscillator. *Journal of the American Chemical Society* **2024**, 146 (50), 34536-34550.
2. G. Agbeworvi et al. An Atom-Precise Approach for Introducing Weak Disorder in First-Order Phase Transitions to Stabilize Broad-Band Neuromorphic Oscillators, submitted for publication.
3. L. Wheeler et al. Tuning Optical and Electrical Properties of Vanadium Oxide with Topochemical Reduction and Substitutional Tin. *Chemistry of Materials* **2024**, 36, 21, 10483–10495.

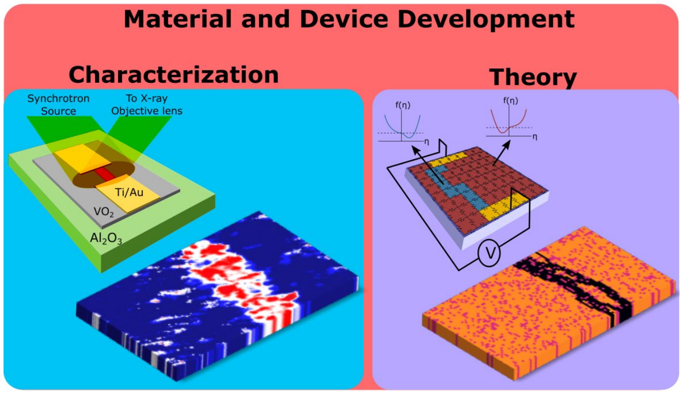
Contributions: J. P.: design, synthesis, characterization; K.A.: simulations; M.S.: electron micrsocopy; J.L.: RIXS and XAS; F. J.: compact model; G.A.: synthesis, magnetism; J.G. RIXS & XAS; X.Q: first-principles modeling; K. J.: electron microscopy; L.W.: topochemistry; P.S.: compact models; S.B.: design and conceptualization

2:50 PM – Team Science Finalist

H-IV-5: INHOMOGENEITIES OF ELECTRICALLY TRIGGERED METAL-INSULATOR TRANSITIONS IN NEUROMORPHIC DEVICES

[EFRC - Q-MEEN-C] Pavel Salev[1], Elliot Kisiel[1], David Alspaugh[1], Oleg Shpryko[1], Marcelo J. Rozenberg[1], Yayoi Takamura[2], Zahir Islam[3], Alex Frano[1], Ivan K. Schuller[1]

[1]University of California, San Diego; [2]University of California, Davis; [3]Argonne National Laboratory



Maximizing the number of operations per energy input in neuromorphic hardware requires taking the full advantage of every functionality offered by materials, which in turn necessitates gaining the comprehensive understanding of the material response to external stimuli. In metal-insulator transition (MIT) quantum materials, applying an above-threshold voltage drives a large resistance change, which can mimic the basic neuronal activation [1,2]. MIT electrical triggering can also be accompanied by transient memory, exhibit pronounced stochasticity and show anomalous magnetic responses [3-5]. These subtle properties accompanying the MIT triggering can offer new exciting opportunities to implement advanced neuronal behaviors, such as adaptation and multimodal spiking, and allow processing and storing information leveraging both charge and spin degrees of freedom. Gaining the basic understanding of such properties, however, is a formidable challenge because of the need for advanced *in-operando* micro- and mesoscale characterization and development of nonequilibrium theoretical frameworks. In our recent works [6,7], we demonstrate that electrical MIT triggering is accompanied by a complex structural response resulting in local lattice states that do not emerge when slowly varying equilibrium control parameters such as temperature or pressure. Utilizing advanced synchrotron x-ray techniques, x-ray microdiffraction and dark-field x-ray microscopy, we observed that driving the electronic MIT by external voltage produces spatially inhomogeneous lattice distortions, including nanoscale monoclinic clusters inside the voltage-induced rutile filament in VO_2 and crystal lattice twinning in $(La,Sr)MnO_3$. We showed that the nominally volatile electrically MIT triggering in VO_2 is accompanied by medium-term memory, which is mediated by local lattice sites that tend to undergo the phase transition at significantly lower threshold voltages after performing electrical cycling. This memory persists even through a brief low-temperature thermal cycle and vanishes after the device relaxes for ~30 minutes. Based on experimental observations, we developed an interacting Mott resistor network model, which showed that point defects can lead to spatially extended phase distribution inhomogeneities and lock the local sites in the low-switching voltage state, leading to the medium-term memory. Overall, our collaborative full-cycle research approach incorporating material synthesis and fabrication, advanced characterization, and theoretical modeling allowed an unprecedented insight into the structural evolution in electrical MIT switches and can lead to the development of novel functionalities in quantum materials neuromorphic electronics.

Contributions: P.S. synthesized materials and fabricated devices, E.K. And P.S. performed the x-ray microscopy measurements, D.A. developed the Mott resistor network analysis.

References: [1] Sci Rep **10**, 4292 (2020), [2] Nat Nanotechnol **16**, 680 (2021), [3] Nature **569**, 388 (2019), [4] PNAS **120**, e2303765120 (2023), [5] Phys Rev B **107**, 054415 (2023), [6] ACS Nano **19**, 15385 (2025), [7] PNAS **121**, e2317944121 (2024).

I. Nuclear

Session II: Monday, August 11, 2025, 1:40 – 3:20 PM, Salon F

1:40 PM – Team Science Finalist

I-II-1: METAL CORROSION UNDER IRRADIATION – EXPLAINING IN SITU X-RAY SPECTROSCOPY WITH EX SITU MICROSCOPY AND ATOM PROBE TOMOGRAPHY

[EFRC - FUTURE] Franziska Schmidt[1], Saikumaran Ayyappan[2], Kayla Yano[3], Matthew Chancey[1], Hyosim Kim[1], Djamel Kaoumi[2], Peter Hosemann[4], Blas Uberuaga[1], Yongqiang Wang[1]

[1]Los Alamos National Laboratory; [2]North Carolina State University; [3]Pacific Northwest National Laboratory; [4]University of California, Berkeley

The FUTURE EFRC targets the behavior of solids under environmental extremes. One aspect of this work is the exposure of simple model systems, such as pure Fe, to the extremes of radiation and corrosion simultaneously in the Irradiation-Corrosion Experiment (ICE III) at LANL. ICE III uses proton irradiation and heavy liquid metals like lead bismuth eutectic (LBE) or molten salts to study the effects of radiation on the corrosion process in these environments. During the experiment, particle-induced x-ray emission spectroscopy (PIXE, from protons hitting the target) provides in situ information about pure Fe corrosion in LBE. The PIXE signal indicates a consistent thinning of the sample that is accelerated by proton irradiation [1]. However, ex situ microscopy images (see Figure 3b) and c)) obtained at NC State and atom probe tomography (APT) results from PNNL paint a more complicated picture. This talk focuses on the Fe-LBE system under proton irradiation, the mechanisms of oxide layer formation and degradation, and the importance of applying a host of analysis tools to unravel the complexities of seemingly simple systems.

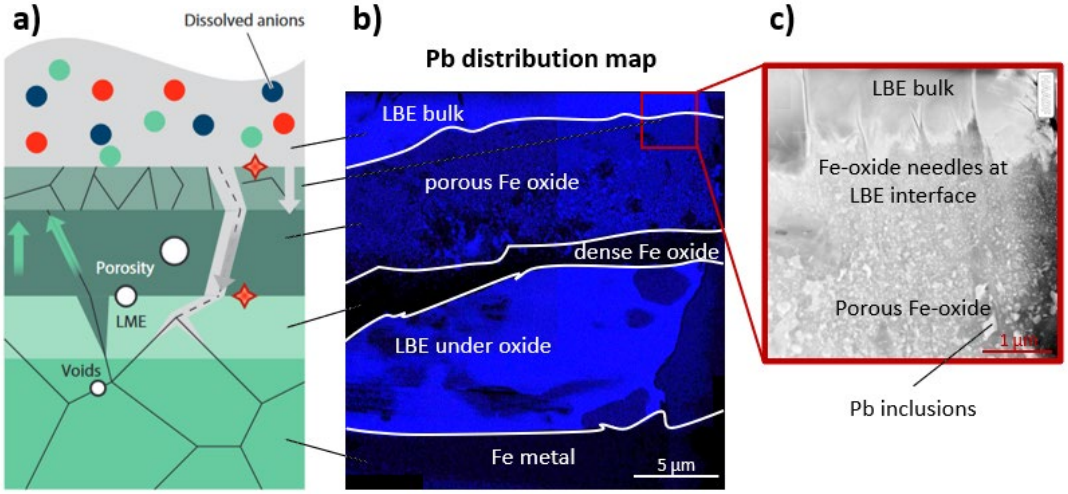


Figure 3 – a) Schematic of corrosion behavior in LBE environments from [2]: In the presence of dissolved O, multiple corrosion layers with varying levels of porosity will form between the LBE (top, grey) and the base metal (green, bottom), which is also affected by liquid metal embrittlement (LME). b) Pb map of broken-off multilayered Fe-oxide floating in LBE near Fe base metal (unpublished). c) Detailed view of Fe-oxide/LBE interface showing mode of oxide growth (needles) into the liquid (unpublished).

Contributions:

PH, YW, BU conceptualized the study; PH contributed the methodology; FS, SA, KY performed formal analysis; FS, MC, HK, YW conducted the investigation; YW provided resources; FS curated data; FS, SA, KY performed visualization; YW, BU, PH, DK supervised the study; BU, PH obtained funding

References

[1] Schmidt, Franziska, et al. "Continuous Monitoring of Pure Fe Corrosion in Lead-Bismuth Eutectic Under Irradiation with Proton-Induced X-ray Emission Spectroscopy." *JOM* 73 (2021): 4041-4050.

[2] Schmidt, Franziska, et al. "Effects of radiation-induced defects on corrosion." Annual Review of Materials Research 51.1 (2021): 293-328.

2:00 PM

I-II-2: Multiscale Investigation of Defects in Oxide Fuels

[EFRC - TETI] Miaomiao Jin[1], Beihan Chen[1], Marat Khafizov[2], Anshul Kamboj[3], Md Minaruzzaman[2], Kaustubh K. Bawane[3], Boopathy Kombaiah[3], Chao Jiang[3], Linu Malakkal[3], Yongfeng Zhang[4], David H. Hurley[1]

[1]The Pennsylvania State University; [2]The Ohio State University; [3]Idaho National Laboratory; [4]University of Wisconsin-Madison

Nuclear fuels present a scientifically intriguing challenge: understanding how radiation-induced defects form and evolve; and how these defects affect thermal transport across scales. This project addresses this challenge through a multiscale investigation methods combining experimental characterization; atomistic modeling and rate theory to gain fundamental insight into the coupling between irradiation-driven microstructural evolution and thermal property degradation.

In oxide fuels; we explore a broad spectrum of defect types; including point defects; small clusters; and dislocation loops using a combination of ab initio methods; molecular dynamics; rate theory; and transmission electron microscopy characterization of irradiated single crystals. To address the limitations of empirical interatomic potentials in modeling complex defect behavior; we developed a machine learning (ML) interatomic potential that enables accurate and efficient simulations of interstitials and their clustering. These atomistic insights inform modeling efforts via molecular dynamics and rate theory; which we used to interpret defect accumulation and recovery kinetics during in-situ annealing and irradiation experiments on irradiated oxide fuels. These combined efforts revealed defect migration; coalescence; and dislocation loop unfaulting; offering valuable insight into thermally and radiation-accelerated recovery mechanisms and improving our understanding of extended defect evolution in fluorite-structured oxides.

2:20 PM

I-II-3: Developing and Validating Multiscale Models of Radiation-Modified Oxide Growth

[EFRC - FUTURE] Aaron A. Kohnert[1], Edward F. Holby[1], Elizabeth A. Peterson[1], Mark Asta[2], Shivani Srivastava[2], Kayla H. Yano[3], Tiffany C. Kaspar[3], Daniel K. Schreiber[3], Blas P. Uberuaga[1]
[1]Los Alamos National Laboratory; [2]University of California, Berkeley; [3]Pacific Northwest National Laboratory

The premise of FUTURE is that irradiation impacts corrosion. In particular, in systems in which an oxide scale forms on the surface of a metal, radiation will impart new defects that may influence the rate at which corrosion mechanisms occur. To understand the fundamental coupling of these two extreme conditions, we have developed a cluster dynamics model that describes the evolution of non-equilibrium radiation-induced point defects and their influence on the overall growth of an oxide scale. Applying this model to hematite, the outer layer of the oxides that forms on iron, we find irradiation typically reduces the overall oxidation rate of the scale, despite the fact that we find radiation-enhanced diffusion in bulk material to be much faster than thermal cases. Ultimately, this reduction is tied to changes in the Fermi level that lead to the suppression of cation interstitial transport processes which mediate hematite growth.

This model explicitly accounts for the multiple charge states that any given defect can adopt, treating each charge state as a unique species in the cluster dynamics equations. This approach allows for charge state transitions and shifts in the Fermi level that impact defect stability and consequently kinetics. Further, this model is validated against various experimental measurements, including our own annealing and irradiation experiments using isotope marker layers quantified with atom probe tomography.

Together, our results highlight the important and sometimes counterintuitive impact of irradiation on corrosion and the importance of considering the coupling between extreme environments.

2:40 PM

I-II-4: Insights into Interfacial Morphological Evolution of Ni Binary Alloys in Molten Salts

[EFRC - MSEE] Yuxiang Peng[1], Xiaoyang Liu[1], Kaustubh K. Bawane[2], Ellery J. Hendrix[3], W. Beck Andrews[3], Ellie M. Kim[4], Phillip W. Halstenberg[4], Xiaoyin Zheng[1], Charles Clark[1], Michael E. Woods[2], Wah-Keat Lee[5], Lu Ma[5], Steven Ehrlich[5], Dmitry S. Maltsev[6], Alexander S. Ivanov[6], Xianghui Xiao[5], Lingfeng He[2], Ruchi Gakhar[2], Sheng Dai[4,6], Mingyuan Ge[5], James F. Wishart[5], Katsuyo Thornton[3], Yu-chen Karen Chen-Wiegart[1,5]

[1]Stony Brook University; [2]Idaho National Laboratory; [3]University of Michigan; [4]University of Tennessee; [5]Brookhaven National Laboratory; [6]Oak Ridge National Laboratory

Understanding the interfacial chemical and morphological evolution of alloys in molten salts is critical for advancing energy systems such as molten salt reactors and concentrated solar power. This work combines in situ synchrotron multimodal characterization, electron microscopy, and phase-field modeling to elucidate the temperature- and chemistry-dependent kinetics governing charge and mass transport in chloride-based molten salts. Specifically, chemical reactions and surface diffusion occur at the interfaces, while long-range diffusion takes place in both the solid and liquid phases, driving the corrosion and coarsening of Ni–20Cr alloys.

We systematically investigated three key factors: (1) the influence of temperature on corrosion morphology, showing distinct mechanisms driving morphological evolution as revealed by synchrotron X-ray nano-tomography involving dealloying and intergranular corrosion; (2) the impact of metal ion additives on modifying reaction chemistry and the resulting morphological changes in the alloys; and (3) the role of salt impurities (e.g., oxygen and water) in shifting corrosion pathways and producing mixed surface oxides.

In addition, phase-field simulations initialized from in situ X-ray tomography provided mechanistic insight into post-corrosion coarsening via surface, solid bulk, and liquid bulk diffusion. Comparisons with experimental data identified surface diffusion as the dominant mechanism, with curvature-driven densification and scaling laws enabling the extraction of diffusivity values consistent with literature.

Together, these results establish a multiscale framework linking salt chemistry, short- and long-range transport, corrosion conditions, interfacial processes, and morphological evolution. This integrated approach supports the predictive design of corrosion-resistant materials and advances the broader understanding of metal degradation in molten salt environments.

3:00 PM

I-II-5: Origin of Reactive Species in Solution Phase Radiolysis of Highly Concentrated Electrolytes

[EFRC - IDREAM] Shuai Li[1], Eleftherios Lambros[2], Aodong Liu[2], Ryan Beck[2], Emily Nienhuis[3], Carolyn Pearce[3], Douglas Garratt[4], Robin Santra[5], Jay LaVerne[6], Thomas Orlando[7], Linda Young[1], Xiaosong Li[2]

[1]Argonne National Laboratory; [2]University of Washington; [3]Pacific Northwest National Laboratory; [4]SLAC National Accelerator Laboratory; [5]Deutsches Elektronen-Synchrotron (DESY); [6]University of Notre Dame; [7]Georgia Institute of Technology

Understanding the elementary steps following ionization in aqueous systems provides a framework for radiation-matter interactions in chemistry and biology. Radiation chemistry has been largely explored on picosecond timescales through pulse radiolysis—a timescale which precludes mechanistic understanding of the origin of reactive species. Synchronized, two-color sub-femtosecond X-ray pulses from X-ray free-electron lasers provide a qualitatively new approach to track the electronic and nuclear dynamics following ionization. To establish methodology, we studied radiation-induced processes in pure liquid water via X-ray transient absorption in the water window, first following outer-valence ionization and then following full-valence ionization. The latter represents the first attosecond pump/attosecond probe experiment on a condensed phase sample and introduced the technique of all X-ray attosecond transient absorption (AX-ATAS). In condensed phase AX-ATAS, we find a strong influence of electron collisional ionization and weaker effects from electronic coherence. Interestingly, the latter study demonstrates the ability of attosecond pump/probe experiments to reveal information on equilibrium properties and resolves a controversy surrounding the interpretation of X-ray emission spectra, as evidence for two structural motifs of liquid water. After establishing the experimental and theoretical methodologies using pure liquid water, we have expanded to the study of aqueous salt solutions. We are now embarking on the investigation of concentrated sodium nitrate solutions, as nitrate is a classic electron scavenger and the dominant species present in legacy radioactive tank waste awaiting retrieval and processing at the Department of Energy's Hanford Site.

Session IV: Tuesday, August 12, 2025, 1:30 – 3:10 PM, Brookside B

1:30 PM

I-IV-1: Comprehensive Analysis of Thermal Transport in Defect-populated ThO_2

[EFRC - TETI] Saqeeb Adnan[1], Amey R. Khanolkar[2], Zilong Hua[2], Kaustubh Bawane[2], Anshul Kamboj[2], Miaomiao Jin[3], Linu Malakkal[2], Md Minaruzzaman[1], Shuxiang Zhou[2], Ella Pek[2], J. Matthew Mann[4], Michael E. Manley[5], Chris Marianetti[6], Boopathy Kombaiah[2], David H. Hurley[2], Marat Khafizov[1]

[1]The Ohio State University; [2]Idaho National Laboratory; [3]The Pennsylvania State University; [4]Air Force Research Laboratory; [5]Oak Ridge National Laboratory; [6]Columbia University

We investigate the impact of irradiation-induced defects on thermal transport in ThO_2 used as a nuclear fuel surrogate. Understanding heat transfer under irradiation conditions is critical to

performance of functional materials in nuclear application. Development of accurate performance analysis codes demands a detailed understanding of how individual nano and sub-nano-scale defect clusters affect heat transfer. We present a comprehensive study of thermal transport in defect-populated ThO_2 that integrates first-principle based modeling with experimental results. Temperature dependent thermal conductivity is modeled by a solution to phonon Boltzmann transport equation (BTE) that captures phonon-phonon and phonon-defects interactions. First-principles description of phonons is validated against inelastic neutron scattering (INS) measurements. The unique low-temperature thermal conductivity trends observed in measurements are analyzed using the BTE model to isolate the impact of individual type of defect. A rate theory (RT) model parametrized based on characterization transmission electron microscopy is used to predict irradiation-induced defect densities which are important input parameters for defect scattering functions in BTE model. Our analysis found a consistent trend of defect scattering parameters from the two different modeling frameworks. However, a resonant-phonon scattering mechanism beyond the traditionally considered Rayleigh scattering is found to significantly influence low-temperature thermal transport in the presence of irradiation-induced point defects. The creation of localized phonon modes due to these point defects is confirmed by Raman spectroscopy. This analysis highlights the impact of various phonon scattering mechanisms on the transport properties in defect-induced nuclear fuels.

1:50 PM

I-IV-2: Overview of FUTURE Salt Effort

[EFRC - FUTURE] Elena Romanovskaia[1], Ho Lun Chan[1], Sean Mills[2], Harjot Singh[1], Valentin Romanovski[1], Kayla Yano[3], Ryan D. Hayes[2], Nathan Bieberdorf[2], Minsung Hong[2], Matthew Chancey[4], Raluca O. Scarlat[2], Yongqian Wang[4], Laurent Capolungo[4], Mark Asta[2], Andrew M. Minor[2], Peter Hosemann[2], John R. Scully[1], Blas Uberuaga[4]

[1]University of Virginia; [2]University of California, Berkeley; [3]Pacific Northwest National Laboratory; [4]Los Alamos National Laboratory

Molten salt environments present several challenges to nuclear reactor structural materials, such as selective dealloying (Cr, Fe, etc.) coupled with the presence of lattice strain, grain boundaries and dislocation substructures that accelerate molten salt corrosion. The corrosion dealloying behavior of Ni-Cr alloy (2-20 wt.%) was investigated in molten LiF-NaF-KF (or FLiNaK) salts at 600°C at a variation of constant potentials. The cold-work effect was studied where NiCr alloys were cold-rolled to achieve reductions of thickness of 10%, 30%, and 50%, introducing a high density of dislocations and their substructures. Separately, model Ni-Cr alloys (5-20 wt.%) were subjected to heavy Ni ion radiation up to a peak damage of 2.2 µm and 60 dpa. STEM-EDS, 4D-STEM and APT analysis were performed to understand the corrosion morphology and mechanisms as well as the nature of precipitates found on the surface of irradiated and corroded NiCr.

The operating temperature is known to have a crucial effect on the materials' durability. The corrosion behavior of Ni-Cr alloys (5-20 wt.%) in FLiNaK over a temperature range of 500-700°C was investigated under a constant electrochemical potential. Post-test surface and cross-sectional analyses were performed using SEM-EDS. Preliminary theoretical mechanisms to explain the observed dealloying behavior were obtained.

Work on impurities effect on Ni-20Cr wt.% alloy uncovered the compositional variations and morphology at multiple length scales in corrosion-damaged samples after exposure to EuF_3 in FLiNaK. Through the development of a 1D phase field model, these results were rationalized by formation energies for the Ni- and Cr-oxidation into the molten salt.

2:10 PM

I-IV-3: Radiation Enhances Gibbsite Dissolution Through Disruption of Ion Networks and Changes to Interfacial Speciation

[EFRC - IDREAM] Xin Zhang[1], Xiaoxu Li[1], Qing Guo[2], Maxime Pouvreau[1], Elias Nakouzi[1], Trent Graham[1], Yifu Feng[1], Jaehun Chun[1], Lili Liu[1], Pravalika Butreddy[1], Zheming Wang[1], James De Yoreo[1], Jay LaVerne[3], Carolyn Pearce[1], Gregory Schenter[1], Gregory Kimmel[1], Aurora Clark[2], Kevin Rosso[1]

[1]Pacific Northwest National Laboratory; [2]University of Utah; [3]University of Notre Dame

The structure and dynamics of ion networks in concentrated aqueous electrolytes are central to controlling particle growth, dissolution, and interparticle interactions. Here, we demonstrate that radiation disrupts these ion networks, leading to significant changes in chemical reactivity and material stability. Building on insights from our previous work—where radiation-induced species were shown to modify the local electrolyte composition in concentrated sodium aluminate solutions—we now reveal how such disruptions enhance the dissolution of the aluminum hydroxide gibbsite ($Al(OH)_3$). By combining high-speed/high-resolution atomic force microscopy (AFM), artificial intelligence/machine learning-assisted image analysis, and ab initio and density functional tight binding molecular dynamics simulations with enhanced sampling, we identify a previously unreported dimer dissolution pathway in alkaline environments. Using a custom-built X-ray atomic force microscope (rad-AFM), along with gamma irradiation experiments on gibbsite suspensions and dry powders, we show that both X-ray and gamma radiation significantly accelerate gibbsite dissolution in alkaline environments. Our results indicate that at the gibbsite/solution interface radiation generates reactive transient chemical species that facilitate nucleophilic attack on bridging oxygens, thereby enhancing aluminum release from gibbsite surfaces. We are actively working to identify key descriptors—including changes in chemical environment, defect generation, and network restructuring—to develop a computational framework for predictive mechanistic simulations of this complex phenomenon. The work will ultimately provide a new foundation for understanding radiation-driven interfacial reactivity across a wide variety of applications, including radioactive waste processing, material degradation and corrosion, and phase transformations in irradiated environments.

2:30 PM

I-IV-4: Structure and Dynamics of Molten Salts: From Reactivity and Speciation to Network Formation

[EFRC - MSEE] Santanu Roy[1], Luke D. Gibson[1], Rajni Chahal[1], Debmalya Ray[1], Alex Ivanov[1], Dmitry Maltsev[1], Phillip Halstenberg[1], Sheng Dai[1], Vyacheslav Bryantsev[1], Matthew Emerson[2], Bichitra Borah[2], Shobha Sharma[2], Hung Nguyen[2], Claudio Margulis[2], Ruchi Gakhar[3], Alejandro Ramos Ballesteros[3], Yang Liu[4], Nirmalendu Patra[4], Nicholas Marcella[4], Kaifeng Zheng[4], Simerjeet Gill[4], Anatoly Frenkel[4], James Wishart[4], Haimeng Wang[5], Edward Maginn[5]

[1]Oak Ridge National Laboratory; [2]University of Iowa; [3]Idaho National Laboratory; [4]Brookhaven National Laboratory; [5]University of Notre Dame

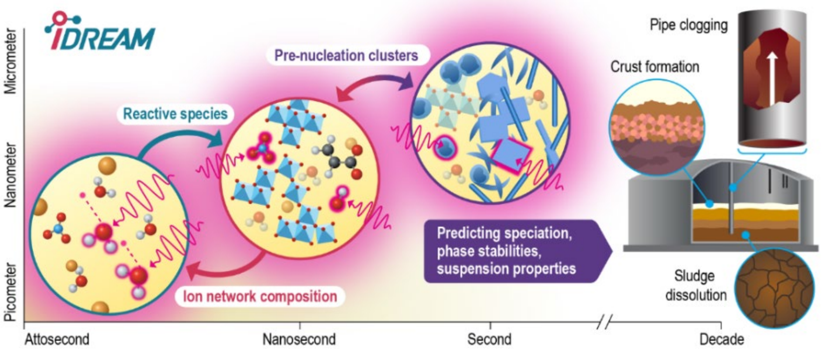
A fundamental understanding of the chemistry and properties of molten salts (MS) is indispensable for enabling their energy-efficient and safe deployment as fuels and coolants in MS-based nuclear reactors. For instance, extremely high temperatures and fission or corrosion reactions result in complex speciation—that is, different metastable ionic complexes or radicals with varying coordination numbers are formed. How and at what rate are these species formed? How are they distributed in the bulk and interfacial environments of different MS solvent compositions? How do the bulk structural and dynamical properties vary from one MS salt to another, influencing speciation events and the solvation and distribution of species to varying extents? These questions remain key to controlling MS behavior under reactor conditions. At our center, Molten Salts in Extreme Environments, we tightly couple the current state-of-the-art theory and computational methods with new, high-precision experiments, aiming at addressing the aforementioned questions regarding MS structures and properties. In this talk, we will elaborate on how we combine molecular dynamics simulations (force field-based or ab initio MD) with modeling Raman, UV-Vis and X-ray absorption spectroscopies, X-ray/neutron scattering, rate theory, and machine learning to determine the structural and dynamical features of chloride-based molten salts. Key points of discussion will range from local ion-exchange mechanisms and dynamics to reactivity, electron localization and transfer, and structural correlations up to the intermediate range. We will highlight the distinct interionic coordination chemistry of actinides and lanthanides, which simple salts of alkali metal ions lack.

2:50 PM – Team Science Finalist

I-IV-5: UNDERSTANDING HOW RADIATION UNIQUELY TRANSFORMS THE PHYSICOCHEMICAL PROPERTIES OF ELECTROLYTES

[EFRC - IDREAM] Ryan Beck[1], Simantini Paul[2], Amita Bedar[3], Greg Felsted[4], Aodong Liu[1], Hemanth Haridas[2], Eleftherios Lambros[1], Maxime Pouvreau[4], Jacob Morton[4], Yifu Feng[4], Pravalika Butreddy[4], Ashley Kennedy[4], William Denman[5], Hossam Elshendidi[6], Shuai Li[7], Emily Nienhuis[4], Trent Graham[4], Xin Zhang[4]

[1]University of Washington; [2]University of Utah; [3]Notre Dame University; [4]Pacific Northwest National Laboratory; [5]Georgia Institute of Technology; [6]Hunter College CUNY; [7]Argonne National Laboratory



We are revealing how attosecond responses to radiolysis ripple across complex ion networks, influencing reactivity of concentrated alkaline radioactive waste suspensions over decades.

The instantaneous, radiation-induced changes to the electronic structure of concentrated electrolytes is central to the retrieval, transport, and treatment of legacy radioactive waste. Based on our new knowledge of the attosecond electronic response of water molecules to radiation, we used the LCLS through our campaign proposal to break new ground by measuring single X-ray pulse resonant inelastic X-ray spectra at the oxygen K-edge in aqueous sodium chloride for the first time. We saw that the generation of an outer valence hole, and the subsequent excitation of a core electron into the hole, was different in the presence of cation traps. To isolate these signatures of short-lived species under radiation, we ran high-accuracy density functional theory (DFT) calculations on water-solute ensembles. Ultrafast proton dynamics also play a pivotal role, and we examined the relaxation of an excess solvated electron in water and with solutes using real-time nuclear electronic orbital (NEO) time dependent DFT calculations. We also pushed our understanding of ultrafast dynamics and structure into more complex high-pH solutions using lab-based two-dimensional infrared (2D-IR) spectroscopy, and we now know that hydroxide preferentially forms solute-solute interactions with other dissolved ions. Classical molecular dynamics (CMD) and graph theory show us how this ion clustering affects transport properties, e.g., viscosity. With ab-initio DFT and our new reactive force field, in combination with Raman and NMR spectroscopy, we are now demonstrating how the strength of these ion networks affects oligomerization of key species in radioactive waste (aluminate and pertechnetate) and the nature of precipitated phases. Using electron paramagnetic resonance and electrochemistry, we tracked the distribution of radicals and redox states that result from radiation-induced changes to local solution structure, so that we can predict reduction of redox active species (pertechnetate and nitrate) and nucleation of aluminum-bearing phases. Through our team science, we are coordinating X-ray, gamma-ray, and electron beam irradiation across multiple institutions to unravel how radiation-induced ultrafast processes in the electrolyte cascade to macroscopic effects, including aggregation, dissolution and hydrogen production.

Contributions: R. Beck, A. Liu: DFT assignment of X-ray signatures. E. Lambros: NEO calculations. S. Paul: CMD/graph theory of ion clustering and solvation. A. Bedar: gamma radiation-induced radical species. G. Felsted: 2D-IR for ultrafast solution dynamics. H. Haridas: RFF modelling of dissolution. T. Graham: NMR and muon spectroscopy. M. Pouvreau: Raman/NMR spectra computation. J. Morton: radiation electrochemistry. X. Zhang: particle synthesis. Y. Feng: atomic force microscopy. P. Butreddy: X-ray imaging of dissolution. A. Kennedy, E. Nienhuis: alkaline electrolyte synthesis. W. Denham: laser spectroscopy measuring gas production. H. Elshendidi: technetium chemistry. S. Li: LCLS experiments

J. Quantum Information Science I

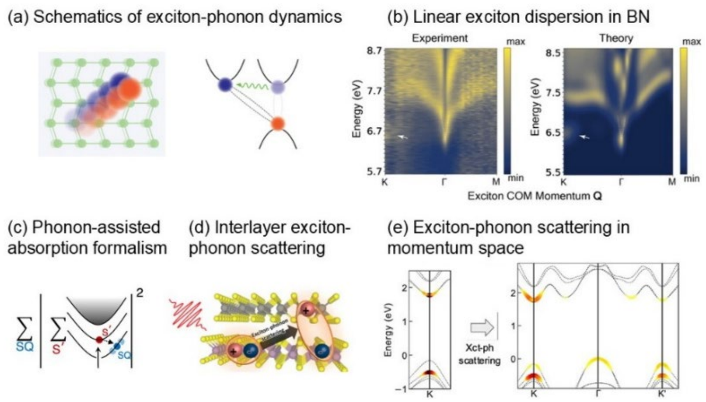
Session I: Monday, August 11, 2025, 9:10 – 10:30 AM, Brookside C

9:10 AM – Team Science Finalist

J-I-1: FIRST-PRINCIPLES ANATOMY OF EXCITON DYNAMICS: FROM DISPERSION TO QUANTUM TRANSPORT

[CMS - C2SEPEM] Luna Liu[1], Gurjyot Sethi[2,3], Jonah Haber[4], Jinyuan Wu[1], Bowen Hou[1], Zhenfa Zheng[5], Jeffrey B. Neaton[2,3], Felipe H. da Jornada[4], Zhenglu Li[5], Diana Y. Qiu[1], Steven G. Louie[2,3]
[1]Yale University; [2]Lawrence Berkeley National Laboratory; [3]University of California, Berkeley; [4]Stanford University; [5]University of Southern California

Exciton dynamics underpin the practical realization of light-matter interactions ranging from the efficiency of energy transport in photovoltaics and photocatalysis to the coherence of quantum information and light-driven quantum phase transitions. The first-principles understanding of exciton dynamics requires a few basic building blocks: 1) The full exciton dispersion to capture the phase space of momentum and energy conserving scattering processes, 2) Interaction of excitons with external perturbations such as electromagnetic fields and lattice vibrations, 3) Exciton scattering matrix elements and self-energies, and 4) An equation of motion describing the dynamical processes. In this talk, we highlight our center's multi-modal developments along these directions, which build synergistically to provide a complete first-principles picture of exciton dynamics spanning from the coherent regime through diffusive transport. We begin by calculating exciton dispersion and validating our theoretical predictions against momentum-resolved electron energy loss spectroscopy measurements (Q-EELS), revealing for the first time the emergence of a massless excitons composed of massive electrons and holes [1]. Building on accurate exciton band structures, we include exciton-phonon scattering from first principles, revealing exciton lifetimes [2], diffusion [3], and relaxation processes [4-5]. We develop the first full quantum theory of exciton orbital magnetic moment [6]. Finally, we implement a real-time quantum master equation, going beyond the secular/Lindblad approximation, that explicitly includes the electron-electron and electron-phonon interactions on the same footing across the Brillouin zone [7]. Our developments put calculations of exciton dynamics in real materials, especially reduced-dimensional systems, within reach through the synergistic combination of novel theoretical developments, innovative algorithmic acceleration, and highly-optimized massively-parallel codes for high performance computing.



[1] L. Liu *et al.*, under review, arXiv:2502.20454v2 (2025). [2] Y.-H. Chan *et al.*, Nano Lett., **23**, 3971 (2023). [3] G. Cohen *et al.*, Phys. Rev. Lett., **132**, 126902 (2024). [4] Y.-H. Chan *et al.*, Nano Lett. **24**, 7972 (2024). [5] Y.-H. Chan *et al.*, Phys. Rev. B, **111**, 184305 (2025). [6] G. Sethi *et al*, in preparation (2025). [7] Z. Zheng *et al.*, in preparation (2025).

Contributions: L.L., J.W., and B.H. performed calculations and experiments on hBN. G.S. developed the theory for exciton orbital magnetic moment. J.H. performed calculations on exciton-phonon coupling. Z.Z. developed the nonequilibrium exciton-phonon dynamics implementation. J.B.N., F.H.J., Z.L., D.Y.Q., and S.G.L. supervised and conceived the research.

9:30 AM – Team Science Finalist

J-I-2: STRONG LIGHT–MATTER INTERACTION IN PLASMONIC ARRAYS ENABLES COHERENT QUANTUM EMISSION

[EFRC - QuPIDC] Zhaoyuan Zheng[1], Jonas Peterson[2], Hanyu Hong[3], Jiwoong Park[3], Libai Huang[2], and Teri Odom[1]
[1]Northwestern University; [2]Purdue University; [3]University of Chicago

Two-dimensional transition metal dichalcogenides (TMDCs) are promising materials platform for scalable quantum emitters due to their strong excitonic resonances and spin-valley physics. However, their photoluminescence is often weak—particularly in multilayer systems—posing challenges for integration into quantum photonic devices. Here, we demonstrate that plasmonic lattices offer a programable photonic platform to enhance and control light emission from TMDCs (Fig.1 a-g). By coupling single and multilayer TMDCs to engineered plasmonic arrays composed of periodically arranged metallic nanoparticles we hybridize localized surface plasmons with diffractive modes to generate surface lattice resonances (SLRs). Through spectral alignment of single-layer WS_2 excitonic transitions with SLR modes, we achieve up to 36-fold Purcell enhancement in radiative rates of excitons at room temperature. Notably, we observe dramatic brightening of multilayer WS_2, with photoluminescence enhanced by more than 3 orders of magnitude. Ultrafast pump-probe microscopy further uncovers the momentum-resolved dynamics of exciton–polariton modes in these hybrid systems, revealing signatures of coherent light–matter interaction. Together, these results highlight plasmonic arrays as a versatile and scalable platform for enhancing emission and coherence in quantum emitters, directly supporting QuPIDC mission to develop room-temperature quantum photonic technologies.

Contributions: Zhaoyuan Zheng fabricated the plasmonic arrays and conducted simulations of light–matter interactions within the system. Jonas Peterson performed the ultrafast optical spectroscopy measurements and carried out kinetic modeling of the data. Hanyu Hong synthesized the two-dimensional materials.

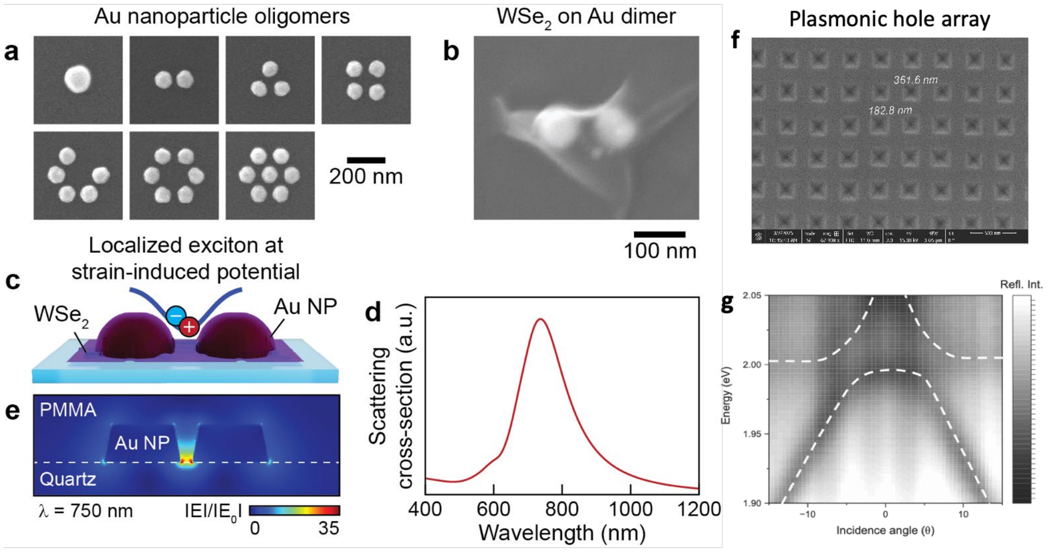


Figure 1: Integration of TMDCs on plasmonic nanoparticle arrays. (a) SEM images of Au oligomers fabricated using soft lithography and reactive ion etching. (b) SEM image of WSe_2 transferred on a Au dimer. (c) Schematics of a TMDC sheet placed on a Au dimer and its exciton trapped in a strain-induced potential. (d-e) Calculated normal scattering spectrum and electric near-field distribution of localized surface plasmon of Au dimer. (f). A SEM image of a plasmonic lattice that can support lattice plasmon. (g) Experimental measured angle-resolved reflectance spectrum showing strong light matter coupling between monolayer WS_2 and lattice plasmon.

9:50 AM

J-I-3: Apparent Circular Dichroism for Improved Chiroptical Control

[EFRC - CMQT] Roel Tempelaar[1], Randall H. Goldsmith[2], Mark C. Hersam[1], Nathaniel Stern[1], Michael R. Wasielewski[1]
[1]Northwestern University; [2]University of Wisconsin–Madison

Photons are envisioned as canonical quantum information carriers with applications ranging from photonic computing to "flying qubits" for long-range information transport. Photonic spin states manifest as circular optical polarization, and the transduction of such spin states to matter-based polarization thus relies on chiroptical interactions. Within the Center for Molecular Quantum Transduction, we have advanced the understanding and application of an emergent chiroptical phenomenon, referred to as "Apparent Circular Dichroism" (ACD), which helps overcoming two major obstacles preventing the application of conventional chiroptics for quantum information purposes: light–matter interactions are too weak, and chiroptical selectivity is too low. Whereas conventional chiroptics relies on minute magnetic dipoles, ACD is driven by electronic dipoles only, allowing for exceptionally-high selectivity. Moreover, it uniquely leads to a chiroptical response that is inverted for oppositely-traveling light, allowing materials to be embedded in optical resonator structures for amplifying light–matter interactions. We have developed a microscopic theory of ACD, harnessed ACD for constructing chiral optical cavities and chiral organic lasing, and created a roadmap for realizing chiral polaritons based on this phenomenon. We have furthermore shown theoretically and experimentally how ACD allows certain inorganic crystals to defy a long-held structure-function relationship by showing a chiroptical response under centrosymmetry, opening up a novel class of materials for the design of enhanced chiroptical responses.

10:10 AM

J-I-4: Using Chirality and Symmetry Breaking to Tailor Hybrid Metal Halide Perovskite Structures and Emerging Properties

[EFRC - CHOISE] David B. Mitzi[1], Rayan Chakraborty[1], Yifan Dong[2], Md Azimul Haque[2], Matthew P. Hautzinger[2], Heshan Hewa-Walpitage[2], Gabrielle Koknat[1], Allan J. Phillips[2], Yi Xie[1], Matthew C. Beard[2], Joseph J. Berry[2], Jeffrey L. Blackburn[2], Volker Blum[1], Joseph M. Luther[2], Seth R. Marder[3], Peter C. Sercel[4], Zeev Valy Vardeny[5]

[1]Duke University; [2]National Renewable Energy Laboratory; [3]University of Colorado Boulder; [4]Center for Hybrid Organic Inorganic Semiconductors for Energy; [5]University of Utah

Hybrid organic-inorganic perovskite (HOIP) semiconductors offer unique opportunities to tailor structure and function through combined organic and inorganic design. This chemical versatility enables tunable properties relevant to a wide range of applications, including photovoltaics, light-emitting devices, detectors, transistors, spintronics, and quantum technologies. This talk highlights how the organic constituent—particularly when chiral—can control lattice distortion and symmetry, influencing optoelectronic and spin-related behaviors. We will discuss recent studies that illustrate the role of hydrogen bonding in driving centrosymmetric-to-noncentrosymmetric structural transitions, and how chiral cation doping (mixing of organic cations) enables control over structural symmetry and spin splitting. Further examples include the observation of giant spin splitting and persistent spin textures driven by secondary ammonium cations, as well as remote chirality transfer using an interfacial organic moiety. These advances underscore the emerging strategy of symmetry engineering through organic molecular design to modulate light, charge, and spin behavior across the HOIP family. Building on this, CHOISE has recently leveraged this tunability to demonstrate, for example, chirality-induced spin selectivity, enhanced circular dichroism, circularly polarized photo and electroluminescence, and room-temperature spin injection at HOIP/III-V semiconductor interfaces—effects with compelling implications for future applications where the interconversion between charge, spin, and light is desired such as opto-spintronic, novel microelectronics, and quantum information.

Session II: Monday, August 11, 2025, 1:40 – 3:20 PM, Brookside C

1:40 PM

J-II-1: Active-space approaches for Ab initio Cavity Quantum Electrodynamics

[CCS - MAPOL] Nam Vu[1], Daniel Mejia Rodriguez[2], Nicholas Bauman[2], Ajay Panyala[2], Edrahl Mutlu[2], Mikulas Matousek[3], Narajan Govind[3], Jay Foley[1]
[1]University of North Carolina at Charlotte; [2] Pacific Northwest National Laboratory; [3]J Heyrovsky Institute of Physical Chemistry

When molecules are placed inside optical cavities, molecular and photonic degrees of freedom become strongly coupled, which can lead to the creation of hybrid light-matter states called polaritons, and the modifications of ground-state properties. The emerging fields of polariton chemistry and molecular cavity quantum electrodynamics have shown that these light-matter interactions can dramatically alter chemical reactivity, opening new pathways to control reactions with light. Recent experimental breakthroughs have achieved optical cavities small enough to reach strong coupling in the single-molecule limit. Plasmonic picocavities and scanning tunneling microscope break-junctions now create mode volumes of 10^{-1} - 10^{2} nm^{3}, where individual molecules experience interaction strengths and electric field fluctuations intense enough to modify their internal structure and intermolecular forces. In this electronic strong coupling regime, the cavity vacuum state alone can alter molecular properties, demanding sophisticated theoretical treatment that goes beyond traditional quantum chemistry. Accurately modeling these complex quantum systems requires computational methods that can handle both the intricate electron correlations within molecules and their interactions with quantized light fields. I will present our recent work developing ab initio cavity quantum electrodynamics methods to model molecules under strong light-matter coupling with high accuracy. Specifically, I'll describe how we've extended complete active space configuration interaction, complete active space self-consistent field theory, and density matrix renormalization group methods to include cavity quantum electrodynamics effects. These active-space approaches allow us to capture the essential physics of strongly correlated electrons while accounting for strong light-matter coupling for one or a few molecules. I'll also discuss our efforts to make these advanced computational tools more accessible through educational materials that introduce students to molecular simulation within the context of cavity-coupled systems, helping train the next generation of researchers in this rapidly growing field.

2:00 PM

J-II-2: Molecular Optical-Spin Interfaces for Quantum Information Applications

[EFRC - CMQT] Sebastian Kopp[1], Shunta Nakamura[1], Yong Rui Poh[2], Kathryn Peinkofer[1], Brian Phelan[1], Joel Yuen-Zhou[2], Matthew Krzyaniak[1], Michael Wasielewski[1]
[1]Northwestern University; [2]University of California, San Diego

We will describe recent work from our laboratory that focuses on using photo-driven processes in molecular materials targeting quantum information applications. Molecular optical-spin interfaces are emerging as promising alternatives to solid state defects such as diamond nitrogen vacancy centers for quantum information science applications. We will report on a new theory-guided approach to molecular color centers that utilizes luminescent stable organic diradicals with triplet ground states. Optical spin polarization of the triplet ground state is achieved by spin-selective excited-state intersystem crossing. The triplet ground state is characterized by pulse electron paramagnetic resonance spectroscopy and shows spin coherence times approaching 30 microseconds at 5 K. Also, we demonstrate coherent microwave manipulation of the spin-polarized ground state populations and coherences using optically detected Rabi nutations, Hahn echo formation, and echo decay measurements at 85 K. This marks a crucial step towards leveraging the favorable spin relaxation times of organic molecules for applications as quantum sensors at temperatures that heretofore have been difficult to achieve by molecular color centers.

2:20 PM

J-II-3: Towards Scalable Generation of Indistinguishable Photons using Solid-State Platforms

[EFRC - QuPIDC] Alisa Javadi[1], Jonathan Hood[2]
[1]University of Oklahoma; [2]Purdue University

The overarching goal of QuPIDC is to develop robust, scalable quantum light sources using solid-state materials platform. In this talk, we present our recent advances in organic molecules and quantum dots as platforms for high-performance single-photon emitters.
We report breakthroughs in permanently tuning pairs dibenzoterrylene defects in anthracene into resonance, enabling the emission of collective quantum states. We also demonstrate the successful integration of these organic emitters with high-quality-factor photonic crystal cavities, achieving strong light-matter coupling. Together, these advances pave the way for on-demand single photon generation, eliminating reliance on the probabilistic nature of spontaneous parametric down-conversion.

We will also discuss our recent advances in droplet-etched epitaxially grown quantum dots, which exhibit near-unity quantum efficiency (>99%), minimal phonon sidebands (<5%), and high photon indistinguishability (>92%). There is a critical gap in quantum emitters compatible with silicon photonics and telecom infrastructure, motivating the development of quantum dots operating at telecom wavelengths. To address this, we are engineering droplet-etched quantum dots that emit near 1350 nm. Toward this goal, we are engineering droplet-etched quantum dots emitting near 1350 nm. These longer-wavelength emitters benefit from low-defect environments, larger physical size, and greater oscillator strength, which together support longer spin and optical coherence times—critical for quantum communication and scalable photonic networks.

Together, these complementary approaches establish a path toward scalable and indistinguishable photon sources, with transformative applications in single-photon spectroscopy, quantum sensing beyond classical limits, and fault-tolerant photonic quantum computing.

2:40 PM

J-II-4: Quantum simulations for quantum technologies

[CMS - MICCoM] Giulia Galli[1,2], Juan de Pablo[3], Maria K. Chan[1], Andrew Ferguson[2], Joseph Heremans[1], Marco Govoni[4], Jie Xu[1], Victor Yu[1], Jonathan Whitmer[5]
[1]Argonne National Laboratory; [2]University of Chicago; [3]New York University; [4]Univerista' di Modena e Reggio Emilia; [5]Notre Dame University

We present the activity of the Midwest Integrated Center for Computational Materials (MICCoM), with focus on advanced methods to study correlated states of defects in solids and the full optical cycle of spin defects for quantum technology applications. MICCoM disseminates interoperable computational tools – open-source software, data, simulation methods, and validation procedures – that enable the community to simulate and predict the properties of functional materials. The Center's focus is on (i) materials for quantum information science and on (ii) materials for low power electronics. MICCoM scientific strategy is based on the premise that the functionality of materials depends critically on the integration of dissimilar, often defective components and on the interfaces that arise between them. Hence the emphasis of the Center's applications is placed on understanding and characterizing defects and interfaces, and on predicting finite-temperature spectroscopic and coherence properties. The description of dissimilar and defective components requires the development of first-principles electronic-structure methods, coupled to appropriate dynamical descriptions of matter and advanced sampling techniques, and requires as well, the ability to predict multiple properties of complex systems. A key success of MICCoM has been the coupling of classical and quantum codes, together with their use on several high-performance computing architectures. In this talk we will describe how the developments of multiple methods and codes has led to the ability to describe defective systems with unprecedented accuracy and efficiency, with numerous predictions, validated experimentally, for materials for quantum technologies.

3:00 PM

J-II-5: 54 Ghz Clock Transition in a Ho^{3+} Spin Qubit Assembled Into a Metal-Organic Framework

[EFRC - M2QM] Linqing Peng[1], Miguel Gakiya-Teruya[2], Robert Stewart[2,3], Shuanglong Liu[4], Chenghan Li[1], Hai-Ping Cheng[4], Stephen Hill[2,3], Garnet K.-L. Chan[4], Michael Shatruk[2]
[1]California Institute of Technology; [2]Florida State University; [3]National High Magnetic Field Laboratory; [4]Northeastern University

A high-symmetry assembly of molecular spin qubits has been achieved in the metal–organic framework (MOF) $[Ho(pzdo)_4](ClO_4)_3$ (1), where the eight-coordinate Ho^{3+} nodes are bridged by pyrazine-1,4-dioxide (pzdo) ligands [J. Am. Chem. Soc. (2025) – DOI:10.1021/jacs.5c07796]. The approximate square-antiprismatic (D_4d) coordination of the Ho^{3+} ion leads to the stabilization of the $m_J = \pm 4$ ground-state doublet due to crystal-field splitting of the J = 8 total angular momentum state. Mixing of the $m_J = +4$ and $m_J = -4$ projection states opens a zero-field energy gap (Δ) resulting in the spin clock transition (SCT) evident in the EPR spectra of 1. The SCTs are known to protect qubits from the surrounding magnetic noise to first order, thus enhancing coherence. Frequency-dependent EPR studies reveal that the Ho^{3+} centers in 1 exhibit a high-frequency SCT with ΔSCT = 54.6 GHz, which can be beneficial to minimizing second-order decoherence effects. To elucidate the crystal field effect that governs the spin clock transition, we developed a novel constrained density functional theory (DFT) to derive effective spin Hamiltonians. Benchmarked against five lanthanide single-ion magnets, our method consistently achieves accuracy comparable to the state-of-the-art from correlated wavefunction methods, but with a significantly reduced computational cost, akin to DFT. This efficiency therefore enables application to this large clock qubit 1. The resulting effective spin Hamiltonian of 1 captures all salient aspects of the magnetic and EPR measurements, providing a detailed and quantitative description of low-energy eigenstates relevant to the spin clock transition.

Session III: Tuesday, August 12, 2025, 9:00 – 10:20 AM, Brookside C

9:00 AM – Team Science Finalist

J-III-1: Enabling Ambient Stability and Quantum Integration of Organometallic Magnonic Ferrimagnets via Atomic Layer Encapsulation

[EFRC - CMQT] Iqbal B. Utama[1], Robert Claassen[2], Srishti Pal[3], Hannah Christianson[4], Donley S. Cormode[2], Dmitry Lebedev[1], Subhajyoti Chaudhuri[1], Qin Xu[3], George C. Schatz[1], Jeffrey R. Long[4], Gregory D. Fuchs[3], Ezekiel Johnston-Halperin[2], and Mark C. Hersam[1]

[1]Northwestern University; [2]The Ohio State University; [3]Cornell University; [4]University of California, Berkeley

Molecule-based spin and magnonic materials are promising for next-generation quantum technologies, offering synthetic tunability beyond what is achievable with fully inorganic counterparts. Magnons, the quanta of spin waves in magnetic materials, are particularly useful in hybrid quantum systems since they bridge electromagnetic and spin degrees of freedom. The magnetic molecular coordination compound vanadium tetracyanoethylene (V[TCNE]$_x$) possesses exceptional magnonic properties but degrades rapidly when exposed to air, limiting its practical use. In this work, we demonstrate a breakthrough in stabilizing V[TCNE]$_x$ by encapsulating it with a sub-100 nm layer of aluminum oxide using atomic layer deposition. This encapsulation substantially enhances the air stability of V[TCNE]$_x$ while preserving its quantum and magnetic properties, thus increasing its viability for practical quantum information technologies. The sub-100 nm thickness of the encapsulation layer enables spectroscopic and surface-sensitive characterization techniques to probe the intrinsic properties of V[TCNE]$_x$ including

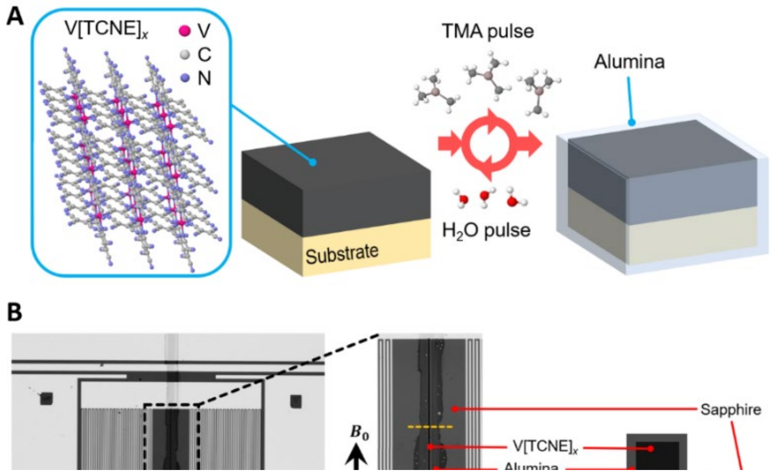


Figure 1. (A) Schematic of ALD alumina encapsulation. (B) Integration of alumina-encapsulated V[TCNE]$_x$ with a microwave resonator.

spatially-resolved magnetometry measurements. Leveraging the optical transparency of the encapsulation layer over a broad electromagnetic spectral range, we performed detailed optical spectroscopy of V[TCNE]$_x$ from deep ultraviolet to mid-infrared energies to resolve the electronic and vibrational excitations of the material. In addition, this encapsulation scheme is compatible with thermal cycling, which allows repeated access to cryogenic temperatures for cavity magnonics, where we observed magnon-photon hybridization at milli-Kelvin temperatures with minimal interference from strain-induced anisotropy effects. Overall, this effective encapsulation scheme enables seamless integration of V[TCNE]$_x$ into advanced quantum devices.

Contributions: M.I.B.U. performed ALD encapsulation, AFM, magnetometry in PPMS, MFM, XPS, UV-vis-NIR, FTIR, ellipsometry, and Raman spectroscopy measurements. R.C. performed CVD growth of V[TCNE]$_x$ and cavity FMR measurements. S.P. fabricated the microwave resonator and performed the cavity magnonics experiments. H.C. performed electrodeposition of V[TCNE]$_x$. M.C.H., E.J.H., G.D.F., J.R.L., and G.C.S. supervised the project.

9:20 AM – Team Science Finalist

J-III-2: CHIRALITY TRANSFER AND SPIN SELECTIVITY IN HYBRID METAL HALIDE SEMICONDUCTORS

[EFRC – CHOISE] Md Azimul Haque[1], Andrew Grieder[2], Steven P. Harvey[1], Roman Brunecky[1], Jiselle Y. Ye[1], Bennett Addison[1], Junxiang Zhang[3], Yifan Dong[1], Yi Xie[4], Matthew P. Hautzinger[1], Heshan Hewa Walpitage[5], Ian A. Leahy[1], Jeiwan Tan[1], Margherita Taddei[1], Pius Markus Theiler[1], Aeron McConnell[6], Andrew H. Comstock[6], Kai Zhu[1], Kirstin Alberi[1], Jeffrey L. Blackburn[1], Zeev Valy Vardeny[5], David B. Mitzi[4], Joseph J. Berry[1,3], Seth R. Marder[1,3], Peter Sercel[7], Dali Sun[6], Joseph M. Luther[1], Yuan Ping[2], Matthew C. Beard[1]

[1]National Renewable Energy Laboratory; [2]University of Wisconsin-Madison; [3]University of Colorado Boulder; [4]Duke University; [5]University of Utah; [6]North Carolina State University; [7]Center for Hybrid Organic Inorganic Semiconductors for Energy

Traditionally, chiroptical properties in hybrid metal halide semiconductors (MHS) arise from symmetry breaking by incorporating chiral A-site organic cations, which restricts compositional flexibility. Furthermore, how structural chirality governs the charge and spin transport has been illusive due to the lack of tunability in traditional chiral semiconductors. Here, we present a new strategy for inducing chirality in MHS through remote chirality transfer, where a proximal chiral molecule selectively interacts with divalent metal cations to impose asymmetric distortions deep into the lattice, as revealed by density functional theory calculations, achieving large circular dichroism dissymmetry factors.[1] Exploiting the tunable chirality of MHS, we demonstrate an exceptionally large room-temperature chirality-induced spin selectivity (CISS)-driven magnetoresistance response exceeding 300% in a spin valve device, where the chiral MHS forms a spin-selective tunneling barrier governed by molecular handedness, generating current dissymmetry factors beyond the limits predicted by conventional models.[2] These findings establish a structure-property relationship between CISS and structural chirality, providing new design principles for controlling charge-to-spin interconversion and advancing chiral opto-spintronic semiconductors.

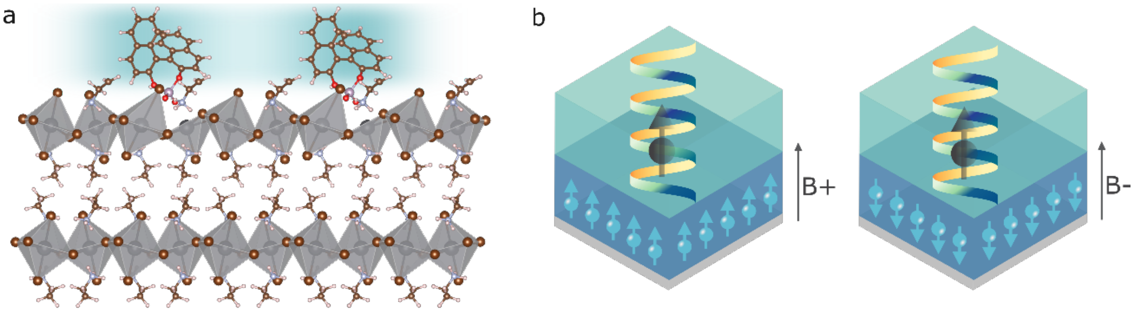


Fig. (a) Schematic showing the structural distortion of CMHS upon interaction with chiral molecules. (b) A low resistance state is observed when the ferromagnet and enantiomorph spins are parallel and high resistance when the spins are antiparallel in a spin valve.

References:
[1] Haque et al., Remote Chirality Transfer in Low-Dimensional Hybrid Metal Halide Semiconductors, Nat. Chem. 17, 29-37, 2025. [2] Haque et al., Chirality-Induced Magnetoresistance in Hybrid Organic-Inorganic Perovskite Semiconductors, Submitted, 2025

Contributions: M.A.H. synthesized the CMHS compositions, fabricated the spin valves and performed characterizations. A.G. developed the chirality transfer model and performed the CCM and DFT calculations.

9:40 AM

J-III-3: Integrating Experiment, Theory and Artificial Intelligence for Discovery and Characterization of Advanced Spin Crossover Complexes

[EFRC - M2QM] Divya Kumar[1], Angel Albavera-Mata[2], Miguel G. Teruya[1], Richard G. Hennig[2], S.B. Trickey[2], and Michael Shatruk[1]
[1]Florida State University; [2]University of Florida

The integration of spin-crossover materials into electronic devices requires their incorporation in ultrathin film architectures. To meet this challenge, we are developing innovative strategies for fabricating Fe(II)-based metal complex films with thicknesses below 20 nm. The films are produced by both sublimation and mechanical exfoliation of molecular layers from bulk crystals. Key to our approach is the design and synthesis of Fe(II) spin-switching complexes that incorporate asymmetric tridentate Schiff-base ligands with tunable substituents. They are chosen strategically to enhance volatility and enable non-covalent thin-film deposition. In this presentation, we examine the effects of Fe(II) oxidation state on the spin-state behavior and crossover transitions. We demonstrate that the spin state is dictated not solely by the metal oxidation state but also by more subtle aspects of the electronic structure of the entire complex. In this vein, we discuss the influence of the topology of peripheral substituents on the spin-crossover characteristics in both Fe(II) and Fe(III) systems, providing insights into their structural and magnetic properties as a function of temperature.

Complementary to the experimental work, we showcase an advanced artificial intelligence tool that enables accurate prediction of the crossover energy of molecular candidates. This theoretical advance significantly streamlines materials discovery. The tool is available as a Python library with a user-friendly interface, to make sophisticated computational techniques accessible to a broader research community. Through the seamless integration of experimental synthesis, modelling, and artificial intelligence, our joint efforts are advancing the development and application of spin switching materials for future device applications.

10:00 AM

J-III-4: Novel Topological States in Thin Films of Topological Matter

[EFRC - CATS] Susanne Stemmer[1], Ivar Martin[2], Anand Bhattacharya[2], Joseph Checkelsky[3]
[1]University of California, Santa Barbara; [2]Argonne National Laboratory; [3]Massachusetts Institute of Technology

Thrust 2 of the CATS EFRC envisions the unique quantum phenomena of topological thin films elevated to the level of "topotronics", with real control over materials, as required for their application in future electronic, spintronic, photonic and quantum information technologies. In this presentation, we will first discuss our approaches to ultrathin, high-quality films of topological matter using molecular beam epitaxy, which allow for electrostatic control of their properties. We will present results that demonstrate that systematic tuning of thin film heterostructures, combined with electric field control, can be used to obtain novel topological ground states that do not exist in bulk materials. We will also discuss the characterization of the hallmark features of topological quantum materials, in particular their boundary states, and new approaches for their detection using quantum point contacts and thermoelectric measurements.

Session IV: Tuesday, August 12, 2025, 1:30 – 3:10 PM, Brookside C

1:30 PM

J-IV-1: Study of novel phenomena in 2D materials with quantum many-body theories and exascale computing

[CMS - C2SEPEM] Steven G. Louie[1,2], James R. Chelikowsky[3], Jack R. Deslippe[1], Naomi Ginsberg[1,2], Felipe H. da Jornada[4], Zhenglu Li[5], Jeffrey B. Neaton[1,2], Diana Y. Qiu[6], Feng Wang[1,2], Chao Yang[1]
[1]Lawrence Berkeley National Laboratory; [2]University of California, Berkeley; [3]University of Texas at Austin; [4]Stanford University; [5]University of Southern California; [6]Yale University

Two-dimensional (2D) van der Waals materials exhibit novel photoexcited states, intriguing field-driven and time-dependent phenomena, and exotic correlated ground states. We present some recent progress in their understanding and predictions using ab initio quantum many-body theories and computational tools developed in the CMS Center for Computational Study of Excited-State Phenomena in Energy Materials (C2SEPEM). Our studies reveal a rich, diverse set of electronic and optical phenomena in these 2D materials and their moiré structures. Recent findings include: a self-driven exciton-Floquet effect (analogous to the optical Floquet effect driven by photons), strong exciton-enhanced linear and nonlinear optical responses (e.g., shift currents and second- or higher-order harmonic generation), as well as formation of light-induced shift current vortex crystals in moiré systems. Moreover, we show exotic correlated ground states may emerge, such as the existence of an unconventional excitonic insulator phase (characterized by emergent k-space spin textures) as well as electron Wigner crystal phases with excitons of unique character in dilutely doped 2D semiconductors. These findings add to the promise of 2D materials for exploration of new science and valuable applications. Many of the recent studies are made possible by efforts within C2SEPEM in the development of new methods and their software implementation for high-performance (e.g., the DOE leadership-class) computers, enabling ab initio calculations of electronic states, excitonic physics, and photo responses in very large and challenging systems, in and out of equilibrium.

1:50 PM

J-IV-2: Topology, band gaps, and magnetic structure of correlated 2D and quasi-2D quantum materials by exascale quantum Monte Carlo

[CMS - CPSFM] P. Kent[1], J. Ahn[1], J. Krogel[1], P. Ganesh[1], H. Shin[2], A. Lopez[3], B. Rubenstein[3], C. Melton[4]

[1]Oak Ridge National Laboratory; [2]Argonne National Laboratory; [3]Brown University; [4]Sandia National Laboratories

We explore the critical nature of structure and stacking of 2D and layered 2D quantum materials in determining their band gaps, magnetic structure, and suitability for topological applications. In these materials, the van der Waals interactions, spin, charge, and lattice degrees of freedom are strongly coupled. Together with a highly sensitive hybridization between layers, this leads to highly composition and configuration dependent properties. Using recently developed Quantum Monte Carlo algorithms which can accurately describe and interpret these phenomena, we give examples of overlooked structure and configuration dependence in multiple materials classes, including for $PtSe_2$ and $MnBi_2Te_4$. We find that the 2D layers in these materials often have nearly degenerate stacking modes, and modifications to the stacking order is an effective mechanism to modify their quantum properties.

2:10 PM

J-IV-3: Real-Time Excitation Dynamics in Out-Of-Equilibrium-Driven Materials with the INQ Code

[CMS - NPNEQ] Jacopo Simoni[5], Jonah Haber[2,3], Wuzhang Fang[5], Andrew C. Grieder[5], Chris Ciccarino[2,3], Kevin Moseni[4], Xavier Andrade[1], Alfredo A. Correa[1], Sheikh Rubaiat Ul Haque[2,3], Sangeeta Rajpurohit[1,4], Aaron M. Lindenberg[2,3], Liang Tan[4], Felipe Jornada[2,3], Yuan Ping[5], Tadashi Ogitsu[1]

[1]Lawrence Livermore National Laboratory; [2]SLAC National Accelerator Laboratory; [3]Stanford University; [4]Lawrence Berkeley National Laboratory; [5]University of Wisconsin-Madison

Recent advances in ultrafast spectroscopic techniques, have created a pressing need for accurate, real-time simulations of non-equilibrium quantum dynamics with atomistic precision. To meet this challenge, we present INQ (DOI: 10.1021/acs.jctc.1c00562): a GPU-accelerated, real-time time-dependent density-functional theory (TDDFT) software capable of simulating orbital, lattice, and spin degrees of freedom in coupled electron-photon-ion systems driven far from equilibrium. In this talk, we first discuss recent developments within INQ enabling real-time, ab initio simulations of spin dynamics in photo-excited materials. We detail our implementation of exchange-correlation magnetic fields, spin-orbit coupling and the coupling with external magnetic fields (arXiv:2506.21908). These provide a foundation for studying non-collinear magnetic phenomena in out-of-equilibrium systems, which we demonstrate on magnetic clusters and in solids. We also highlight applications, including real-time magnon dynamics, ultrafast spin response to circularly and linearly-polarized light, and spectroscopic signatures such as magnetic circular dichroism and pump-probe Kerr rotation, as well as reduced-complexity electronic structure methods to capture strong-field phenomena.

We also showcase a center-wide theory-experiment collaboration to interpret nonlinear optical responses in terahertz-pumped layered van-der-Waals magnets, revealing an intricate interplay of spins, electrons, and phonons. Further motivated by experiments, we address the robustness of photoexcited phenomena—particularly Floquet-driven topological phase transitions in photo-irradiated graphene—when the driving field displays a finite coherence. We conclude with an outlook of future INQ developments, highlighting how such a GPU-first, exascale software package can capture physics of non-equilibrium materials from first principles.
Part work was performed at LLNL under Contract DE-AC52-07NA27344.

2:30 PM

J-IV-4: First-principles open quantum dynamics and transport for solids based on density-matrix formalism

[CCS - ADEPTs] Jacopo Simoni[1], Mayada Fadel[2], Mayank Gupta[1], Joshua Quinton[2], Andrew Grieder[1], Christian Multunas[2], Junting Yu[1], Gabriele Riva[1], Shihao Tu[1], Mani Chandra[2], Kejun Li[1], Ravishankar Sundararaman[2], Yuan Ping[1]
[1]University of Wisconsin-Madison; [2]Rensselaer Polytechnic Institute

The theoretical prediction of materials' properties driven out of equilibrium is critical in various fields from semiconductor spintronics to quantum information science. Here we will introduce our recently developed Exascale GPU-accelerated real-time first-principles density-matrix dynamics (FPDMD) method. We derive this theory based on the evolution of the electronic density matrices capable of treating electron-environment interactions and electron-electron correlations at the same level of description. Electron-electron interactions can be formally derived using the nonequilibrium Green's function plus generalized Kadanoff-Baym ansatz. We further extend this framework with Wigner functions for simulating spatial-temporal quantum dynamics and transport accounting for a range of quantum degrees of freedom (e.g., electron, spin, orbital, phonon).

We show our methods can accurately predict spin and carrier lifetime, spin diffusion length, pump-probe Kerr-rotation, and nonlinear optical signatures for disparate solids, from 2D materials to halide perovskites. In particular, we show our recent study of how g factor fluctuations lead to spin dephasing in solids under an external magnetic field, and the distinct electron-phonon contributions to spin and carrier relaxations and the crucial dependence on crystal symmetry.

Finally, we will present recent work on first-principles prediction of spatial-temporal spin transport properties in graphene and chiral materials, where we show spin and orbital angular momentum generation and dephasing in both coherent and incoherent transport, and discuss the distinction between chirality induced spin selectivity and colinear Edelstein effects. Our results provide important insights for spin-optotronic properties and spin and orbital transport in solids.

2:50 PM

J-IV-5: Numerically-Exact Treatment of Dirac and Schrodinger Electrons in Molecules and Solids

[CCS - NEREST] Edward Valeev[1], Robert Harrison[2], Deborah Penchoff[3], Jonathon Misiewicz[1], Erica Mitchell[1], Charles Peterson[4]

[1]Virginia Polytechnic Institute and State University; [2]Stony Brook University; [3]University of Central Florida; [4]University of California, Los Angeles

CCS Center "Numerically-Exact Relativistic many-body Electronic Structure Theory" (NEREST) innovates novel numerical representations for simulating the many-body electronic structure with rigorous control of the numerical errors necessary for predictive description of structures, energetics, and spectra of heavy-element compounds. The use of adaptive multiresolution real-space numerical representations pioneered by the Center members allows to treat valence and core electrons without uncontrolled errors (such as introduced by pseudopotentials) and without poor conditioning in the high-accuracy regime of atomic orbital representations. Key highlights of project year's developments include the first numerical multiconfiguration Dirac solver applicable to general molecules and first numerical solver for all-electron simulation of periodic solids with robust control of numerical error and optimal rate of convergence to the thermodynamic limit.

K. Quantum Information Science II

Session I: Monday, August 11, 2025, 9:10 – 10:30 AM, Glen Echo

9:00 AM

K-I-1: Observation of the Axion Quasiparticle in Condensed Matter

[EFRC - CATS] Jian-Xiang Qiu[1], Barun Ghosh[2], Jan Schütte-Engel[3], Tiema Qian[4], Michael Smith[5], Yueh-Ting Yao[6], Junyeong Ahn[1], Yu-Fei Liu[1], Anyuan Gao[1], Christian Tzschaschel[1], Houchen Li[1], Ioannis Petrides[4], Damien Bérubé[1], Thao Dinh[1], Tianye Huang[1], Olivia Liebman[4], Emily Been[4], Joanna Blawat[7], Kenji Watanabe[8], Takashi Taniguchi[8], Kin Chung Fong[2], Hsin Lin[9], Peter Orth[10], Prineha Narang[4], Claudia Felser[11], Tay-Rong Chang[6], Ross McDonald[7], Robert McQueeney[10], Arun Bansil[2], Ivar Martin[5], Ni Ni[4], Qiong Ma[12], David Marsh[13], Ashvin Vishwanath[1], Su-Yang Xu[1]
[1]Harvard University; [2]Northeastern University; [3]University of California, Berkeley; [4]University of California, Los Angeles; [5]Argonne National Laboratory; [6]National Cheng Kung University; [7]Los Alamos National Laboratory; [8]National Institute for Materials Science; [9]Institute of Physics; [10]Ames National Laboratory; [11]Max Planck Institute for Chemical Physics of Solids; [12]Boston College; [13]King's College London

Axion, which is the coherent oscillation of the theta field, is an elusive particle that can solve multiple fundamental questions including the strong CP problem of QCD and the dark matter. However, its detection is challenging because it has almost no interaction with existing particles. Similar theta field has been introduced to condensed matter and so far studied as a static, quantized value to characterize topology of materials. We report the observation of the Axion quasiparticle in the 2D topological antiferromagnet $MnBi_2Te_4$. Specifically, we directly observe a coherent oscillation of the theta angle in $MnBi_2Te_4$ at 44 GHz, therefore proving the existence of the Axion quasiparticle by its definition. This Axion quasiparticle is induced by the out-of-phase magnon, which strongly couples to the Berry curvature of the electrons therefore dynamically controlling the theta angle. In terms of condensed matter, the Axion quasiparticle enables novel light-matter interaction and coherent antiferromagnetic spintronics. More broadly, the Axion quasiparticle serve as a conceptually novel approach to detect of the dark matter Axion particle in the critically-lacking meV regime. We estimate the sensitivity of this detector based on our data.

9:20 AM

K-I-2: Time-Lapsed Treasure Maps for Finding Programmable Quantum Materials

[EFRC - Pro-QM] Yiping Wang[1], Jeongheon Choe[1], Eric Anderson[2], Weijie Li[2], Julian Ingham[1], Eric A. Arsenault[1], Yiliu Li[1], Chaowei Hu[2], Xiaodong Hu[2], Takashi Taniguchi[3], Kenji Watanabe[3], Xavier Roy[1], Dmitri Basov[1], Jiun-Haw Chu[2], Di Xiao[2], Raquel Queiroz[1], James C. Hone[1], Xiaodong Xu[2], Xiaoyang Zhu[1]
[1]Columbia University; [2]University of Washington, Seattle; [3] National Institute for Materials Science, Japan

The Pro-QM EFRC aims to discover, characterize, and deploy new forms of quantum matter controllable by gating, magnetic proximity and nano-mechanical manipulation. In a joint experimental/theoretical effort between the east coast (Zhu, Querioz, Hone, Roy, Basov) and the west coast (Xu, Xiao, Chu), a Pro-QM team demonstrated a time-domain pump-probe approach as hitherto the most sensitive experiment in detecting quantum phases at moiré interfaces of 2D van der Waals crystals [Nature 2025, 641, 1149]. A pump laser pulse excites charge across a many-body gap or disrupts correlation in a doped moiré interface; a probe pulse tracks subsequent melting and recovery dynamics from exciton sensing. This is essentially a background-free technique when the pump photon energy is below quasi-particle gaps and perturbs only the correlated states. The team applied the approach to the twisted $MoTe_2$ bilayer ($tMoTe_2$) for its richness of quantum phases, as exemplified by the landmark demonstrations of the fractional quantum anomalous Hall effect (FQAH) [Nature 2023, 622, 63; Nature 2023, 622, 74]. In addition to known states in $tMoTe_2$, the team discovered a zoo of hitherto unknown correlated states at fractional fillings of the moiré superlattice, including six new states at fractional hole fillings of the 1st and 2nd Chern bands, two of which have now been confirmed in independent transport measurements. Some of these states are potential candidates for the coveted fractional topological insulators and/or non-abelian anyons. The Pro-QM discovery represents time-lapsed treasure maps for finding new quantum matter in the programmable moiré system.

10:00 AM

K-I-3: Measurement of the dynamic charge susceptibility near the charge density wave transition in $ErTe_3$

[EFRC - QSQM] Dipanjan Chaudhuri[1], Qianni Jiang[2], Xuefei Guo[1], Jin Chen[1], Caitlin S. Kengle[1], Farzaneh Hoveyda-Marashi[1], Camille Bernal-Choban[1], Niels de Vries[1], Tai-Chang Chiang[1], Eduardo Fradkin[1], Ian R. Fisher[2], Peter Abbamonte[1]

[1]University of Illinois Urbana-Champaign; [2]Stanford University

A charge density wave (CDW) phase, observed in many materials with a highly anisotropic electronic structure, is characterized by a periodic modulation of valence electron density coupled with lattice distortion. The formation of a CDW ground state is closely tied to the dynamical charge susceptibility, $\chi(q,\omega)$, which reveals the collective behavior of charge carriers in materials. However, $\chi(q, \omega)$ near a CDW transition had never been measured at nonzero momentum transfer with ~meV energy resolution, despite decades of extensive studies.

In this talk, I will present our results on the investigation of a canonical CDW transition in $ErTe_3$, using momentum-resolved electron energy loss spectroscopy (M-EELS), a technique uniquely sensitive to valence band charge excitations. Unlike phonons, which soften via Kohn anomaly, we find that the electronic excitations exhibit purely relaxational dynamics well described by a diffusive model, with the diffusivity peaking just below the ordering temperature. Additionally, we report, for the first time, a divergent behavior in the real part of $\chi(q, \omega)$ in the static limit ($\omega \rightarrow 0$), a long-predicted hallmark of CDWs. Unexpectedly, this divergence occurs as $T \rightarrow 0$, with only a weak thermodynamic signature at the ordering temperature. Our study necessitates a reexamination of the traditional description of CDW formation and demonstrates the power of M-EELS as a versatile probe of charge dynamics in correlated quantum materials.

9:40 AM

K-I-4: Entanglement and Coherence from Quantum Emitters in hBN

[EFRC - QuPIDC] Souvik Biswas[1], Tongcang Li[2]
[1]Stanford University; [2]Purdue University

Optically active spin defects in solids have long served as a cornerstone for quantum sensing. With the advent of spin qubits in low-dimensional materials, it is imperative to develop optimal quantum control strategies to enhance coherence and enable entanglement for improving sensitivity and resolution.

In this talk, we will present our recent work on boron vacancy (VB-) ensembles and single carbon-related spin defects in hexagonal boron nitride (hBN). First, by employing magnetic-field-based eigenstate engineering, we demonstrate how a single quantum sensor can be programmed to detect both magnetic and electric fields. This reconfigurability enables complete Hamiltonian tomography, revealing rich hyperfine interactions and anisotropic gyromagnetic ratios. Next, we use dynamical decoupling to extend the electron spin coherence time (T_2) to nearly 100 µs—the longest reported for an electronic spin in a van der Waals material.

We also demonstrate atomic-scale nuclear magnetic resonance (NMR) and coherent control of individual ^{13}C nuclear spins in hBN. Using a combination of microwave and radiofrequency pulse sequences, we generate electron–nuclear spin entanglement at room temperature, achieving a Bell-state fidelity of 0.89. The nuclear spin acts as a long-lived quantum memory, enhancing frequency resolution for AC field sensing.

Together, these results establish new directions for quantum sensing in emerging van der Waals platforms.

L. AI/ML

Session I: Monday, August 11, 2025, 9:10 – 10:30 AM, Salon G

9:10 AM

L-I-1: Multiscale Computational Framework for Biomolecular Energy Transduction: from Electrons to the Mesoscale

[CCS - CMSET] Scott Kaiser[1], Siva K. Dasetty[1], Chenghan Li[2], Hezhou Zhang[1], Tomasz Skora[3], Jiangbo Wu[1], Jong Ho Choi[1], Thomas Qu[1], Sahithya Sridharan Iyer[1], Garnet K. L. Chan[2], Tamara Bidone[3], Andrew Ferguson[1], Gregory Voth[1]
[1]University of Chicago; [2]California Institute of Technology; [3]University of Utah

Biomolecular energy transduction couples degrees of freedom over a wide range of time and length scales. Examples involve chemical reactions where the catalysis is activated by localized electronic factors that are themselves coupled to the slow macromolecular dynamics taking place over much larger scales. One example is the microtubule, involving many hundreds of tubulin proteins, which undergoes large conformational rearrangements controlled by GTP hydrolysis of the β-tubulin. CMSET develops scalable methods capable of bridging this range of length and time scales. By leveraging advances in GPU technology, the Chan group has optimized a multigrid DFT implementation which improves upon existing QM/MM methods, especially for hybrid functionals. This is implemented in a QM/MM coupling between PySCF and LAMMPS, and is employed, e.g., in QM/MM studies of nucleotide hydrolysis and amino acid protonation equilibria. This work in turn facilitates the parameterization of a physics-based machine learning approach for multiscale reactive molecular dynamics (MS-RMD), which is three orders of magnitude faster than typical QM/MM. MS-RMD makes the sampling of much longer reactive MD time scales more accessible. Connecting to the all-atom scale, the Ferguson group has addressed the challenge of slow relaxation dynamics in biomolecules using a neural network-based equation free approach, which allows an all-atom MD configuration to take large leaps forward in time. To access even longer length and time scales, Voth and Bidone bridge all of the aforementioned work to new coarse-graining methods and algorithms. Important predictions have already been made in this project and experimentally validated by others.

9:30 AM

L-I-2: Physically Constrained 3D Diffusion for Inverse Design of Fiber-Reinforced Polymer Composite Materials

[EFRC - AIM] Pei Xu[1], Yunpeng Wu[1], Alireza Zarei[2], Shahriar Ahmed[1], Srikanth Pilla[2], Gang Li[1], Feng Luo[1]
[1]Clemson University; [2]University of Delaware

Designing fiber-reinforced polymer composites (FRPCs) with a tailored nonlinear stress-strain response is crucial for applications such as energy absorption in crash structures, flexible robotics, and impact-resistant protective gear. However, the inherent complexities of composite materials and the multitude of parameters involved, render traditional design and optimization methods inadequate for achieving effective inverse design of composites. In this paper, we present an AI-based inverse design framework that effectively and efficiently generates FRPCs with targeted nonlinear stress-strain responses. We introduce a physically constrained diffusion model (PC3D_Diffusion) capable of managing the complexities of composite materials and producing detailed, high-quality designs. We propose a loss-guided, learning-free approach to generate physically feasible microstructure designs by explicitly enforcing physical constraints during the generation process. For training purposes, 1.35 million FRPC samples were created, and their corresponding stress-strain curves were computed using established physics-based computational models. The results show that PC3D_Diffusion consistently generates high-quality designs with tailored mechanical behaviors, while guaranteeing compliance with the physical constraints. PC3D_Diffusion advances FRPC inverse design and may facilitate the inverse design

of other 3D materials, offering potential applications in industries reliant on materials with custom mechanical properties.

9:50 AM

L-I-3: Machine Learning Approaches to Energy Materials and Devices

[EFRC - CABES] Peter Frazier, Tomas Arias
Cornell University

This presentation will present machine learning (ML) approaches for the design and characterization of energy materials and devices. We will present data on catalyst design through minimum energy pathways, predicted onset potentials and high entropy catalysts. We will discuss the use of applied Bayesian optimization of composite functions (BOCF) to accelerate the search for optimization of electron microscopy images. We will also discuss prediction of block copolymer MEA properties.

10:10 AM

L-I-4: Energy Storage Research Alliance - Accelerating Materials Discovery, Synthesis, Characterization, and Understanding with AI/ML and advanced characterization

[Hub - ESRA] Gerbrand Ceder[1,2], Maria Chan[3], Ruozhu Feng[4], Ethan Crumlin[1], Kamila Wiaderek[3], James Burrow[3,5], Wei Wang[4], Shirley Meng[3,5]
[1]Lawrence Berkeley National Laboratory; [2]University of California, Berkeley; [3]Argonne National Laboratory; [4]Pacific Northwest National Laboratory; [5]University of Chicago

The Energy Storage Research Alliance (ESRA) aims at tackling fundamental science challenges in beyond-Li-ion energy storage systems. Underlying the scientific thrusts are the crosscutting efforts which aim at developing cutting-edge capabilities, namely: 1) Materials Acceleration Platform (MAP) and 2) Correlative Characterization. The MAP crosscut leverages and contributes towards the advances in artificial intelligence/machine learning (AI/ML) and automation to accelerate the discovery, synthesis, and characterization of new and existing energy storage materials, especially for Na and Zn. Under the MAP crosscut, we use AI to enable and accelerate physics-constrained information extraction from characterization, combine computational discovery and design with autonomous synthesis with closed-loop feedback, create autonomous electrochemical characterization laboratories, and make possible large-scale predictions of dynamic systems with ML interatomic potentials (MLIPs). The correlative characterization crosscut develops and leverages advanced characterization capabilities including vibrational, x-ray, and optical spectroscopies; x-ray and neutron scattering; analysis of gas and liquid phases; electron, x-ray, and optical microscopy; and nuclear magnetic resonance. The integration of AI/ML is critical for data tracking, prevention of information loss, and automation of experimentation. Together, these crosscut efforts make possible new capabilities to support the scientific endeavors in ESRA.

Session II: Monday, August 11, 2025, 1:40 – 3:20 PM, Salon G

1:40 PM

L-II-1: Autonomous Manufacturing and Automated Materials Exploration for 3D Ferroelectric Microelectronics Manufacturing

[EFRC - 3DFeM2] Ichiro Takeuchi[1], Gilad Kusne[1,2], Haotong Liang[1], Stanislav Udovenko[3], Darren Pagan[3], Jon-Paul Maria[3], Yu Liu[4], Sergei Kalinin[4], Rama Vasudevan[5]
[1]University of Maryland; [2]National Institute of Standards and Technology; [3]The Pennsylvania State University; [4]University of Tennessee-Knoxville; [5]Oak Ridge National Laboratory

Within the 3DFeM2 Center, we have a research thrust dedicated to pursuing various approaches to accelerate the discovery and optimization of ferroelectric materials as well as their manufacturing processes at large. A particular emphasis is to develop autonomous systems which operate on self-driving modes where AI/ML are making the decision as to what experiment to perform next after each iteration. Enlisting Bayesian active learning, autonomous systems can lead to significant reduction in amount of time and resources needed to arrive at the best solutions with minimal to no human intervention. We have a concerted effort to develop automated synthesis and processing tools to advance next-generation manufacturing techniques including thin-film deposition as well as etching. As an example, we have developed a thin film fabrication system, where in-situ characterization of a film being grown is dynamically monitored through electron diffraction, and computer vision is used to determine the quality of the film on the fly. The system steers itself in a multi-dimensional process parameter space in search of the best synthesis condition. In the materials exploration front, we are fabricating combinatorial libraries of various ferroelectric materials which are being probed using piezo-force microscopy (PFM) techniques. There have been significant advances in automating PFM techniques, and we are also pushing towards fully autonomous screening of the thin film libraries, while optimizing multiple physical properties at the same time.

2:00 PM

L-II-2: Orchestrating Interfacial Control: AI-Driven Insights for Advanced Power Electronics

[EFRC - APEX] Steven R. Spurgeon[1,2], Michelle Smeaton[1], Danny Sallis[1], Krishna Acharya[2], Emerson Liu[1], Madeline Hoffman[1,2], Renae Gannon[1], Vladan Stevanovic[2], Andriy Zakutayev[1]
[1]National Renewable Energy Laboratory; [2]Colorado School of Mines

Mastery of emerging wide bandgap power electronics, a core focus of the APEX EFRC, is critically predicated on understanding and precise control of thin-film interfaces, exemplified by systems such as NiO/Ga_2O_3. These interfaces present significant challenges for stabilization due to the inherent reactivity of their constituent components under non-equilibrium synthesis conditions. Emerging artificial intelligence (AI)-guided characterization approaches offer an unprecedented opportunity to interrogate these complex interfaces, leading to a richer, more predictive understanding of synthesis pathways. Here, we describe the development of a comprehensive workflow designed to classify interface structures and defects. This workflow leverages a powerful combination of atomic-resolution scanning transmission electron microscopy (STEM), deep learning techniques, and high-fidelity atomistic simulations. We show how the synergistic integration of experiment and theory, powerfully guided by AI, can provide novel and actionable insights into critical device interfaces, thereby enabling the rational design and synthesis of next-generation power electronics.

2:20 PM

L-II-3: Accelerating the discovery and design of advanced functional materials using AI/ML and exascale computing

[CMS - MLAMD] Cai-Zhuang Wang[1], Ying Wai Li[2], Feng Zhang[1], Yongxin Yao[1], Vladimir Antropov[1], Ryan Richard[1], Zhuo Ye[1], Weiyi Xia[1], Maxim Moraru[2]
[1]Ames National Laboratory; [2]Los Alamos National Laboratory

High-performance functional materials are critical for technological innovation and sustainable development. However, the pace of discovery and design of novel functional materials is far behind the demands. The major goal of this CMS center is to develop a series of exascale-capable computational strategies and codes to dramatically speed up discovery and synthesis of novel advanced functional materials. We accomplish this goal by developing computational frameworks and workflows to efficiently integrate materials theories and methods with AI/ML tools, materials databases, and high-performance/exascale computing to predict new materials in new composition-structure-property spaces and identify synthetic pathways for the new materials. Along with software development, we aim to discover and design novel ternary or quaternary compounds with desirable and experimental validated magnetic or superconducting properties. Studies on the discovery of high performance rare-earth free magnetic materials and novel complex quantum materials will be presented. The power of AI/ML and high-performance computing for significantly reducing the time-to-solution in energy and advanced technology innovations is demonstrated. Limitations of current ML approaches for materials discovery and challenges in closing the feedback loop between computational prediction and experimental synthesis will also be discussed. The AI/ML integrated open-source community codes and associated databases produced by this CMS center are widely applicable for enabling science-based predictive discovery and design of a wide range of functional materials that would otherwise be impractical or impossible to perform within reasonable timeframes due to their complexity.

2:40 PM

L-II-4: Learning at Scale: AI-Driven Design and Discovery of Moiré Superlattices and Complex Quantum Materials

[CMS - HeteroFAM] Ting Cao[1], Yueyao Fan[1], Thomas Huang[1], Kaichen Xie[1], Eric J. Bylaska[2], Daniel Mejia Rodriguez[2], Niranjan Govind[2], Jenna Pope[2], Nicholas Bauman[2], Peter Sushko[2], Juan Carlos Idrobo[1,2], Di Xiao[1,2]
[1]University of Washington; [2]Pacific Northwest National Laboratory

The HeteroFAM project addresses the challenge of rational materials design by developing computational tools to explore an extensive design space exemplified by heterostructures comprising two-dimensional (2D) materials and transition metal oxides. By including machine learning and automation, HeteroFAM enables breakthroughs in areas such as moiré materials, correlated electron physics, and magnetic materials.

Simulating moiré superlattices in 2D materials, where large supercells (>10,000 atoms) and intricate atomic reconstructions make traditional first-principles methods intractable. We developed a generalizable machine learning force field (MLFF) framework capable of simulating twisted multilayer heterostructures with varying twist angles, stacking, and layer numbers. Demonstrated on 2+2 $MoTe_2$, our model captures topology-driven band transitions and provides a scalable solution for studying correlated moiré phenomena.

We innovated a fine-tuning protocol that adapts the pretrained foundation MLFF models—both invariant and equivariant—with < 10 DFT-computed structures per material combination. These models achieve force accuracies that outperform scratch-trained models and offer a path toward accurate simulations of systems containing over 100,000 atoms.

This framework enables materials design with complexity and at scale that were previously out of reach. We identified new moiré structures and emergent electronic features, such as flatter Chern bands. Our learning loop draws from a curated dataset of moiré systems, which further incorporates magnetic descriptors into the model architecture, allowing the prediction of spin-lattice coupled metastable states. This hybrid quantum/ML strategy, supported by localized motif embedding and high-level benchmarks, forms a powerful platform for high-throughput exploration and design of moiré materials with novel topological and magnetic properties.

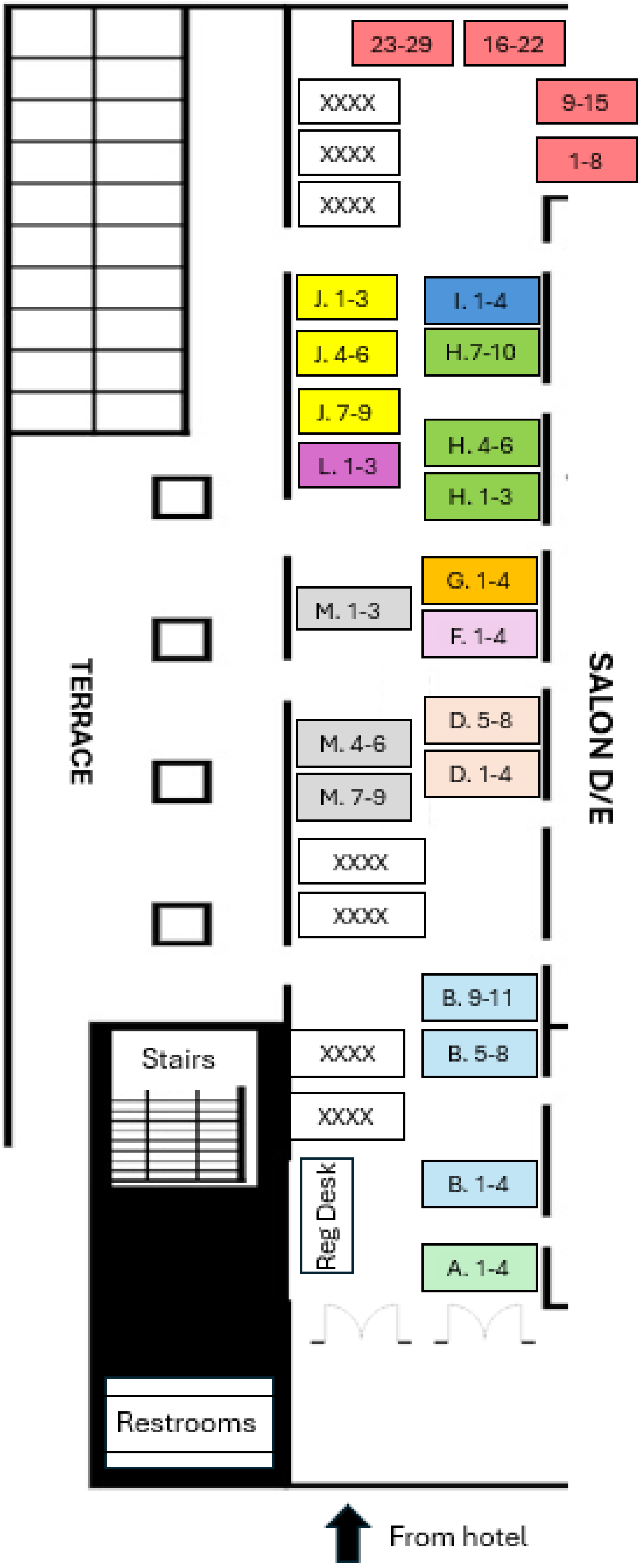
3:00 PM

L-II-5: QMC-HAMM: High accuracy multiscale models from quantum Monte Carlo

[CMS - QMC-HAMM] David Ceperley, Yueqing Chang, Elif Ertekin, Shubhang Goswami, Kevin Kleiner, Kitthithat Krongchon, Harley Johnson, Tawfiqur Rakib, Lucas Wagner
University of Illinois Urbana-Champaign

Much of our understanding of materals is based on density functional theory (DFT), an approximate but highly useful model of quantum mechanical behavior. Since the microscopic behavior of nuclei and electrons is known to very high precision, DFT is often used to perform so-called first principles calculations at that scale to help guide experiments and interpret results. However, DFT often has significant errors that make it difficult to rectify theory and experiment. Using exascale resources, we will show that quantum Monte Carlo (QMC) offers a way forward to learn more accurate potential energy surfaces with applications to the phase diagram of hydrogen, graphene-boron nitride, and battery materials, in which we find that the ion pathways computed by DFT are inaccurate. We will also show how to use QMC to address excited states, which allows us to evaluate interacting coarse-grained electronic models, which enable detailed study of many systems, including strongly correlated light-emitting defects. As our project is part of Computational Materials Sciences, we will discuss software and data products that are an integral part of this work.

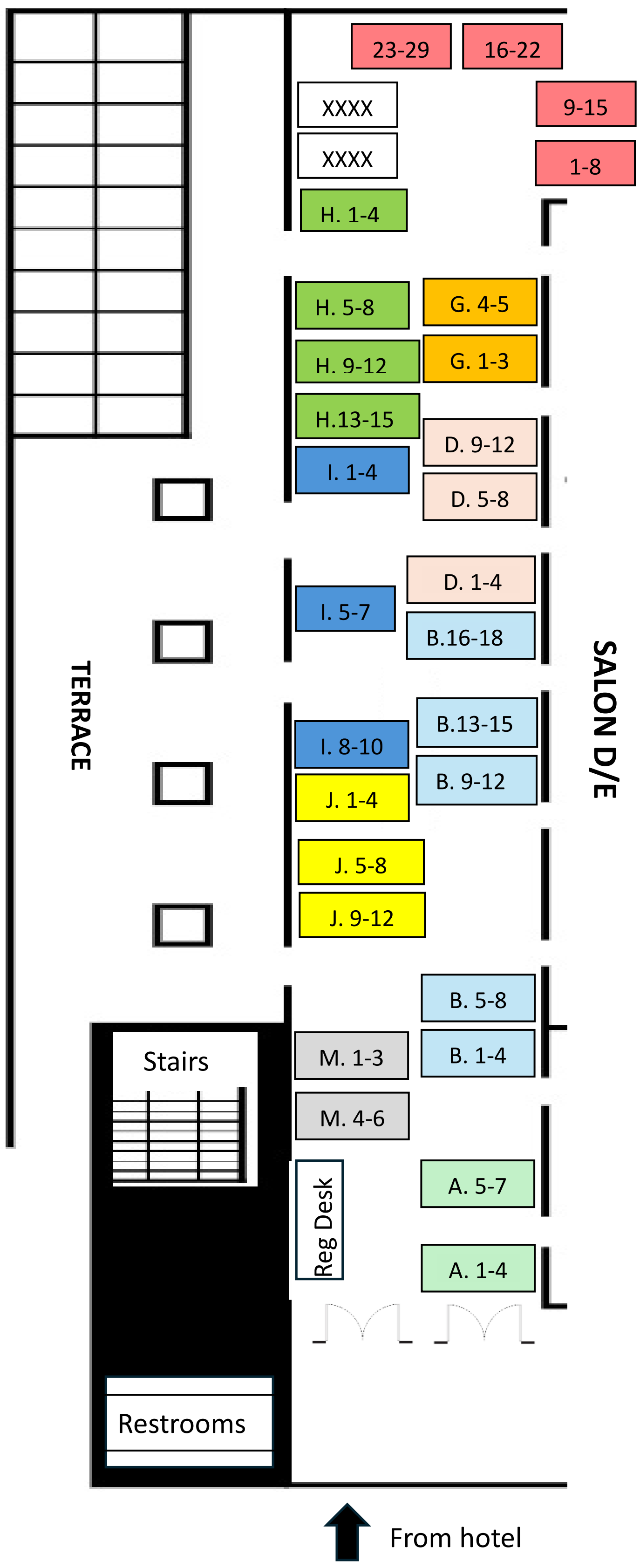
MAP OF POSTER SESSIONS



Overview Poster Session

Monday, August 11, 2025
10:40 – 12:10 PM, Grand Foyer

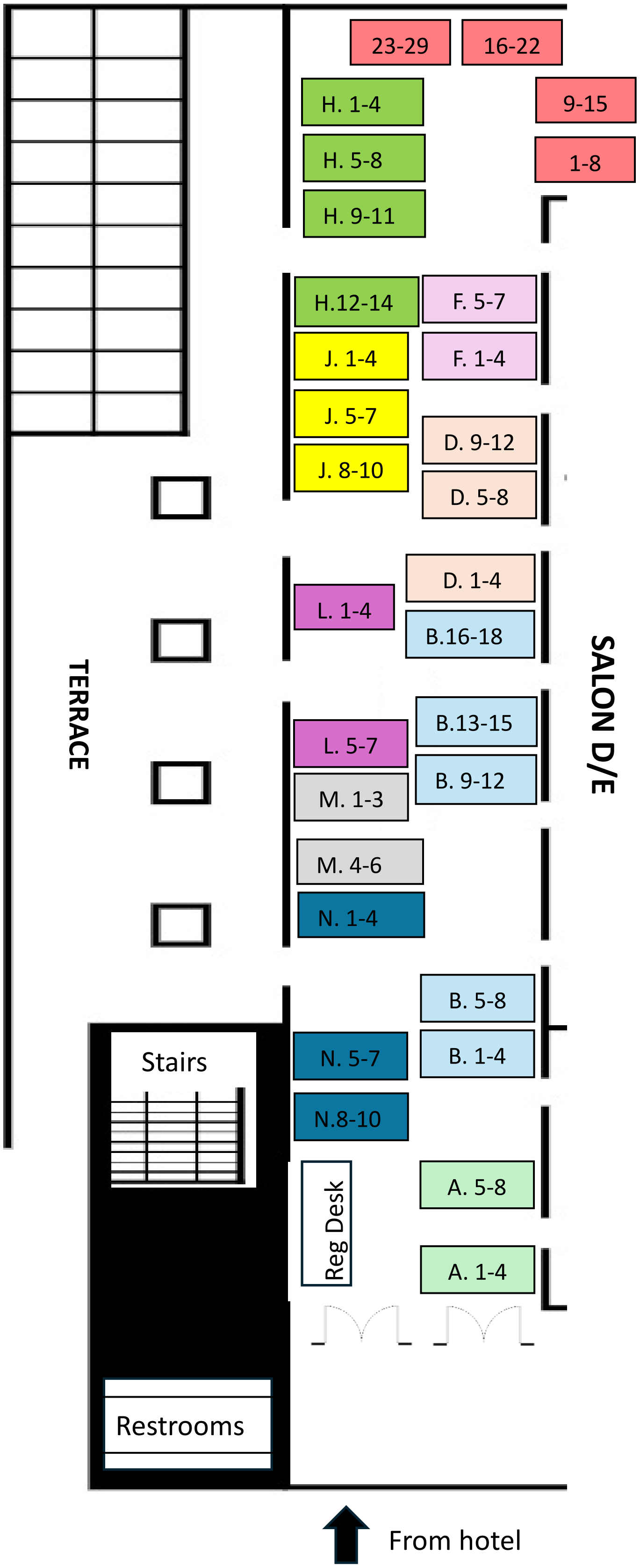
- **A. Advanced Manufacturing**
- **B. Catalysis**
- **D. Energy Storage**
- **F. Energy-Water**
- **G. Hydrogen**
- **H. Microelectronics**
- **I. Nuclear**
- **Art of Science Image**
- **J. Quantum Information Science**
- **L. AI/ML**
- **M. Research at the Exascale**



Technical Poster Session I

Monday, August 11, 2025
3:30 – 5:00 PM, Grand Foyer

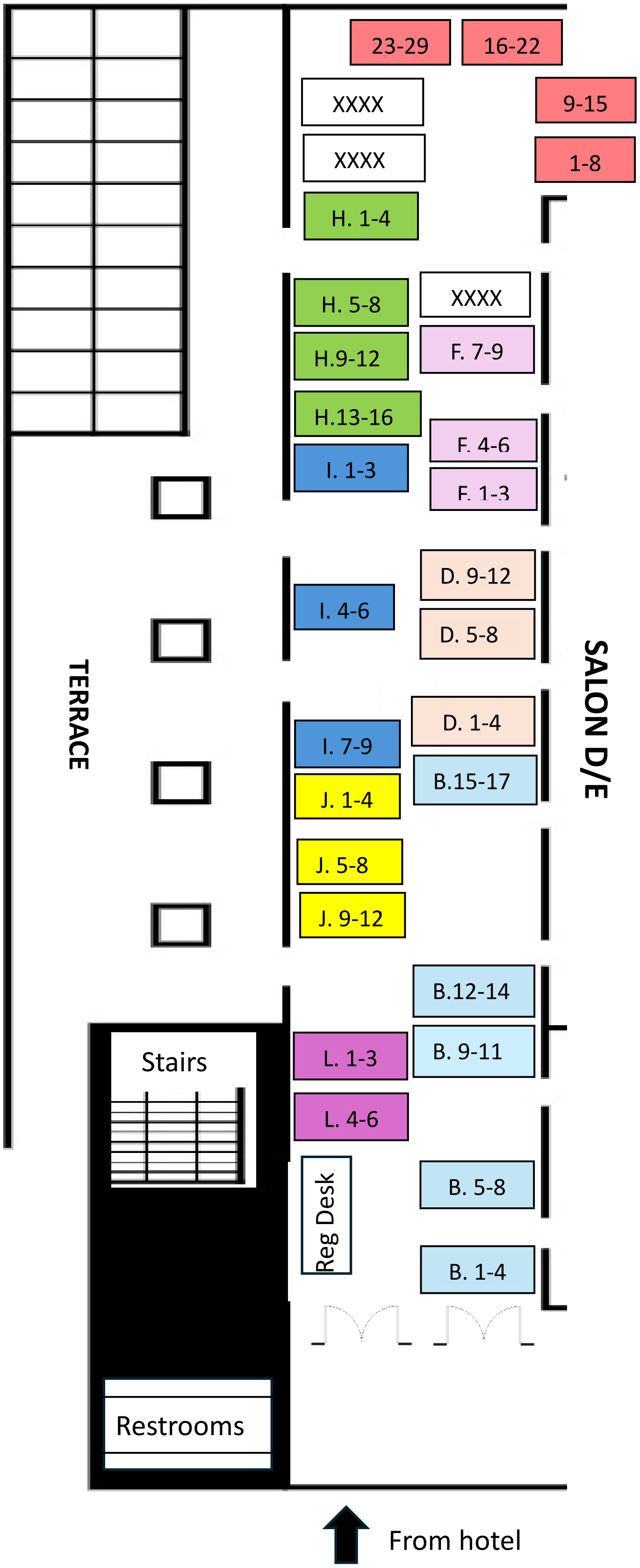
A. Advanced Manufacturing
B. Catalysis
D. Energy Storage
G. Hydrogen
Art of Science Image
H. Microelectronics
I. Nuclear
J. Quantum Information Science
M. Research at the Exascale



Technical Poster Session II

Tuesday, August 12, 2025
10:30 – 12:00 PM, Grand Foyer

A. Advanced Manufacturing
B. Catalysis
D. Energy Storage
F. Energy-Water
Art of Science Image
H. Microelectronics
J. Quantum Information Science
L. AI/ML
M. Research at the Exascale
N. Operando Techniques



Technical Poster Session III

Tuesday, August 12, 2025
3:20 – 5:00 PM, Grand Foyer

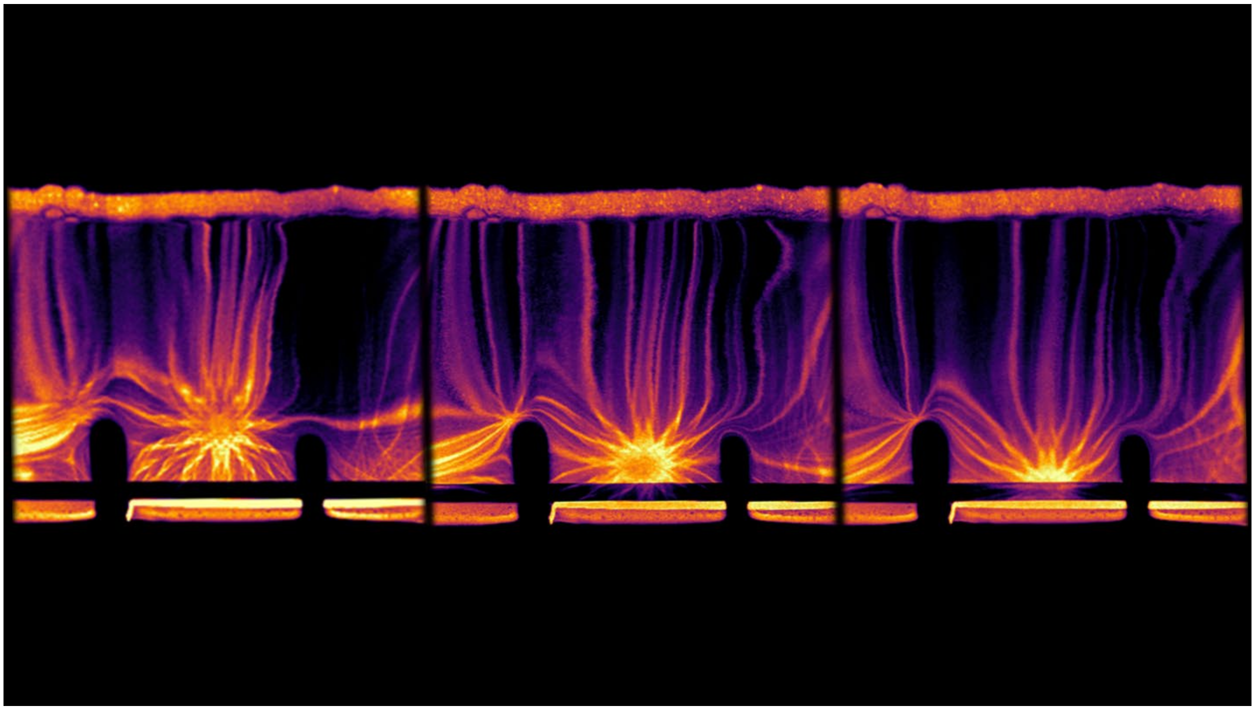
B. Catalysis
D. Energy Storage
F. Energy-Water
H. Microelectronics
Art of Science Image
I. Nuclear
J. Quantum Information Science
L. AI/ML

ART OF SCIENCE IMAGE CONTEST

As part of the 2025 EFRC-Hub-CMS-CCS Principal Investigators' Meeting, the Department of Energy's Office of Basic Energy Sciences (DOE BES) sponsored the *Art of Science Image Contest*. Following the BES tradition, during each meeting there is an optional contest designed to educate, inspire, and entertain an intelligent but not expert audience about the extraordinary science, innovation, and people in the Energy Frontier Research Centers (EFRCs), Energy Innovation Hubs (Hubs), Computational Materials Sciences (CMS), and Computational Chemical Sciences (CCS) Centers. The groundbreaking research conducted at BES-funded collaborative centers results in dozens of beautiful and impactful scientific images every year. This year's *Art of Science Image Contest* aimed to showcase the stunning imagery that arises from the cutting-edge research across the EFRCs, Hubs, CMS and CCS Centers, while providing a glimpse into the world of energy research for those beyond the scientific community. Participants were asked to submit images that were the product of experimental measurements, imaging techniques, modeling, simulation, or combinations thereof, that were rooted in scientific data and displayable in a static format.

BES received 29 excellent entries. The winners, selected by a panel of illustrious judges, will be announced at the Virtual Plenary Session on August 6, 2025 at 3:45pm. The 29 submissions are available at https://www.energyfrontier.us/art-of-science-image-contest, and they are reproduced below listed alphabetically by Center.

1. A Crystal Sunset



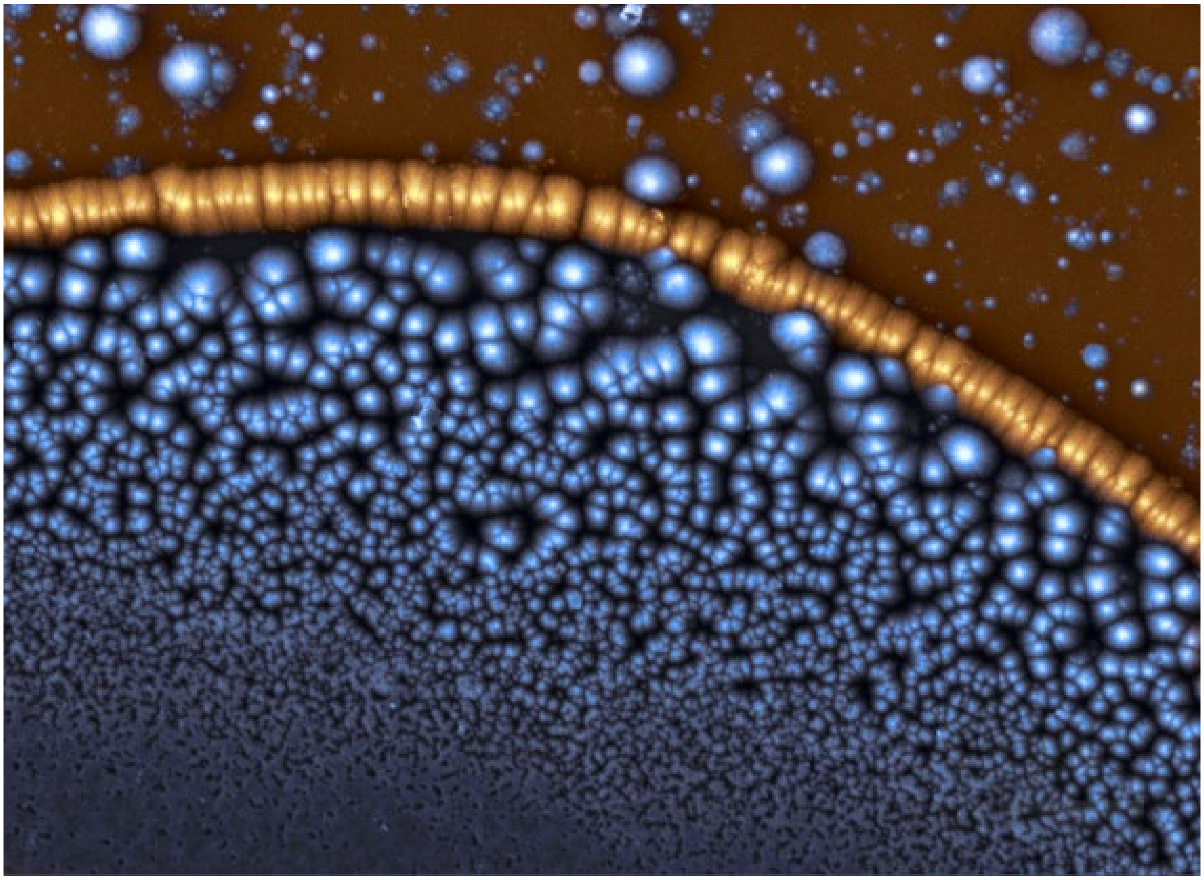
Bend contour contrast, formed by the electron scattering through a GaN/AlBScN/Pt stack used in the design of novel memory devices, unfolds like a sunset across the GaN crystal, shifting and shimmering as the lattice tilts under the electron beam—revealing the interplay between structure and strain in delicate gradients of contrast.

Creator: Sebastian Calderon (Carnegie Mellon University)

Graphic created by Center for 3D Ferroelectric Microelectronics Manufacturing (3DFeM^2) for the Art of Science Image Contest at the 2025 DOE EFRC-Hub-CMS-CCS Principal Investigators' Meeting.

Center: 3DFeM^2

2. When the Levee Breaks



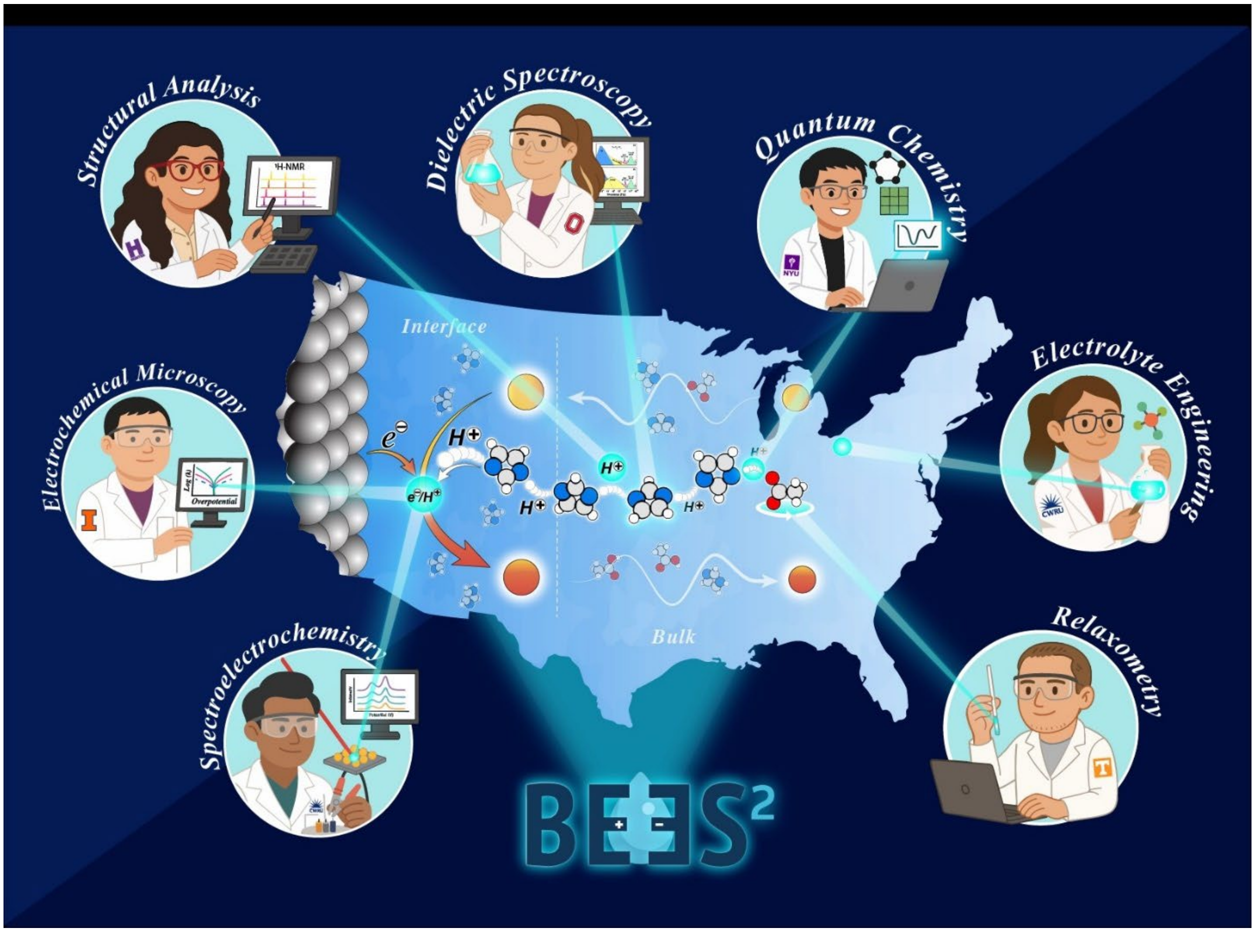
Some materials have hidden talents that are discoverable when one looks in the right place. An example of this is aluminum nitride, which for many years was thought to only be a polar material, meaning it maintains an internal dipole. However, 6 years ago it was found that when combined with elements like scandium or boron, this internal dipole becomes reorientable. This class of materials are called ferroelectric where the dipoles can stably be oriented in different states and are extremely exciting for non-volatile memory in computing. This image shows individual regions of dipoles called domains in aluminum boron nitride. When aluminum nitride was discovered to be ferroelectric this opened the floodgates to a myriad of other materials that were also discovered to be ferroelectric under the right conditions. This is why this image is named “When the Levee Breaks”.

Creator: Ian Mercer (The Pennsylvania State University)

Graphic created by Center for 3D Ferroelectric Microelectronics Manufacturing (3DFeM^2) for the Art of Science Image Contest at the 2025 DOE EFRC-Hub-CMS-CCS Principal Investigators’ Meeting.

Center: 3DFeM^2

3. The Chemistry of Collaboration: Designing Electrolytes for Large Scale Energy Storage



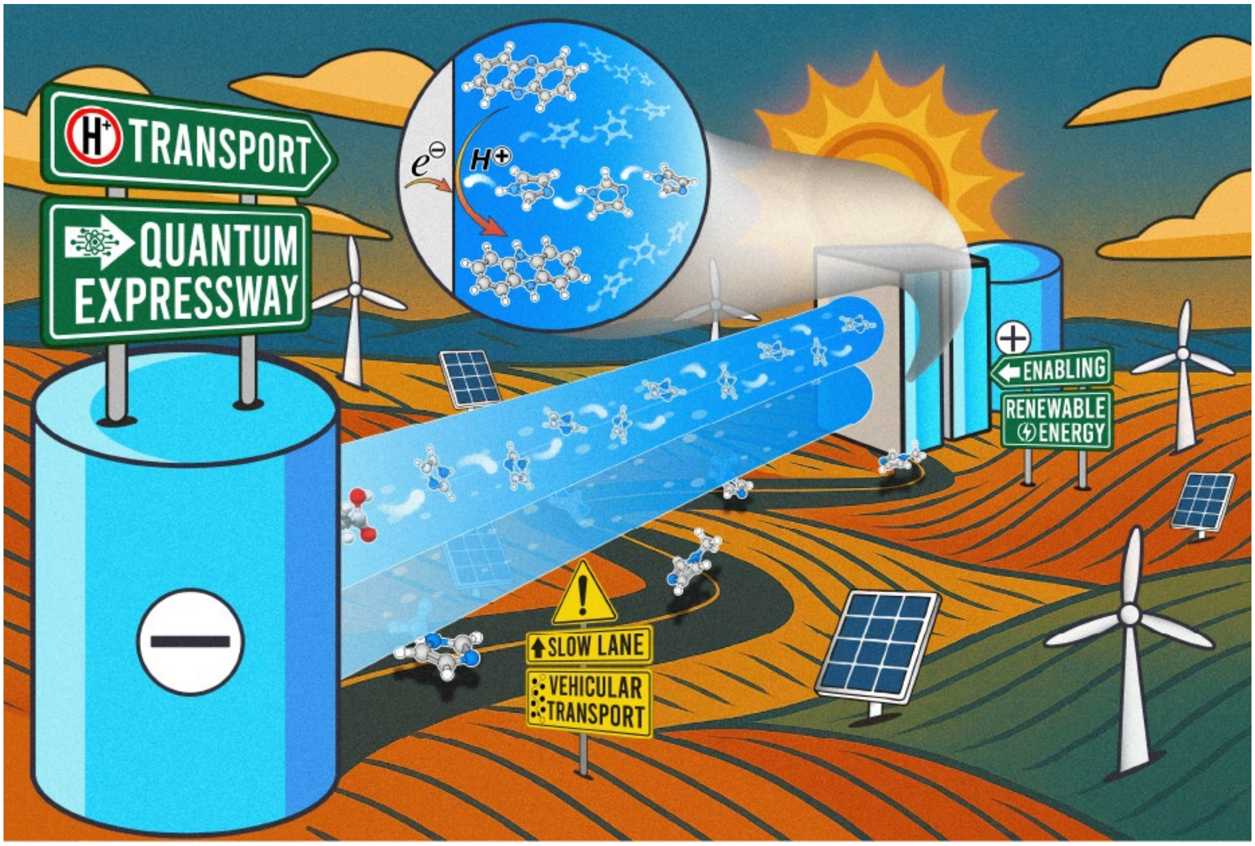
This image celebrates the collaborative spirit of the BEES2 Energy Frontier Research Center, where diverse scientific expertise converges to decode the liquid structure, transport mechanisms, and interfacial reactions in structured electrolytes. Each illustrated researcher represents a team member who specializes in a certain technique or analysis, from advanced spectroscopy to electrokinetics to theory calculations; the collective approach unveils fundamental processes at play in electrolytes engineered for large scale energy storage systems. The central U.S. map highlights how the collaborative research framework is built from individual efforts to advance science. The artwork visually narrates the essence of "team science," where innovative tools and minds align to solve energy challenges that are too complex for any one discipline alone to solve.

Creators: Miguel Muñoz (creator/artist and student researcher), Burcu E. Gurkan (ideation and editing) and Robert Savinell (review and feedback)

Graphic created by Breakthrough Electrolytes for Energy Storage Systems (BEES2) for the Art of Science Image Contest at the 2025 DOE EFRC-Hub-CMS-CCS Principal Investigators' Meeting.

Center: BEES2

4. The Quantum Shortcut: Proton Hopping in Structured Electrolytes



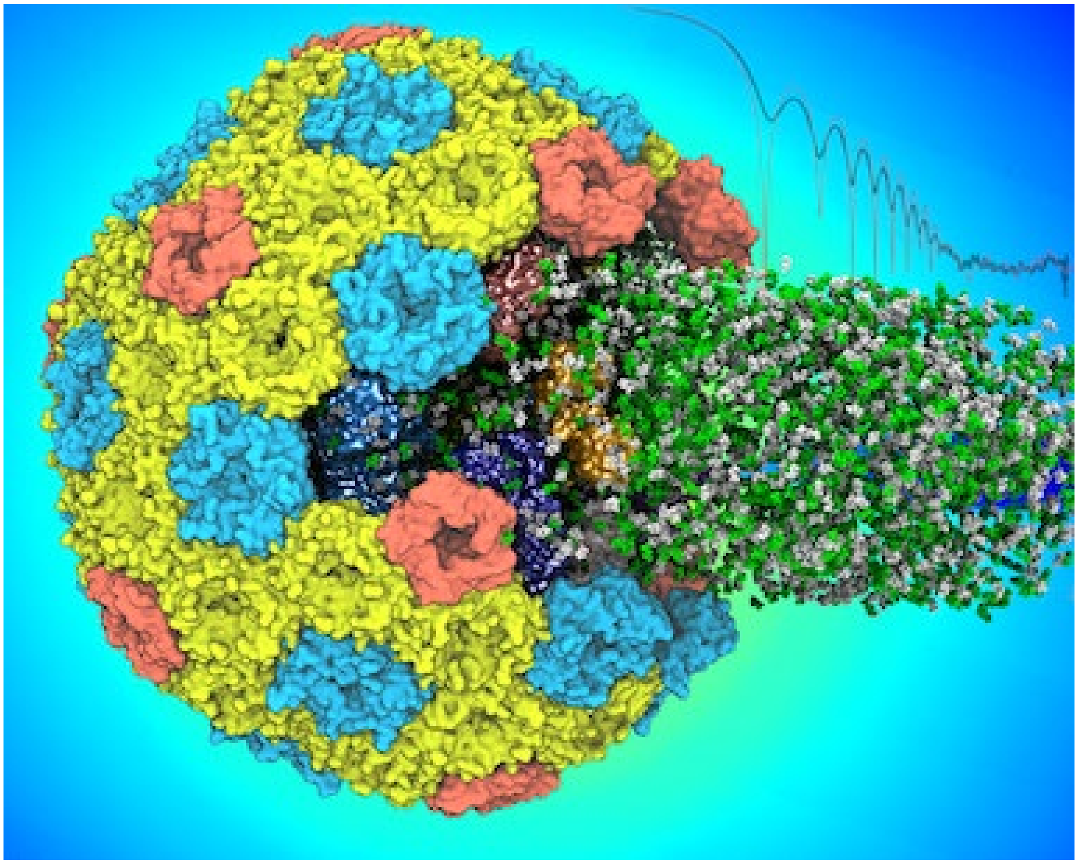
Inspired by the BEES2 EFRC research and by overlaying molecular models, reaction schemes, and landscape analogies, the image highlights how the fundamental research plays a crucial role in advancing safer electrolytes for large scale energy storage from renewable sources such as the sun and the wind. As the center focuses on electrolytes, in which the redox active species and ions move to enable electron transfer reactions at the electrodes hence store energy, the understanding of the transport mechanisms is a central mission. In particular, structured electrolytes are less-volatile and highly tunable alternatives to conventional aqueous and volatile organic electrolytes. BEES2 EFRC develops structured electrolytes where the hydrogen bonding network of the bulk liquid is leveraged for quantum-like proton hopping (represented by a transparent expressway) — a faster route compared to the more common vehicular transport— for proton conduction and proton coupled electron transfer reactions.

Creators: Miguel Muñoz (creator/artist and student researcher), Burcu E. Gurkan (ideation and editing) and Robert Savinell (review and feedback)

Graphic created by Breakthrough Electrolytes for Energy Storage Systems (BEES2) for the Art of Science Image Contest at the 2025 DOE EFRC-Hub-CMS-CCS Principal Investigators' Meeting.

Center: BEES2

5. The Bacterial Microcompartment Catalysis Arcade



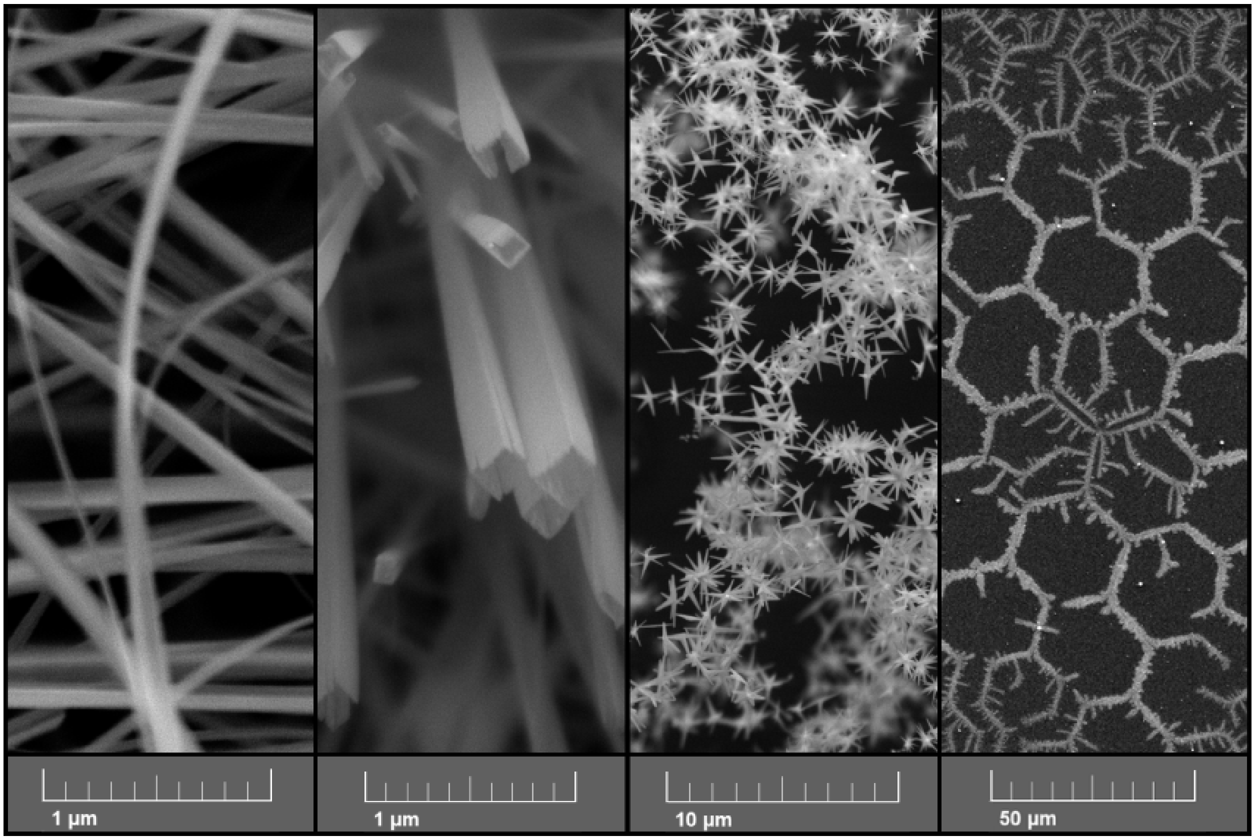
The bacterial microcompartments that the Center for Catalysis and Biomimetic Confinement works with encapsulate enzymes to accelerate catalysis. One way to visualize how these microcompartments work is to imagine Pac-Man eating the little substrate dots as it moves around in space, converting them into tailored products and metabolites. In this image, we use this idea to show the inner workings of a catalytic microcompartment, cutting away tiles in the outer shell to create a microcompartment at home in a 1980s arcade specifically to show the shell interior filled with proteins. While the substrates are usually uniformly distributed, we emphasize the Pac-Man heritage by showing two substrates entering the microcompartment in a line. The center has demonstrated that shell proteins encapsulate the shell by small angle x-ray scattering experiments, which contribute the underlying color gradient to the molecular Pac-man model, as well as the scattering profile shown in the upper right.

Creators: Josh Vermaas and Saad Raza (simulation, molecular visualization ,and image assembly), Alexander Jussupow and Michael Feig (packed model construction), Xiaobing Zuo, Nina Ponomarkenko, and David Tiede (SAXS profiles)

Graphic created by the Center for Catalysis and Biomimetic Confinement (CCBC) for the Art of Science Image Contest at the 2025 DOE EFRC-Hub-CMS-CCS Principal Investigators' Meeting.

Center: CCBC

6. RuO_2 Morphologies for Splitting Water



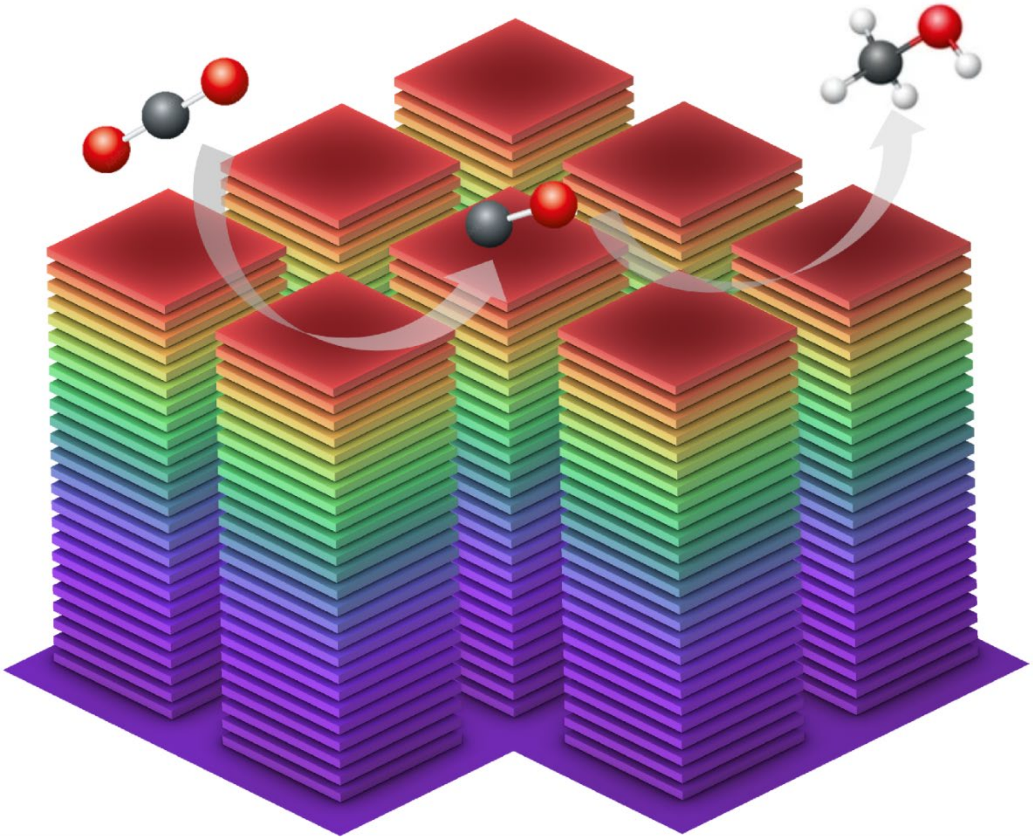
Welcome to Catalyst Survivor: RuO_2 Island, where four fierce tribes battle for electrocatalytic dominance in the oxygen evolution reaction (OER) through morphological control. On Team Nanowire, crystalline RuO_2 wires play to their strengths, leveraging the highly regarded (110) facets for greater stability while boasting high surface area and strong connectivity. Team Nanotube follows, wrapping mechanical toughness into their strategy. Team Nanostar, bold and unpredictable, plays with diverse crystal facets, but will their instability get them voted/corroded off the electrode? And finally, the wild card: Team Hexagon, forged in harsh 600+°C conditions, bringing long-range order and an unconventional 2D strategy to the table. All seek the ultimate prize: stability and activity of during the OER. However, only the strongest morphology will survive the harsh electrochemical trials. Who will outlast and outreact? Stay tuned for the next episode of Catalyst Survivor.

Creators: Austin Reese, Jin Suntivich

Graphic created by the Center for Electrochemical Dynamics and Reactions on Surfaces (CEDARS) for the Art of Science Image Contest at the 2025 DOE EFRC-Hub-CMS-CCS Principal Investigators' Meeting.

Center: CEDARS

7. Harnessing the Sun: CO_2 Conversion Through Tandem Catalysis



On a single electrode plane,
CO_2 tandem cascades form a chain—
Sequential steps, each finely tuned,
with catalysts in concert, placed,
where local pH a main role plays by
shifting the equilibrium towards bicarbonate.

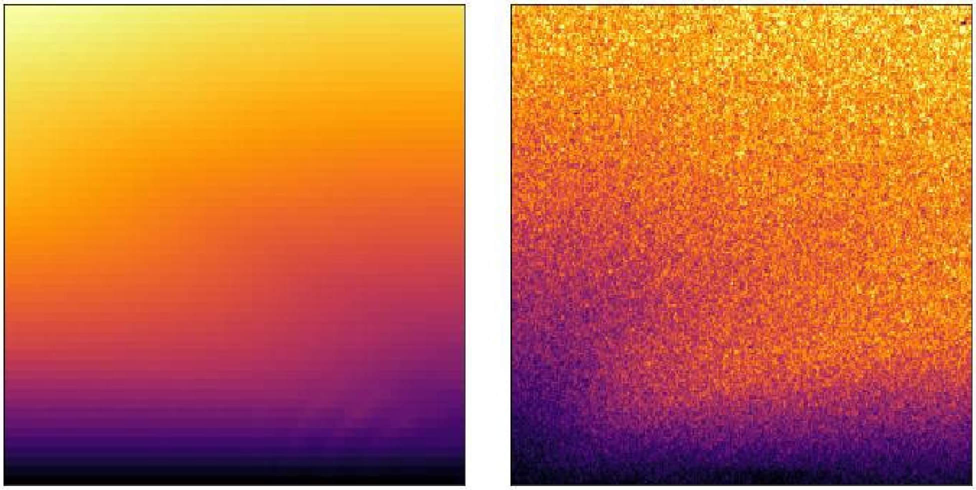
Modeling now refines our scope,
using mass transport and kinetics rates,
It maps how intermediates arise and accumulate
—their transformation, stage by stage,
Toward solar fuels to drive the modern age!

Creators: Marisé Garcia-Batlle and Pablo Fernandez, using COMSOL.

Graphic created by the Center for Hybrid Approaches in Solar Energy to Liquid Fuels (CHASE) for the Art of Science Image Contest at the 2025 DOE EFRC-Hub-CMS-CCS Principal Investigators' Meeting.

Center: CHASE

8. Simulation & Experiment



What is the shape of the grating?

We don’t yet know—
It’s too small to touch, too fragile to show.
Could X-rays help? They’re swift and bright...
But we seek shape with softer light.

Let’s place a CCD, firm and still,
And watch fluorescence form at will.
The structure bends each photon’s flight—
It guides them through the angled night.

Measurement takes patient care,
Simulation too—precision, flair.
A solver hums through Maxwell’s page,
Tracing fields from grating’s cage.

At last, two glowing maps appear—
One measured close, one modeled clear.
If they align in form and trace,
We’ve glimpsed the grating’s hidden face.

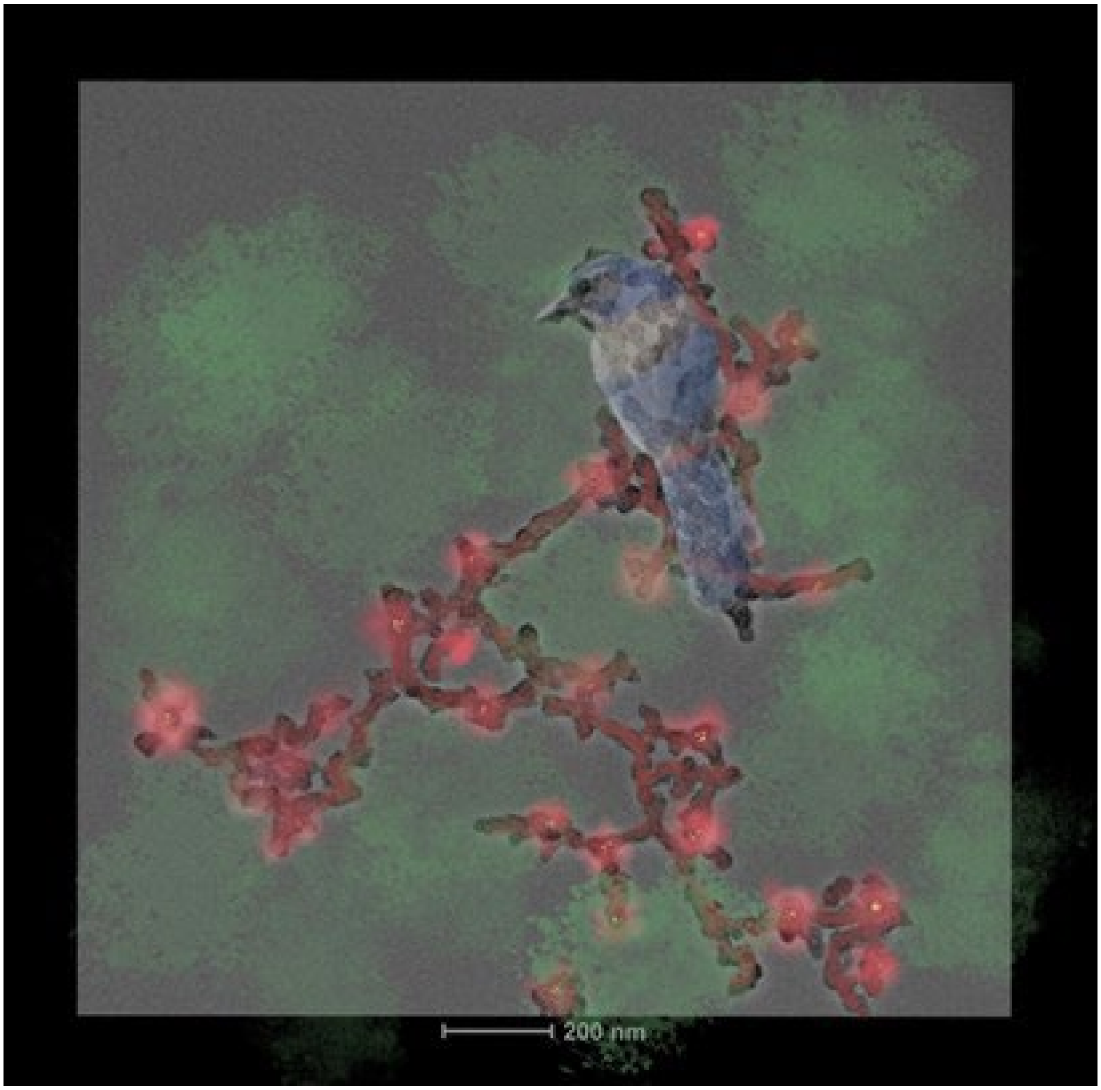
Repeat the sim, refine the light—
Each match a step toward structural insight.
From photons, fields, and patterned intent,
Comes truth through **Simulation & Experiment**.

Creators: Kas Andrle and Thomas Ferron

Graphic created by the Center for High Precision Patterning Science (CHiPPS) for the Art of Science Image Contest at the 2025 DOE EFRC-Hub-CMS-CCS Principal Investigators' Meeting.

Center: CHiPPS

9. Enzyme on a Helix: Spring in a Birdsong



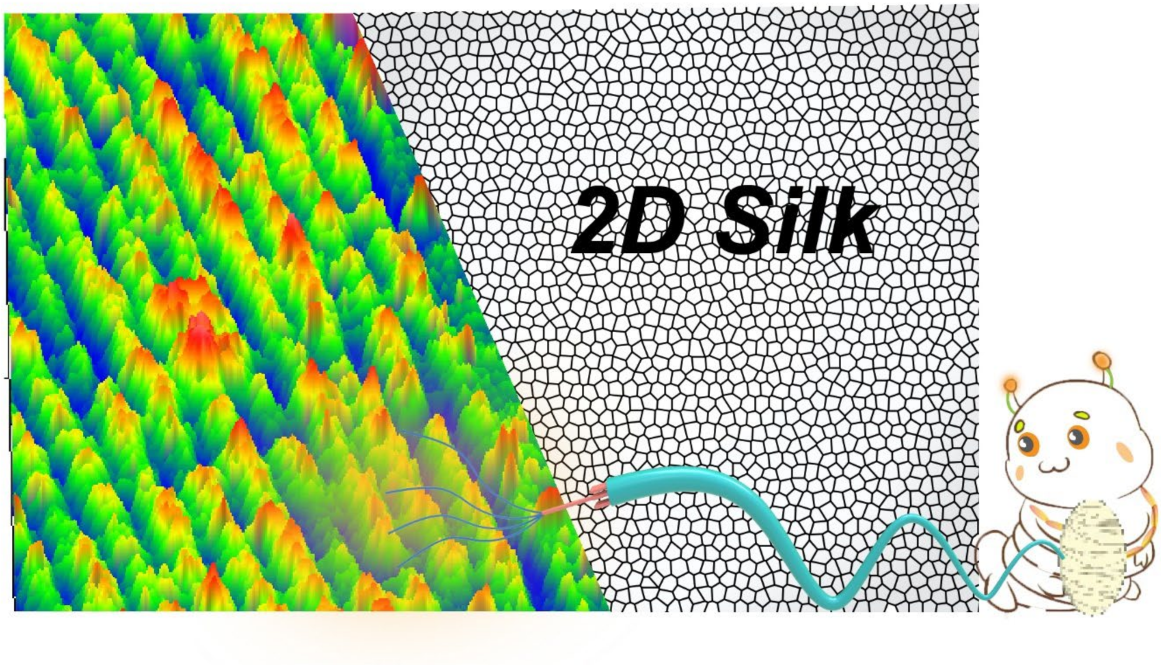
A bird perches on a blooming branch—or so it seems — a view of DNA-folded octahedra decorated with enzyme CD38, a key regulator of immune response, calcium signaling, and aging. The DNA octahedra here serve as nano-scaffolds to organize and enhance CD38 enzymatic activity. The DNA-enzyme blocks form a complex nanoscale pattern, as captured through transmission electron microscopy (TEM). The picture is reimagined with a touch of watercolor to revitalize the nanoworld. It reminds us of the intricate connection between science and art: here, science calls for spring, the invisible becomes art, and logic finds harmony with emotion.

Creators: Daphne Shen, Oleg Gang

Graphic created by the Center for the Science of Synthesis Across Scales (CSSAS) for the Art of Science Image Contest at the 2025 DOE EFRC-Hub-CMS-CCS Principal Investigators' Meeting.

Center: CSSAS

10. Flattening Nature's Thread: Weaving the Future in Two-Dimensional Silk



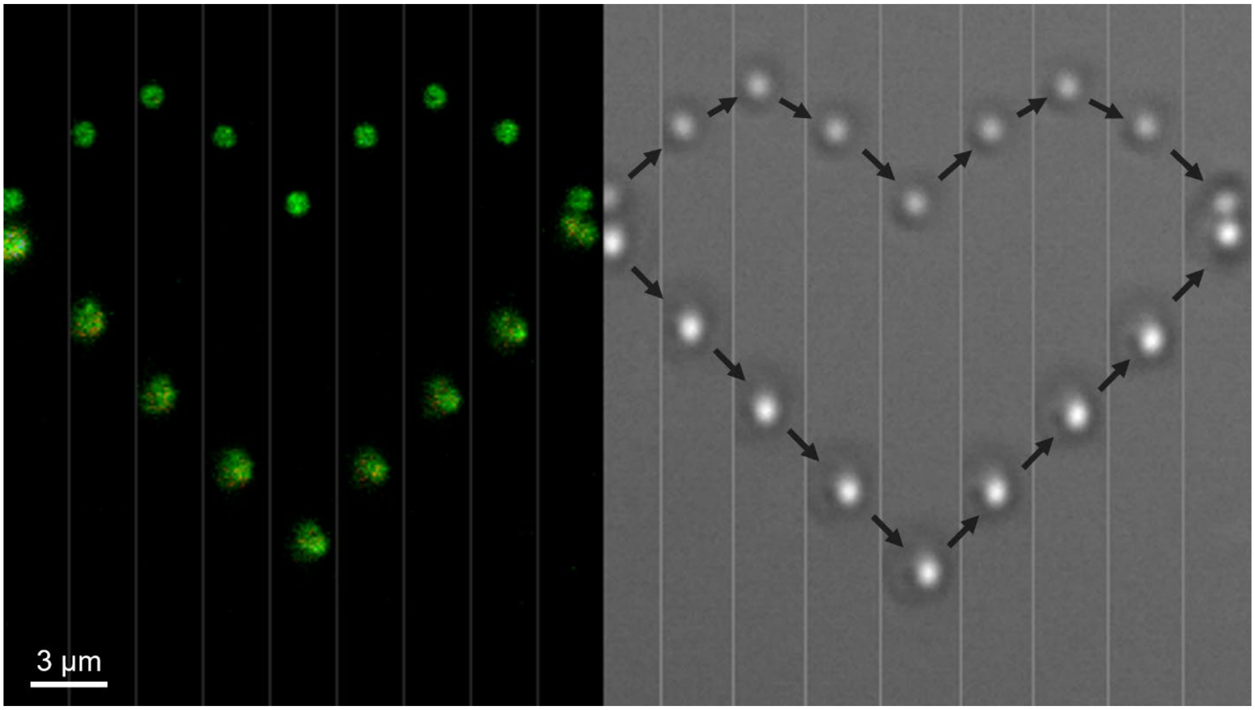
In this imaginative re-visioning of silk production, a humble silkworm spins not its usual cocoon, but a gleaming, ultra-thin 2D silk sheet—layer by layer, like nature's own nanoprinter. Inspired by cutting-edge research into protein self-assembly and material flattening, this artwork captures the surreal beauty of biomolecular precision at the interface of biology and technology. The lamellar silk film shown here hints at the next generation of bioelectronics and sustainable nanomaterials—engineered not through brute force, but by decoding and redirecting nature's own blueprint. Just as the silkworm evolved to protect itself with 3D fibers, science now guides it to serve new functions in two dimensions. This visual metaphor invites viewers to imagine a future where the oldest textile meets the frontiers of materials science—where silkworms may help us weave circuits, sensors, and memory devices, one nanosheet at a time.

Creator: Chenyang Shi

Graphic created by the Center for the Science of Synthesis Across Scales (CSSAS) for the Art of Science Image Contest at the 2025 DOE EFRC-Hub-CMS-CCS Principal Investigators' Meeting.

Center: CSSAS

11. For the Love of Photocatalysis



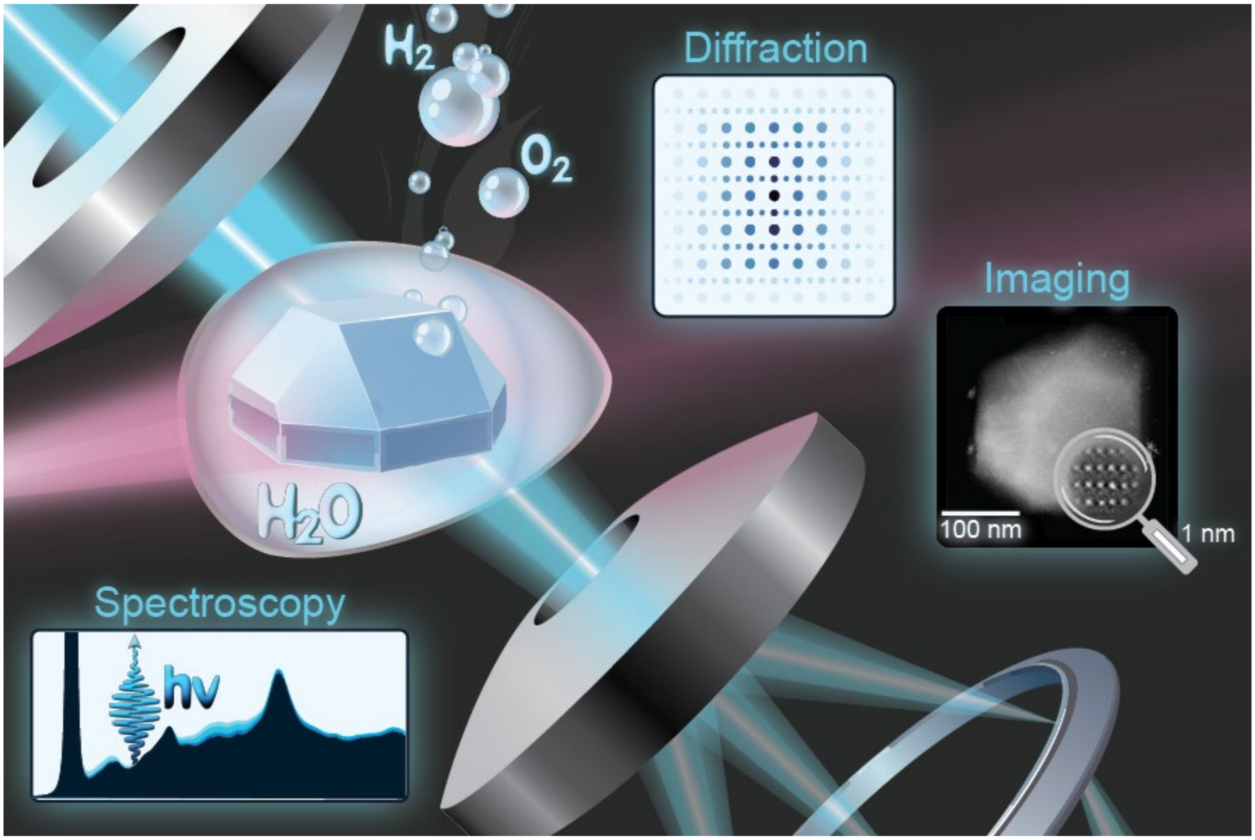
A pair of phosphorus-doped $BiVO_4$ microparticles, suspended in an aqueous solution initially in close proximity, are forcibly separated by the intense infrared trapping lasers of the optical tweezers in which they are contained, as indicated by the sequence of confocal microscopy images (right image). While illuminated by the bright blue light shining from above, the excited microparticles photoluminesce a primarily verdant green (left image) while simultaneously splitting water to create similarly green hydrogen fuel. The nanoreactors are ultimately brought back together, where they are now influenced by each other's presence once again. The heart-felt journey of this adorable $BiVO_4$ couple sets the stage for performing groundbreaking *operando* measurements for a large cast of photosynthetic nanoreactors, utilizing both optical tweezers and EPN's extensive correlative microscopy network to elucidate their structure-property relationships in the presence and absence of neighboring nanoreactors.

Creators: Kevin Dunn, Daniel Esposito, and Shane Ardo

Graphic created by Ensembles of Photosynthetic Nanoreactors (EPN) for the Art of Science Image Contest at the 2025 DOE EFRC-Hub-CMS-CCS Principal Investigators' Meeting.

Center: EPN

12. Fueling Life on Earth, Atom-by-Atom



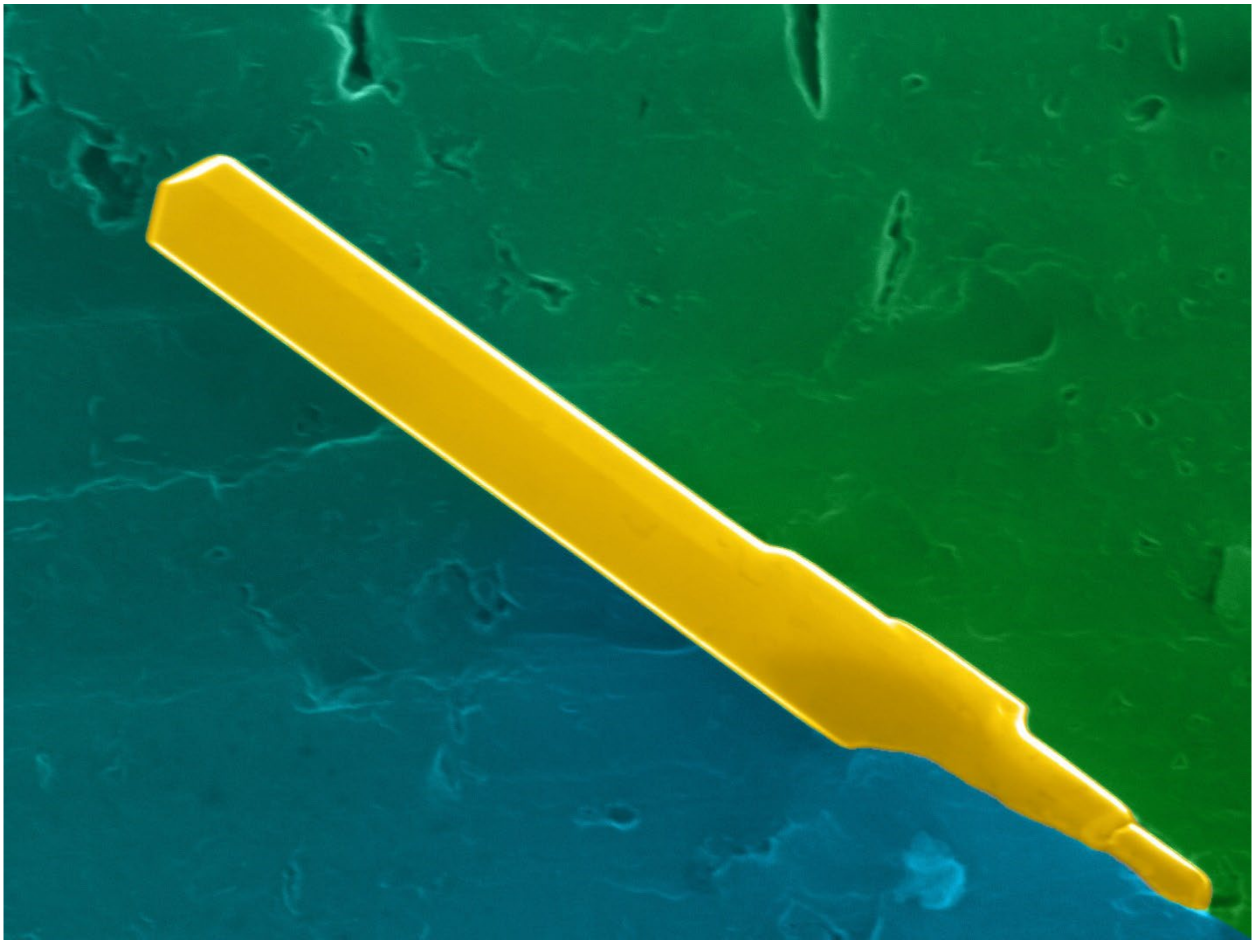
The water, warmth, and light received by life on Earth is unlike the offerings of any other planet. Humanity has always drawn energy originating from these gifts, but now, our growing needs demand more. We are driven to generate an energy harvesting process that can sustain us into the future. Our Center harvests energy from the water, warmth, and light sources that fuels us. Suspended in a water droplet within our electron microscope, a single nanoparticle begins its work. Powered by sunlight, tiny bubbles emerge as evidence of hydrogen gas forming from water. As our microscope's electrons pass through, we measure the effects that light has on the particle's atomic structure, diffraction patterns, and spectral signatures, all captured in a moment of catalytic transformation. We witness life's most essential molecule becoming a limitless fuel, built atom by atom from Earth's simplest elements.

Creators: Levi Palmer, Avishek Banik, and Shane Ardo

Graphic created by Ensembles of Photosynthetic Nanoreactors (EPN), a DOE EFRC, for the Art of Science Image Contest at the 2025 DOE EFRC-Hub-CMS-CCS Principal Investigators' Meeting.

Center: EPN

13. Shattered Sodium Sword



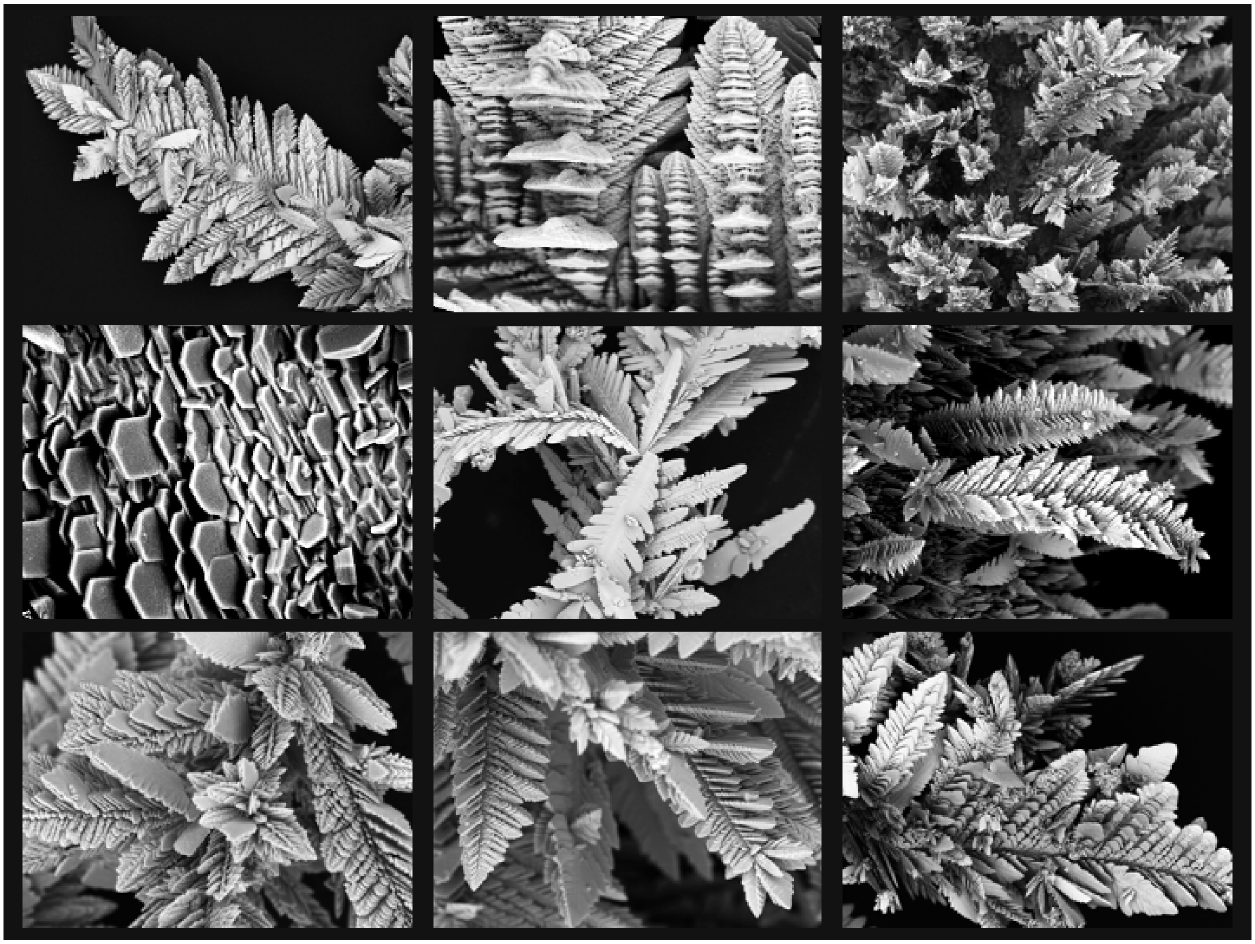
Scanning electron microscopy (SEM) image of $Na_2(B_{10}H_{10})$ solid state electrolyte and a growing Na crystal. The bias of the electron beam on a solid-state electrolyte generates excess positive surface charge which is abated by the mobility of Na^+ ions to the surface where they reduce into beautiful Na Metal crystals. Here, a Na crystal is seen protruding from the surface like a sword blade left behind on a forgotten battlefield. Many years having erased all other remnants of the battle save this sharp reminder. Scientifically, this project is aimed at understanding the rate at which the electron beam interacts with the $Na_2(B_{10}H_{10})$ for interfacial characterization of solid electrolyte / anode interfaces in solid-state batteries. The SEM image is false colored.

Creators: Thomas S. Marchese, James N. Burrow, and Y. Shirley Meng

Graphic created by the Energy Storage Research Alliance (ESRA) at the Advanced Electron Microscopy OSRF core facility at University of Chicago for the Art of Science Image Contest at the 2025 DOE EFRC-Hub-CMS-CCS Principal Investigators' Meeting.

Center: ESRA

14. Zinc Fern Garden



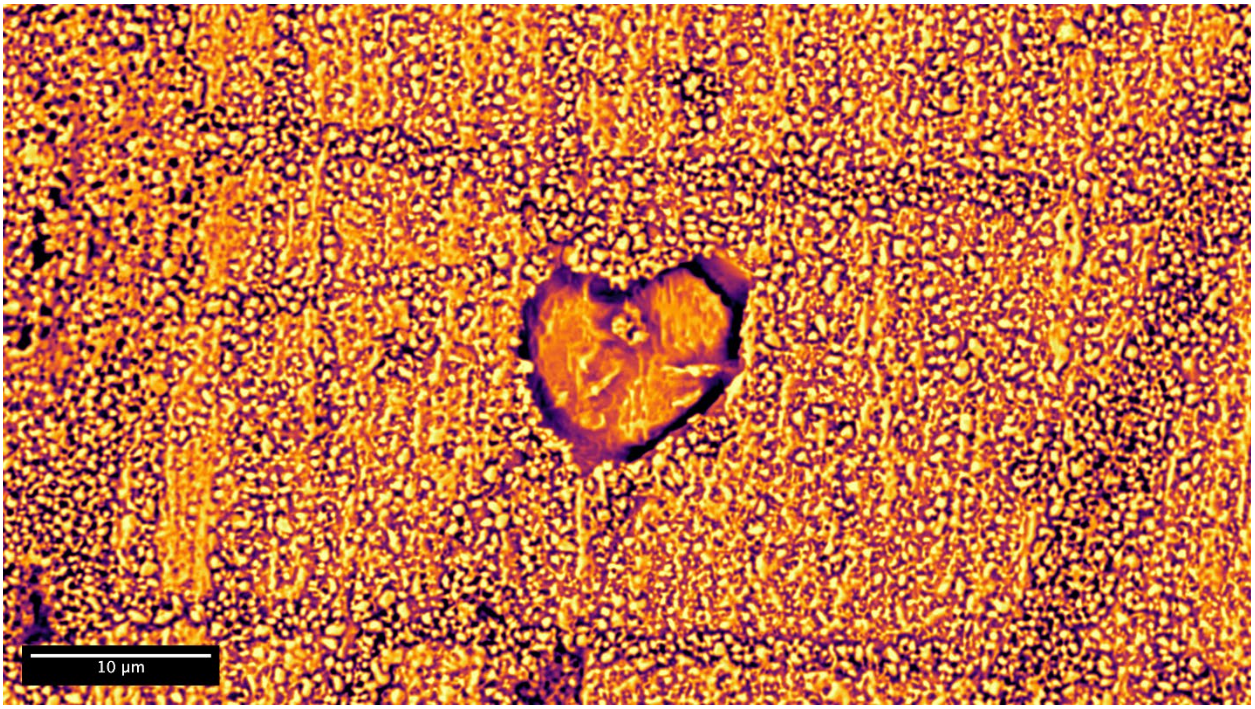
Fractals surround us, from arms growing from snowflakes to the leaves branching off trees. These endless patterns of layers building on layers often seem like each piece was placed in its spot by hand. Yet, we see these fractals every day in nature like the swirling conch shell and the spirals in a pinecone. Even my work in electrochemistry has been touched by these mesmerizing patterns. This work is a collage of micrographs taken with Scanning Electron Microscopy (SEM) of dendritic zinc from alkaline electrodeposition. As these zinc structures form, dendrites branch from one another, giving rise to generation after generation, eventually leaving behind a garden of ferns.

Creators: Diana Oh, Lauren Marbella, and Dan Steingart

Graphic created by the Energy Storage Research Alliance (ESRA) for the Art of Science Image Contest at the 2025 DOE EFRC-Hub-CMS-CCS Principal Investigators' Meeting.

Center: ESRA

15. Salt and Sediment



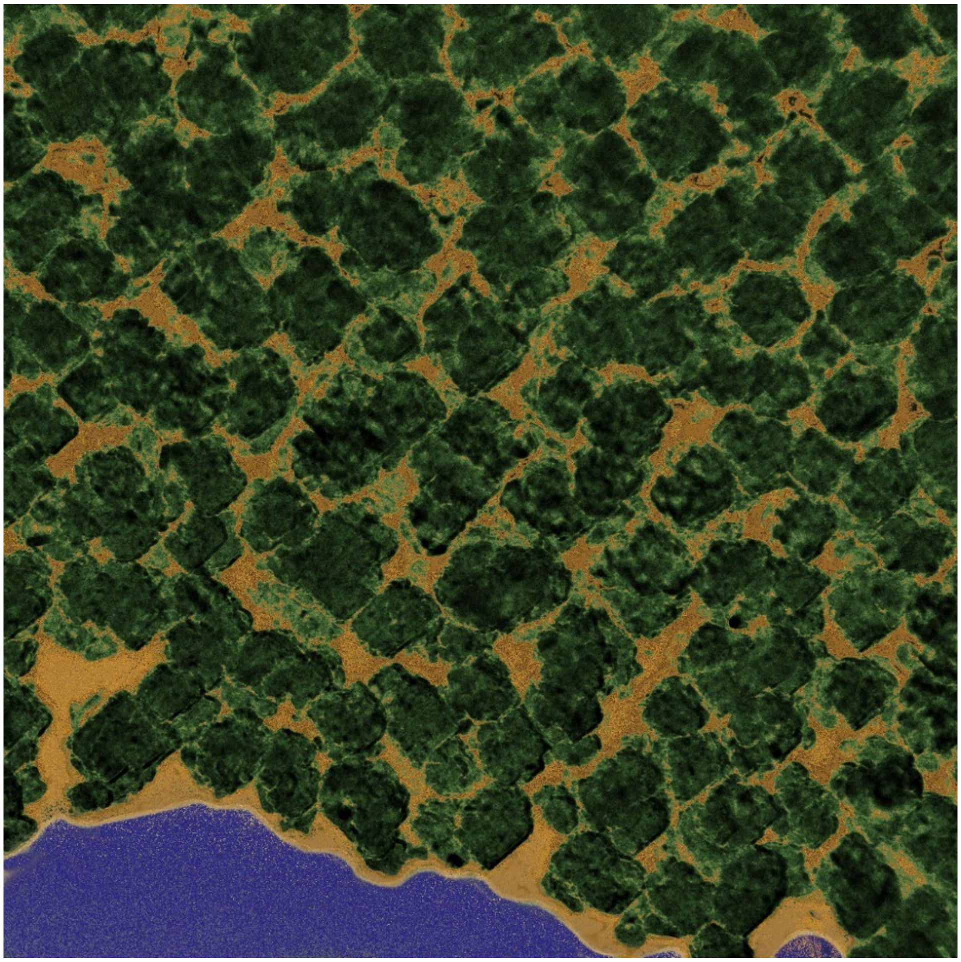
A sprinkle of salt, a world of sentiment. At first glance, this heart shaped void appears to symbolize warmth or tenderness. In reality, it is a scar etched by corrosion. This feature formed on the surface of a Ni-20Cr (wt%) sample that was held potentiostatically at 1.75 V vs. K^+/K for 10,000 seconds in molten FLiNaK. Captured via scanning electron microscopy, the image reveals the sting of materials degradation: elements stripped away, structures hollowed, a heart corroded from within. The surrounding texture reflects a landscape of dealloying-driven porosity. Yet amid this harsh environment, a distinctly human symbol emerges, unintended and poetic, offering more than data—a moment of reflection.

Creators: Harjot Singh, Ho Lun Chan, Elena Romanovskaia, Valentin Romanovski, and John R. Scully

Graphic created by the Fundamental Understanding of Transport Under Reactor Extremes (FUTURE) EFRC for the Art of Science Image Contest at the 2025 DOE EFRC-Hub-CMS-CCS Principal Investigators' Meeting.

Center: FUTURE

16. Nanocomposite Forest



This “Nano-Composite Forest” reveals a hidden world of engineered materials critical to sustainable energy. Far from a natural scene, this image originated as a plan-view transmission electron microscopy (TEM) image of a vertically aligned nanocomposite (VAN). These VANs, composed of different materials precisely engineered at the nanoscale, are designed and studied for their role in hydrogen energy technologies. The TEM captured the intricate architecture of these tiny structures, but this microscope blueprint has been transformed into a vibrant forest. The trees and lakeshore are reminiscent of Lake Michigan, on which Northwestern University--where the image was captured—sits. This image highlights the unexpected beauty and parallels between human ingenuity and the artistry of nature.

Creators: Elizabeth Griffin, Gabriel Trindade dos Santos, Yong-Yun Hsiau. YH synthesized the vertically aligned nanocomposite sample, GTS acquired the plan-view transmission electron microscopy image, and EG created the nanocomposite forest image.

Graphic created by the Hydrogen in Energy and Information Sciences (HEISs) EFRC for the Art of Science Image Contest at the 2025 DOE EFRC-Hub-CMS-CCS Principal Investigators’ Meeting.

Center: HEISs

17. The Beration of Adam

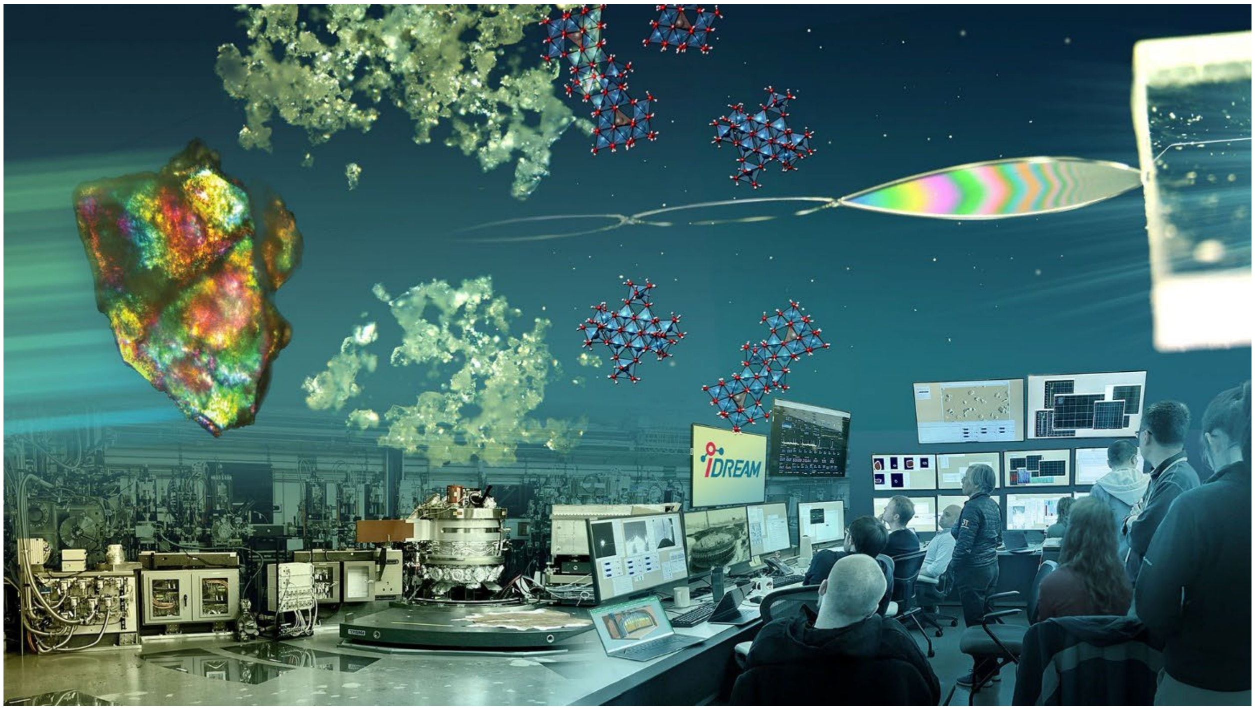
This drawing by Aven Peters, titled “The Beration of Adam”, depicts the hands of Adam and God from “The Creation of Adam” by Michelangelo. However, Adam is dropping a plastic bottle onto a heap of plastic garbage, while God asks him “Are you planning to recycle that?” The cover reminds us that our dominion over the earth has littered it with plastic waste, and that we have a responsibility to find sustainable recycling solutions. The image appeared as supplementary cover art for the iCOUP authored review article: “Population Balance Models for Catalytic Depolymerization: From Elementary Steps to Multiphase Reactors”, in Accounts of Chemical Research (2025).

Creator: Aven Peters

Graphic created by the Institute for Cooperative Upcycling of Plastics (iCOUP) for the Art of Science Image Contest at the 2025 DOE EFRC-Hub-CMS-CCS Principal Investigators’ Meeting.

Center: iCOUP

18. The Stars Align: Revealing the Earliest Radiation-Driven Reactions in Complex Ion Networks



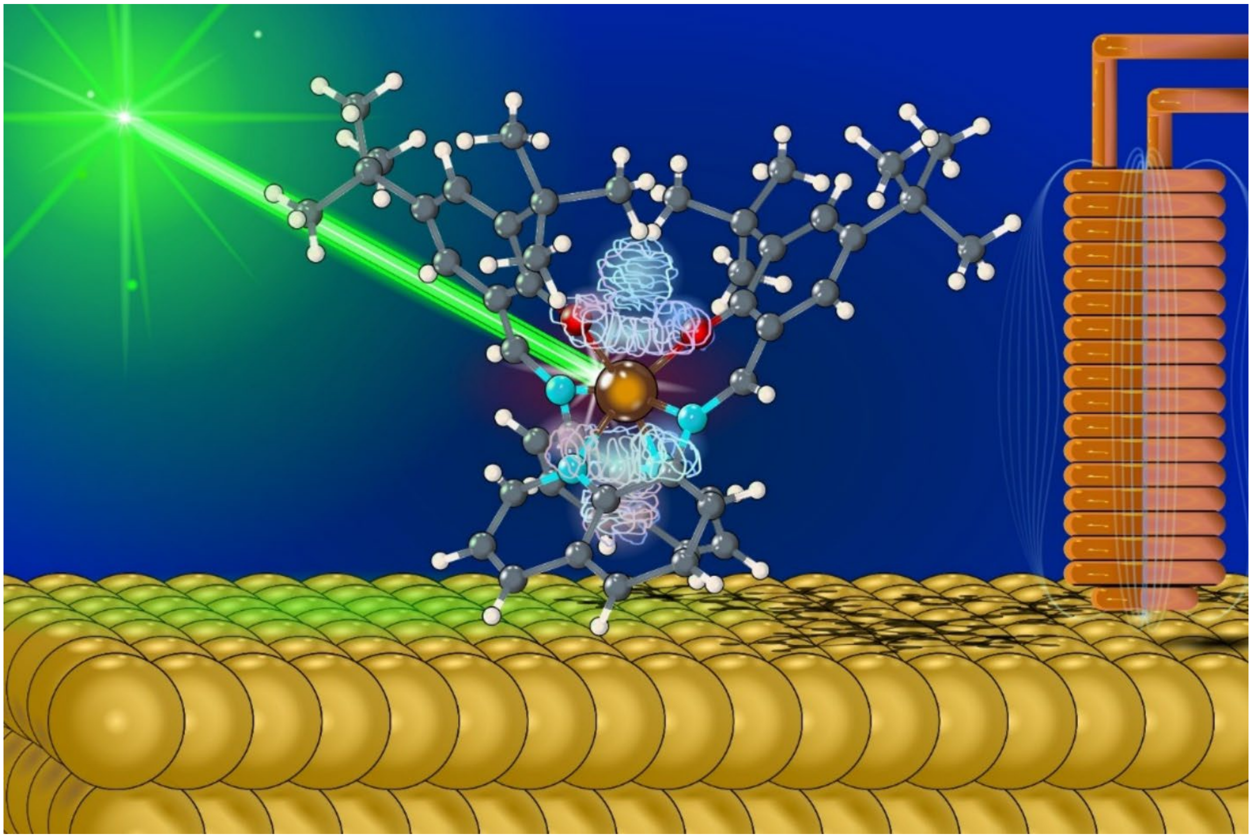
Ion Dynamics in Radioactive Environments and Materials (IDREAM) researchers are exploring the extraordinary universe of chemical bond making and breaking under irradiation, furthering our knowledge of how the availability of water shapes us all. With a multi-disciplinary approach, IDREAM studies the structure and dynamics of how water interacts with dissolved electrolytes following ultrafast irradiation. In this image, a thin sheet jet of water (top right) is irradiated and probed with attosecond resolution using an X-ray free-electron laser (bottom left) - the Linac Coherent Light Source - a Department of Energy user facility. The initial changes in the water affect the formation of ion clusters and the precipitation of crystals (top left). The layers of staff, laboratory equipment, and data show the teamwork and effort the IDREAM Energy Frontier Research Center uses to study the cascading effects of ionized water on chemistry critical to energy, material science, environmental management, and more.

Creator: Robert Felsted

Graphic created by the Ion Dynamics in Radioactive Environments and Materials (IDREAM) EFRC for the Art of Science Image Contest at the 2025 DOE EFRC-Hub-CMS-CCS Principal Investigators' Meeting.

Center: IDREAM

19. Molecular Spins for Quantum Information Technologies



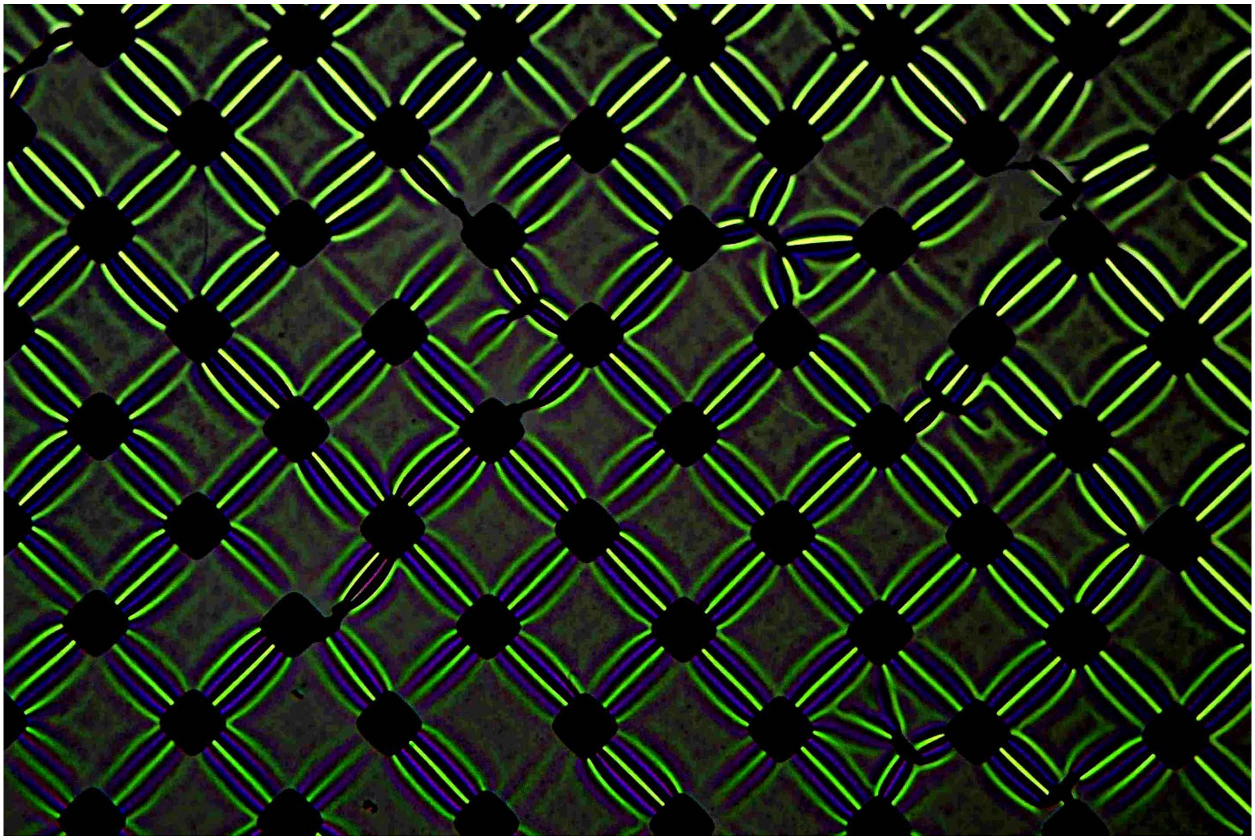
The figure showcases the potential of molecular spins for quantum information technologies. Those spins can encode information or perform gate operations, thus showing a novel way into the future of quantum computing and data processing. The image highlights the intriguing quantum states of photoactive molecular materials (surface-deposited molecules) that are coherently tunable and manipulable by an external electromagnetic field. This precise control is crucial for the development of reliable, efficient quantum systems. M2QM's innovative approach exploits synergy among theoretical models, artificial intelligence algorithms, and cutting-edge experimental techniques to design, realize, and improve quantum materials. This collaborative effort both enhances current prospects and opens modes of discovery of candidates with exceptional properties for target quantum applications. By integrating these diverse disciplines, we bridge the gap between theoretical possibilities and practical implementations. The figure was created meticulously using solely circles, rectangles, and lines on Inkscape.

Creator: Angel Albavera-Mata

Graphic created by the Center for Molecular Magnetic Quantum Materials (M2QM) for the Art of Science Image Contest at the 2025 DOE EFRC-Hub-CMS-CCS Principal Investigators' Meeting.

Center: M2QM

20. Strain-relaxed, Defect-free SiGeSn Thin Films via Epitaxial Lift-off Transfer



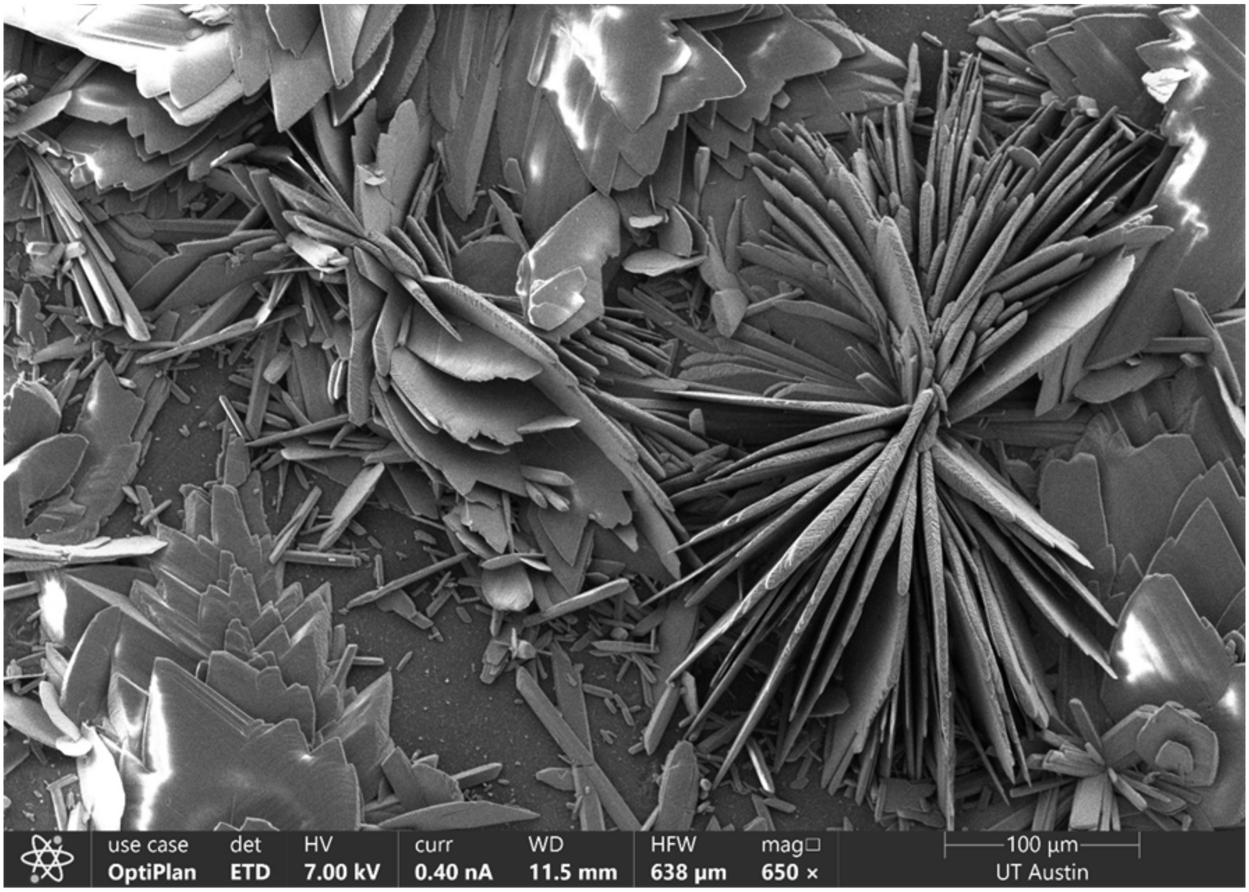
This image highlights the flower-like morphology resulting from SiGeSn lattice relaxation after epitaxial lift-off transfer. SiGeSn compound semiconductors hold strong promise for next-generation optoelectronic devices due to their tunable quasi-direct bandgap, offering advantages over conventional Si-based materials. However, direct epitaxy on Si substrates suffers from significant biaxial compressive strain, which distorts conduction band alignment. While Ge buffer layers mitigate this strain, they introduce high densities of defects and dislocations, degrading carrier transport and causing parasitic leakage. We successfully lifted off ~40 nm SiGeSn films from defective Ge/Si onto PDMS stamps. Despite poor etch selectivity between SiGeSn and Ge/Si, clean film transfer was achieved. Upon release, the contracted SiGeSn lattice relaxed to its intrinsic dimensions, forming overlapping regions along the pattern geometry and resulting in characteristic petal-like structures. The transferred films were free from strain and defects, providing an ideal platform to explore the intrinsic properties of SiGeSn.

Creators: Suho Park, Jifeng Liu, Fisher Yu, Yuping Zeng

Graphic created by the Center for Manipulation of Atomic Ordering for Manufacturing Semiconductors (μ-ATOMS) for the Art of Science Image Contest at the 2025 DOE EFRC-Hub-CMS-CCS Principal Investigators' Meeting.

Center: μ-ATOMS

21. Under the Sea



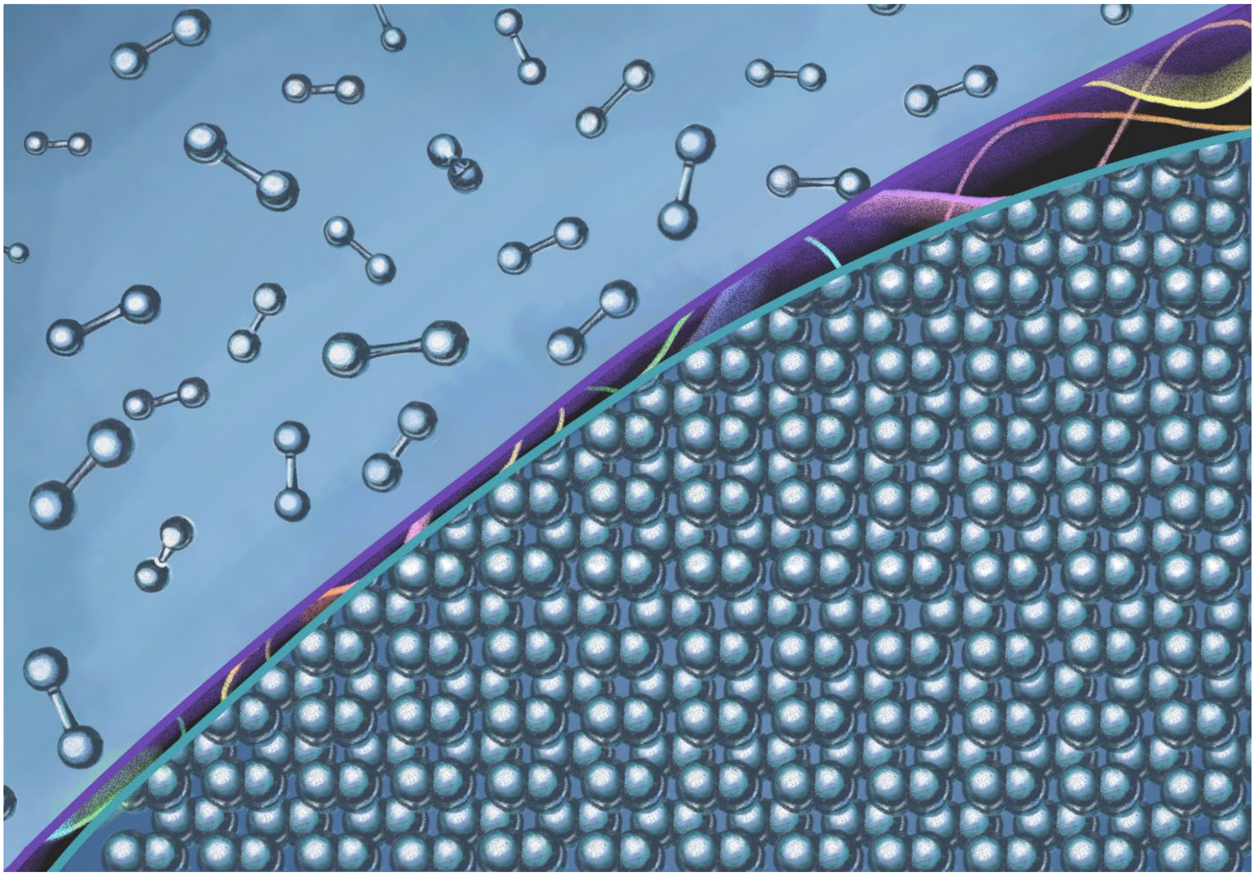
Precipitating gypsum typically forms needle-like structures. Interferences from large organic macromolecules during reverse osmosis operations force precipitating gypsum crystals to deviate from the typical structure and form flat sheet-like structures which can also appear needle-like. Some have noted that these crystals look like starfish, sea urchins, and coral, with the whole image resembling the sea floor.

Creators: Cameron McKay (SEM operator and research scientist), and David Bollinger (resolution manager)

Graphic created by the Center for Materials for Water and Energy Systems (M-WET) for the Art of Science Image Contest at the 2025 DOE EFRC-Hub-CMS-CCS Principal Investigators' Meeting.

Center: M-WET

22. Quantum motion shapes the melting line of dense hydrogen



Hydrogen, despite being the simplest element in the universe, has a rich phase diagram with lots of exciting quantum phenomena. Particularly, hydrogen has significant macroscopic quantum behavior because of its really high quantum zero point motion (ZPM). Our research showed that for molecular hydrogen, at pressures larger than 150 GPa, the ZPM has large effects on the macroscopic thermodynamics—lowering the melting temperature by as much as 100 K! To put this into perspective, if you were to carry the weight of the entire US population on your body, then you would experience about 150 GPa of pressure.

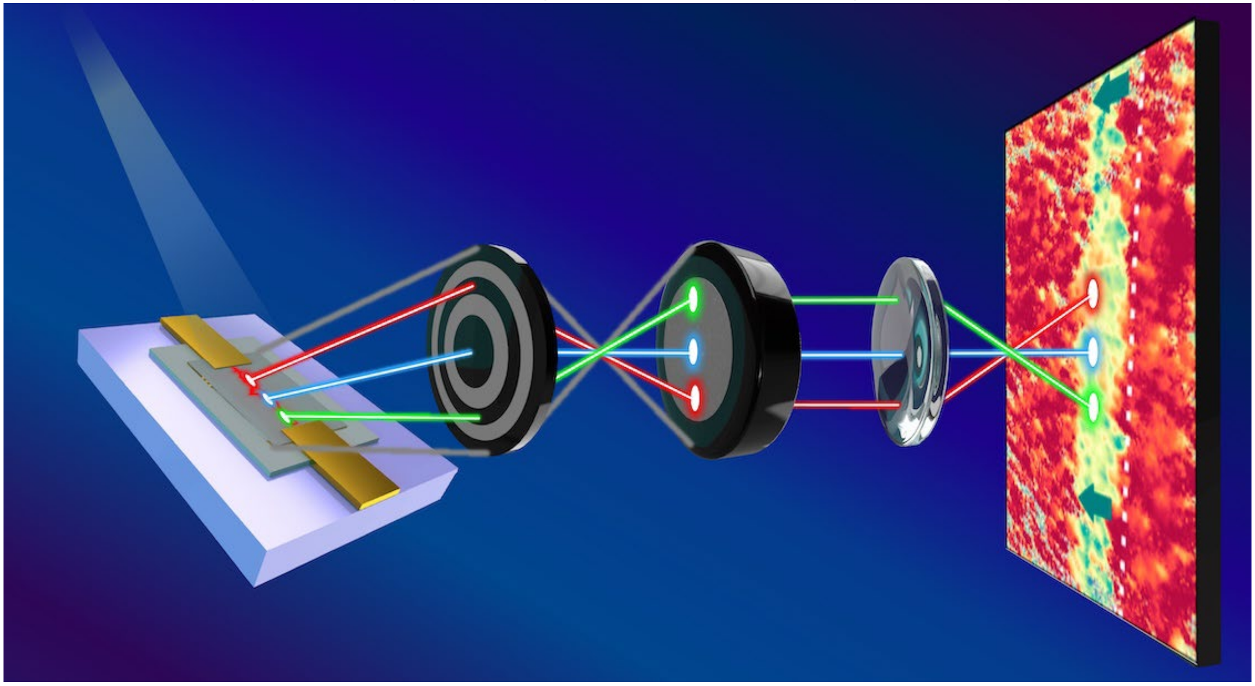
The image depicts the melting line of molecular hydrogen in temperature-vs-pressure from 50 to 175 GPa and 800 to 2000 K with the quantum effects depicting the shift in the melting line caused due to ZPM.

Creator: Isabel Zhou

Graphic created by the High-Accuracy Multiscale Models Using Quantum Monte Carlo (QMC-HAMM) CMS for the Art of Science Image Contest at the 2025 DOE EFRC-Hub-CMS-CCS Principal Investigators' Meeting.

Center: QMC-HAMM

23. Dark Field X-ray Microscopy: a new synchrotron tool to study neuromorphic devices



This image illustrates how we use a new technique, Dark Field X-ray Microscopy (DFXM), to see inside neuromorphic devices made from quantum materials. Deployed in collaboration with Argonne National Laboratory under this EFRC, DFXM lets us observe where new crystalline phases emerge as the device operates.

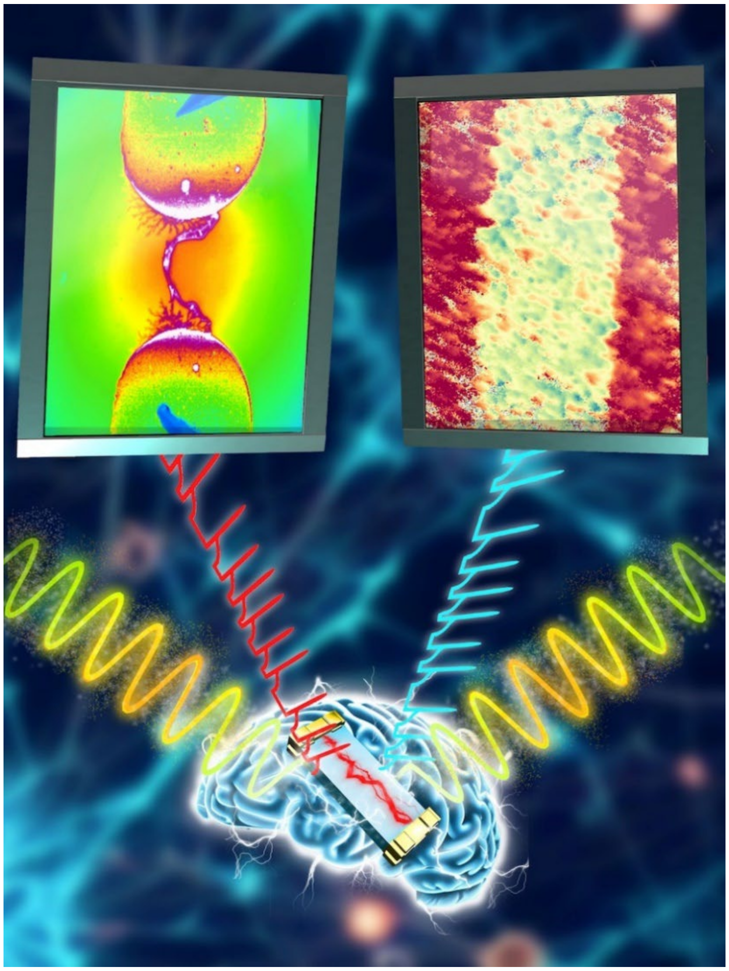
Here's how it works: a focused x-ray beam shines on the sample, where different regions scatter the beam depending on their crystal structure. These scattered beams (red, green, and blue) represent scattering from different parts of the device. After passing through a lens system, each beam is focused to a specific point on a detector screen. This transforms a traditional diffraction experiment into a real-space image. Remarkably, this reveals exactly where inside the material these structural changes are happening.

Creators: Mario Rojas, Alex Frano, and Ivan Schuller

Graphic created by the Quantum Materials for Energy-Efficient Neuromorphic Computing (Q-MEEN-C) EFRC for the Art of Science Image Contest at the 2025 DOE EFRC-Hub-CMS-CCS Principal Investigators' Meeting.

Center: Q-MEEN-C

24. Illuminating Filaments: Light-Matter Interactions in Quantum Neuromorphic Devices



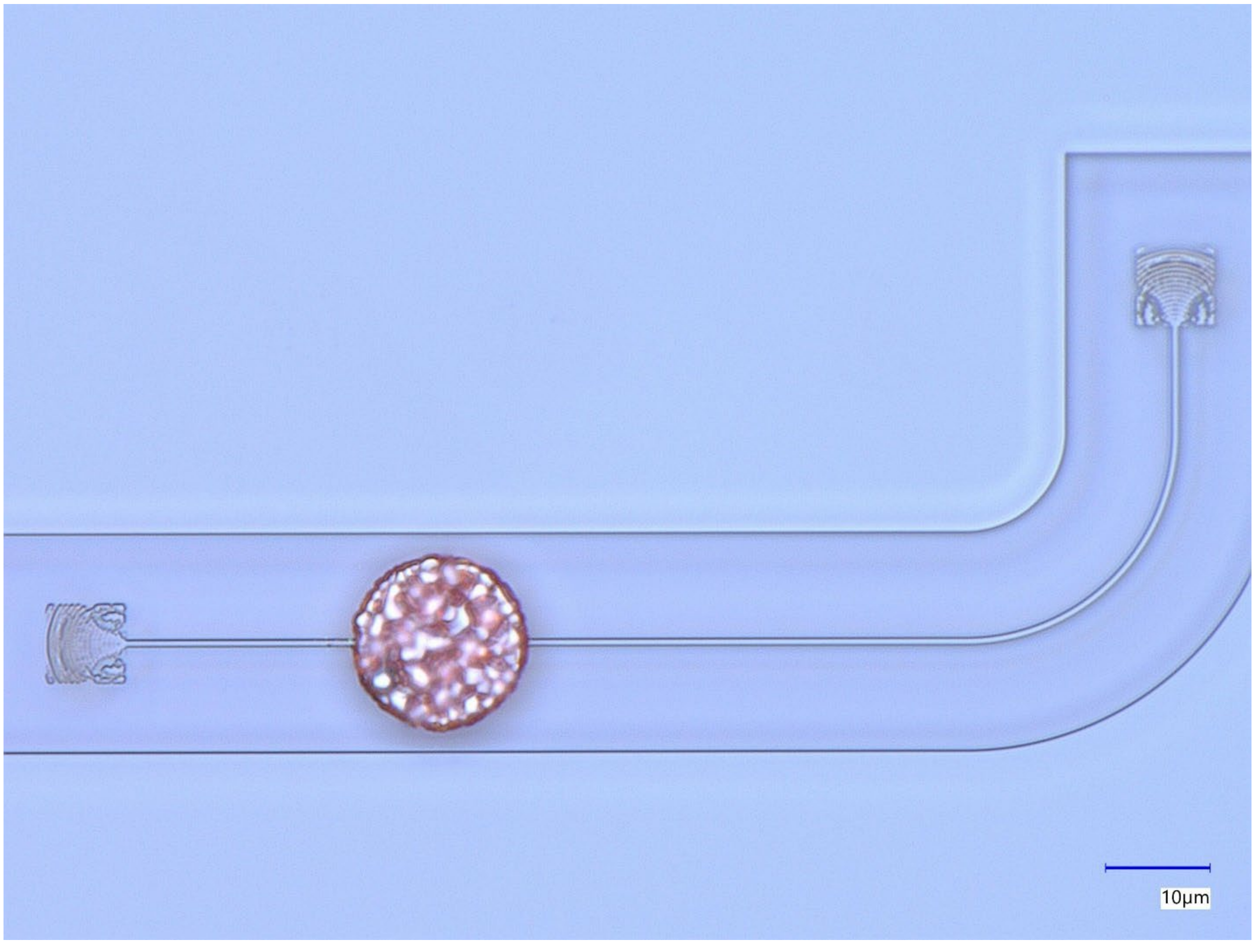
Making brain-like computers more energy efficient starts with understanding how tiny conductive threads, called filaments, form inside devices made of advanced quantum materials. This image shows two different ways scientists use light to explore that process. On the right, x-rays from a powerful and novel synchrotron microscope (deployed for the first time on such devices under this EFRC) reveal the *crystal structure* of these filaments inside a neuromorphic vanadate device. On the left, infrared light shined on similar devices helps us see that filaments are essentially regions of different temperatures. Though both methods use light, they uncover different pieces of the puzzle: one structural, one thermal. Together, they offer a richer picture of how these devices work, and this information guides efforts to build faster, smarter, and more efficient computing technologies inspired by the brain.

Creators: Mario Rojas, Alex Frano, and Ivan Schuller

Graphic created by the Quantum Materials for Energy-Efficient Neuromorphic Computing (Q-MEEN-C) EFRC for the Art of Science Image Contest at the 2025 DOE EFRC-Hub-CMS-CCS Principal Investigators' Meeting.

Center: Q-MEEN-C

25. Caramel Candy on the Monorail en route from point A to point B



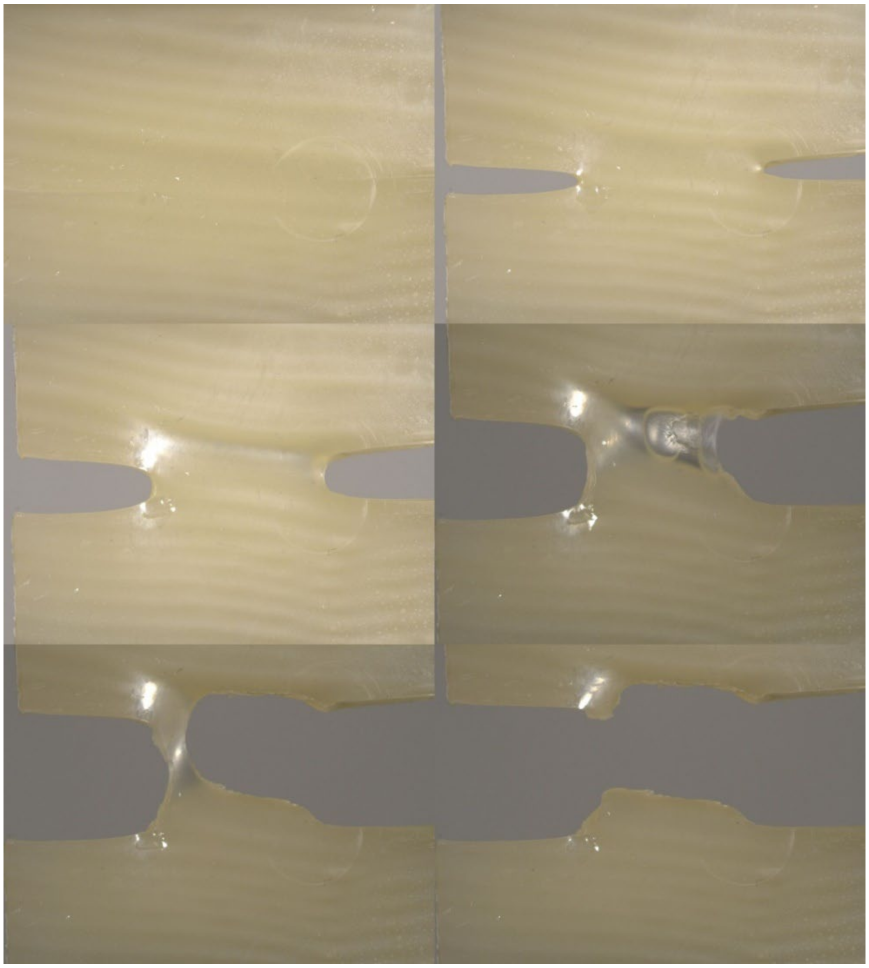
A whimsical take on a real microscopy image, this artwork depicts a lithographically defined Cu_2O micro-pillar – fabricated via electron beam lithography and positioned ~700 nm above a curved silicon nitride waveguide – as a caramel candy cruising along a monorail. The waveguide features asymmetry to allow both co-polarized and cross-polarized output coupling, with topologically optimized gratings guiding the path. This nanophotonic platform is engineered to probe the coupling of Rydberg excitons to guided modes at cryogenic temperatures, blending fundamental quantum optics with visual storytelling.

Creator: Artem Kryvobok

Graphic created by the Quantum Photonic Integrated Design Center (quPIDC) EFRC for the Art of Science Image Contest at the 2025 DOE EFRC-Hub-CMS-CCS Principal Investigators' Meeting.

Center: quPIDC

26. The Beauty in Failure, Crack Propagation Motion of Cyclooctadiene (COD) & Ethylidene-norbornene (ENB)



This collage captures the progression of a polymeric specimen composed of Cyclooctadiene (COD) & Ethylidene-norbornene (ENB) during Double Edge Notch Tension (DENT) testing. The stripes or 'patterns' that you see are varying crystalline and amorphous regions that occur autonomously during polymerization that self-organize via reaction-diffusion processes similar to what is seen in nature. Each frame encapsulates key stages of mechanical failure. These patterns are not just visual artifacts but tell a story of material processing, structure and performance. Similar to life, failure can reveal more than our successes. The beauty in breaking, we begin to understand.

Creators: Amyra Black, Anna Cramblitt, Luis Rodriguez, and Nancy Sottos

Graphic created by the Regenerative Energy-Efficient Manufacturing of Thermoset Polymeric Materials (REMAT) EFRC for the Art of Science Image Contest at the 2025 DOE EFRC-Hub-CMS-CCS Principal Investigators' Meeting.

Center: REMAT

27. Helix of Growth

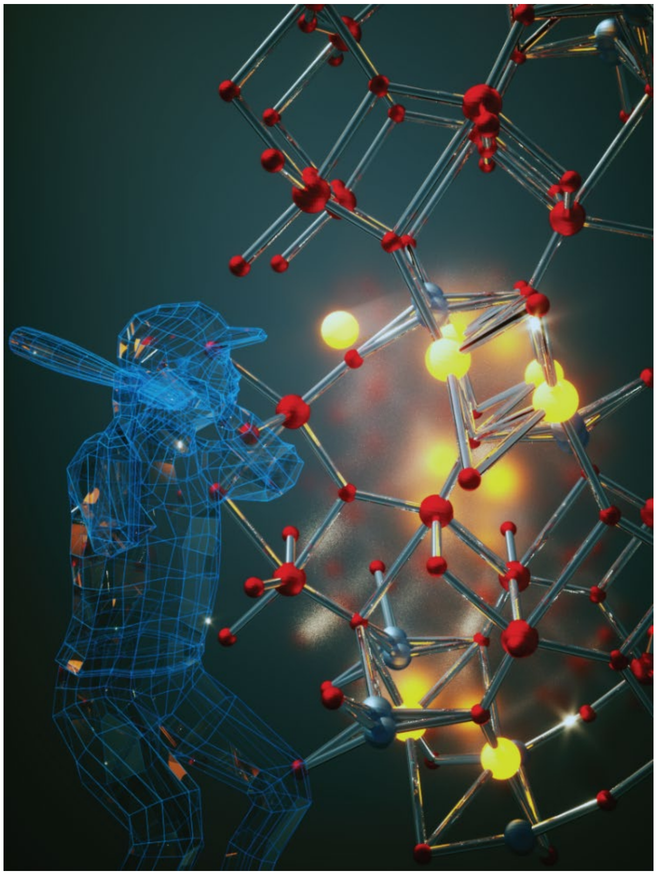
Emerging from an earthy foundation, the twisting helix in this image represents our research journey from potential to realization. Fabricated through “growth printing,” a novel additive manufacturing process we developed, the helix draws inspiration from natural growth in plants and organisms—where chemical reactions interact with environmental conditions to guide development. Using chemistry that converts liquid resin into solid plastic, we ‘grew’ this structure with the help of a motion stage. Growth printing is powered by frontal ring-opening metathesis polymerization (FROMP), a self-sustaining exothermic reaction that rapidly cures a resin mixture of dicyclopentadiene (DCPD) and polybutadiene (PBD) into a thermoset polymer at speeds around 1 mm/s. This process requires no continuous external energy input, making it significantly faster and more energy-efficient than traditional additive manufacturing methods. The resulting helix embodies the potential of merging nature’s design logic with cutting-edge materials science—opening new avenues for sustainable, efficient manufacturing technologies.

Creators: Mohammad Tanver Hossain, Yun Seong Kim, Sameh H. Tawfick and Randy H. Ewoldt

Graphic created by the Regenerative Energy-Efficient Manufacturing of Thermoset Polymeric Materials (REMAT) EFRC for the Art of Science Image Contest at the 2025 DOE EFRC-Hub-CMS-CCS Principal Investigators’ Meeting.

Center: REMAT

28. reMIND's Called Shot



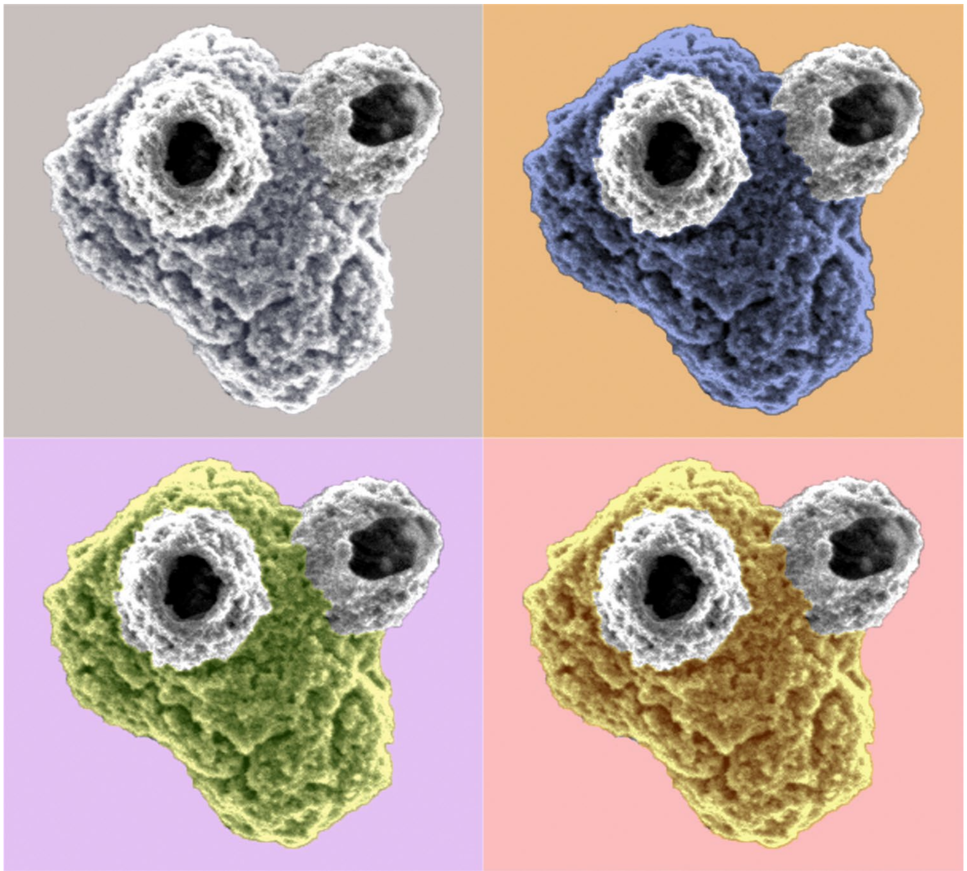
In Game 3 of the 1932 World Series, Babe Ruth pointed and "called his shot" at Wrigley Field, yielding an iconic moment in baseball history. reMIND has effectively repeated the gesture in the field of ion insertion chemistry, accurately positioning Li-ions using topochemical methods in four distinct interstitial sites of a ζ-V_2O_5 framework, thereby precisely modulating electronic structure and neuromorphic function for brain-inspired computing. Each of the sites have been identified through single crystal diffraction. The results suggest an effective strategy for atom-precise positioning of cations, accessing metastable insertion regimes, selectively redirecting diffusion pathways, and precisely modulating instabilities underpinning neuronal emulation. From: Joseph V. Handy, Wasif Zaheer, Ryan Albers, George Agbeworvi, Teak D. Boyko, Vladimir Bakhmoutov, Nattamai Bhuvanesh, Sarbajit Banerjee, Protecting Groups in Insertion Chemistry: Site-Selective Positioning of Lithium Ions in Intercalation Hosts. *Matter* **2023**, *6*, 1125-1139 https://doi.org/10.1016/j.matt.2023.01.028.

Creators: Joseph Handy, Sarbajit Banerjee, and Ella Maruschenko

Graphic created by the Reconfigurable Electronic Materials Inspired by Nonlinear Neuron Dynamics (reMIND) EFRC for the Art of Science Image Contest at the 2025 DOE EFRC-Hub-CMS-CCS Principal Investigators' Meeting.

Center: reMIND

29. It’s Not Easy Bein’ Green



After an attempt to fabricate an electrochemical memory device using ruthenium hexacyanoruthenate Prussian blue analog (RuPBA) by chemical deposition, interrogation by scanning electron microscopy revealed that the as-grown material formed a porous sponge-like structure with dimensions of several micrometers that resembles the head of the beloved Muppet character “Kermit the Frog.”

The four quadrants resemble colors commonly adopted by the RuPBA, which is tuned by electrochemical redox and ion insertion. The RuPBA changes from colorless/white [the fully reduced Ru(II) state] to dark blue [the mixed valence Ru(II:III) state], and then yellow [the unstable fully oxidized Ru(III) state]. RuPBA even becomes green as it is oxidized from the blue to yellow states, but the instability leads our Kermit to lament, “It's not easy bein' green!” Electrochemical charging also modulates the material’s conductivity, a key working principle for synaptic nonvolatile electrochemical random-access memory (ECRAM).

Creator: Donny Robinson

Graphic created by the Reconfigurable Electronic Materials Inspired by Nonlinear Neuron Dynamics (reMIND) EFRC for the Art of Science Image Contest at the 2025 DOE EFRC-Hub-CMS-CCS Principal Investigators’ Meeting.

Center: reMIND

CENTER OVERVIEW POSTER SESSION

A. Advanced Manufacturing

A-O-1: Artificially Intelligent Manufacturing Paradigm for Composites

[EFRC - AIM] Srikanth Pilla[1] (Director), Gang Li (Associate Director)[2], Farhang Pourboghart[3], George Karniadakis[4], Kevin Simmons[5], Qiong Zhang[2], Zhen Li[2], James Sternberg[2], Feng Luo[2], Michael Carbajales-Dale[2], Yong Huang[6], Nikunja Swain[7], Dale Hitchcock[8], Sai Aditya Pradeep[1]
[1]University of Delaware; [2]Clemson University (lead institution); [3]The Ohio State University; [4]Brown University; [5]Pacific Northwest National Laboratory; [6]University of Florida; [7]South Carolina State University, [8]Savannah River National Laboratory

The mission of this EFRC is to build an AI-enabled inverse design approach for fundamental understanding and integrated material-manufacturing design of advanced polymer composites. While uncovering these fundamental insights, this EFRC also aims to build Inverse Design Software (InDeS) tools that accelerate the discovery of advanced polymer composites for improved performance and energy-efficient manufacturing, thereby enabling a smaller carbon footprint, lower structural weight, and lower cost.

A-O-2: EFRC for Regenerative Energy-Efficient Manufacturing of Thermoset Polymeric Materials

[EFRC - REMAT] Nancy R. Sottos[1] (Director), Leah Appelhans[2], Jeff Baur[1], Adam W. Cook[2], Randy H. Ewoldt[1], Philippe H. Geubelle[1], Rafael Gomez-Bombarelli[3], Jeremiah A. Johnson[3], Samuel Leguizamon[2], Jennifer Lewis[4], Jeffrey S. Moore[1], Matthew Sigman[6], Sameh H. Tawfick[1]
[1]University of Illinois Urbana-Champaign (lead institution); [2]Sandia National Laboratories; [3]Massachusetts Institute of Technology; [4]Harvard University; [5]Stanford University; [6]University of Utah

REMAT's mission is to advance the science of thermochemical reaction-diffusion processes in additive and morphogenic manufacturing and accelerate a transformative, circular strategy for thermoset polymeric and composite materials with programmed end-of-life.

A-O-3: Center for the Science of Science of Synthesis Across Scales

[EFRC - CSSAS] François Baneyx[1] (Director), James J. De Yoreo[1,2], Christopher J. Mundy[1,2], Brandi M. Cossairt[1], Lilo Pozzo[1], David Baker[1], Chun-Long Chen[1,2], Andrew L. Ferguson[3], Oleg Gang[4], David Ginger[1], Sergei V. Kalanin[5], Jim Pfaendtner[6], Wendy Shaw[2], F. Akif Tezcan[7], Shuai Zhang[1,2]
[1]University of Washington; [2]Pacific Northwest National Laboratory; [3]University of Chicago; [4]Columbia University; [5]University of Tennessee-Knoxville; [6]North Carolina State University, [7]University of California, San Diego

To harness the complex functionality of hierarchical materials by mastering the design of high-information-content building blocks that predictively self-assemble into responsive, reconfigurable, self-healing materials, and direct the formation and organization of inorganic components.

A-O-4: Center for Plastics Innovation

[EFRC - CPI] LaShanda T.J. Korley[1] (Director), Thomas H. Epps, III[1], Gwendolyn J. Gregory[1], Juan J. de Pablo[2], Hui Fang[1], Marianthi Ierapetritou[1], Aditya M. Kunjapur[1], Daeyeon Lee[3], Frank Leibfarth[4], Dongxia Liu[1], Raul F. Lobo[1], Joshua K. Michener[5], Eleftherios T. Papoutsakis[1], Stuart J. Rowan[6], Brent Sumerlin[7], Dionisios G. Vlachos[1], John Vohs[3], Mary P. Watson[1]

[1]University of Delaware (lead institution); [2]New York University; [3]University of Pennsylvania; [4]University of North Carolina at Chapel Hill; [5]Oak Ridge National Laboratory; [6]University of Chicago; [7]University of Florida

To develop energy-efficient, selective, and tolerant chemo- and bio-catalytic and synthetic pathways to valorize diverse plastics waste streams and dramatically increase circularity

B. Catalysis

B-O-1: Institute for Cooperative Upcycling of Plastics

[EFRC - iCOUP] Mahdi Abu-Omar, Susannah Scott[1], Russ Bowers[2], Geoffrey Coates[3], Anne LaPointe[3], Massimiliano Delferro[4], David Kaphan[4], Byeongdu Lee[4], Megan Fieser[5], Andreas Heyden[6], Wenyu Huang[7], Frédéric Perras[7], Aaron Sadow[7] (Director), Erik Luijten[8], Ken Poeppelmeier[8], Anne McNeil[9], Baron Peters[10]

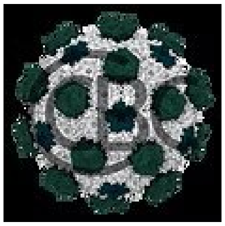
[1]University of California, Santa Barbara; [2]University of Florida; [3]Cornell University; [4]Argonne National Laboratory; [5]University of Southern California; [6]University of South Carolina; [7]Ames National Laboratory (lead institution); [8]Northwestern University; [9]University of Michigan; [10]University of Illinois Urbana-Champaign

iCOUP's Scientific Mission is to establish the molecular and macromolecular scientific principles governing deconstruction and reconstruction of polymers to enable manufacturing from energy-rich plastics.

B-O-2: The Center for Catalysis in Biomimetic Confinement

[EFRC - CCBC] Cheryl A. Kerfeld[1,2] (Director), David M. Tiede[3], Michael Feig[1], Robert Hausinger[1], Lisa Utschig[3], Michaela TerAvest[1], Eric Hegg[1], Karen Mulfort[3], Oleg Poluektov[3], Paul Ashby[2], Kristen Parent[1], Joshua Vermaas[1], Xiaobing Zhuo[3], Markus Sutter[1,2]

[1]Michigan State University (lead institution); [2]Lawrence Berkeley National Laboratory; [3]Argonne National Laboratory



To understand the means by which Nature spatially organizes catalysis across scales using compartmentalization within selectively permeable protein-based membranes, and to use these principles to develop a modular platform for spatially organizing catalysis

B-O-3: Center for Programmable Energy Catalysis

[EFRC - CPEC] Paul Dauenhauer[1] (Director), Susannah Scott[2] (Deputy Director), Eranda Nikolla[3], Phillip Christopher[2], Daniel Frisbie[1], Yuriy Roman[4], Rachel Getman[5], Matthew Neurock[1], Lars Grabow[6], Aditya Bhan[1], Kelsey Stoerzinger[1], Bharat Jalan[1], Omar Abdelrahman[6], Michael Gordon[2]

[1]University of Minnesota (lead institution); [2]University of California, Santa Barbara; [3]University of Michigan; [4]Massachusetts Institute of Technology; [5]The Ohio State University; [6]University of Houston

The mission of the DOE Center for Programmable Energy Catalysis (CPEC) is to transform how catalysts convert energy-rich molecules to enable a large-scale implementation of distributed energy. Through innovative research and diverse partnerships, the CPEC team aims to invent catalytic processes that are programmed to change on the timescale of an individual catalytic reaction, leading to dramatic enhancements in rate, selectivity, and conversion. By laying a foundation for a complex distributed energy ecosystem, CPEC will increase energy efficiency and promote future economic development while reducing the manufacturing challenges associated with chemical energy conversion.

B-O-4: Bio-inspired Light-Escalated Chemistry

[EFRC - BioLEC] Gregory Scholes[1] (Director), Gabriela Schlau-Cohen[2], Matthew Bird[3], Felix Castellano[4], Amy Cordones-Hahn[5], Paul Chirik[1], Sijia Dong[6], Abigail Doyle[7], Kelly Gaffney[5], Todd Hyster[1], Elena Jakubikova[4], Robert Knowles[1], David MacMillan[1], James McCusker[8], Ana Moore[9], Thomas Moore[9], Barry Rand[1], Obadiah Reid[10,11], Garry Rumbles[10,11], Hannah Sayre[6]

[1]Princeton University (lead institution); [2]Massachusetts Institute of Technology; [3]Brookhaven National Laboratory; [4]North Carolina State University; [5]SLAC National Accelerator Laboratory; [6]Northeastern University; [7]University of California, Los Angeles; [8]Michigan State University; [9]Arizona State University; [10]National Renewable Energy Laboratory; [11]University of Colorado Boulder

An emerging technological paradigm is to use the energy of light to boost substantially the power of the reactions enabled by molecular catalysts. Magnifying this opportunity, the mission of BioLEC is to combine light harvesting and advances in solar photochemistry to enable more powerful editing, building, and transforming of abundant materials to produce energy-rich feedstock chemicals. By developing new supercharged light-powered catalysts and reactions and deepening our understanding of existing ones, valuable products can be generated from plentiful molecules such as those extracted from waste and renewable resources.

B-O-5: Ensembles of Photosynthetic Nanoreactors (EPN)

[EFRC - EPN] Shane Ardo[1] (Director), Rohini Bala Chandran[2], Scott K. Cushing[3], Gordana Dukovic[4], Daniel V. Esposito[5], Nien-Hui Ge[1], Shu Hu[6], Katherine E. Hurst[7], Kenneth A. Miller[8], Tadashi Ogitsu[9], Xiaoqing Pan[1], Joseph P. Patterson[1], Oluwaseun I. Salako[10], Justin B. Sambur[11], Young-Seok Shon[12], A. Alec Talin[13], Jenny Y. Yang[1]

[1]University of California, Irvine (lead institution); [2]University of Michigan, Ann Arbor; [3]California Institute of Technology; [4]University of Colorado Boulder; [5]Columbia University; [6]Yale University; [7]National Renewable Energy Laboratory; [8]Fort Lewis College; [9]Lawrence Livermore National Laboratory; [10]The City University of New York – Medgar Evers College; [11]Colorado State University; [12]California State University, Long Beach; [13]Sandia National Laboratories

Our scientific mission is to understand, predict, and control the activity, selectivity, and stability of solar water splitting nanoreactors in isolation and as ensembles, via concerted efforts spanning the four research thrusts of electronic selectivity, reactant accumulation, chemical selectivity, and ensemble effects.

B-O-6: Beyond-DFT Electrochemistry with Accelerated and Solvated Techniques (BEAST)

[CCS - BEAST] Ravishankar Sundararaman[1] (Director), Derek Vigil-Fowler[2], Mauro Del Ben[3], Charles Musgrave[4], Christopher Sutton[5]

[1]Rensselaer Polytechnic Institute; [2]National Renewable Energy Laboratory; [3]Lawrence Berkeley National Laboratory; [4]University of Colorado Boulder; [5]University of South Carolina

We aim to develop accurate and efficient exascale-ready solvated beyond-DFT methods for computational electrochemistry by (1) making key advances in atomic-scale electrolyte solvation models that capture the equilibrium effect of electrolyte in the electronic structure calculation of a single configuration by DFT, (2) making GW many-body perturbation theory and the random phase approximation (RPA) total energy beyond-DFT calculations practical for electrochemistry by integrating them with solvation techniques and optimizing them for exascale computing, and (3) integrating all these advances within a grand canonical scheme to fundamentally describe the effect of solvation and bias on the electrochemistry, and facilitating ML approaches for first-principles electrochemistry, including 'Δ-learning' approaches to make RPA-quality predictions at

DFT cost, by developing a beyond-DFT electrochemical database. Together, the BEAST team aims to deliver exascale-ready solvated beyond-DFT methods and ML acceleration using an electrochemical database to make truly ab initio electrochemistry accessible and ubiquitous.

B-O-7: Liquid Sunlight Alliance

[Hub - LiSA] Harry A. Atwater[1,2] (Director), Theo Agapie[1,2], Marco Bernardi[1,2], Scott Cushing[1,2], William Goddard[1,2], John Gregoire[1,2], Joel Haber[1,2], Ryan Hadt[1,2], Carrie Hofmann[1,2], Karthish Manthiram[1,2], Jonas Peters[1,2], Kimberly See[1,2], Chengxiang Xiang[1,2], Peter Agbo[1,3], Joel Ager[1,3], Alexis Bell[1,3], Shannon Boettcher[1,3,8], Walter Drisdell[1,3], Naomi Ginsberg[1,3], Martin Head-Gordon[1,3], Frances Houle[1,3], Jeff Neaton[1,3], Kristin Persson[1,3], Adam Weber[1,3], Peidong Yang[1,3], Junko Yano[1,3], Ann Greenaway[1,4], Wilson Smith[1,4], Myles Steiner[1,4], Bill Tumas[1,4], Emily Warren[1,4], Andriy Zakutayev[1,4], Frank Abild-Pedersen[1,5], Michal Bajdich[1,5], Amy Cordones-Hahn[1,5], Thomas Jaramillo[1,5], Adam Nielander[1,5], Shane Ardo[1,6], and Cliff Kubiak[1,7]

[1]Liquid Sunlight Alliance; [2]California Institute of Technology (lead institution); [3]Lawrence Berkeley National Laboratory; [4]National Renewable Energy Laboratory; [5]SLAC National Accelerator Laboratory; [6]University of California, Irvine; [7]University of California, San Diego; [8]University of Oregon

The mission of the Liquid Sunlight Alliance (LiSA) is to establish the science principles by which durable coupled microenvironments can be co-designed to efficiently and selectively generate liquid fuels from sunlight, water, carbon dioxide, and nitrogen. These principles will guide the creation of microenvironment assemblies co-designed to harness diverse sunlight-driven phenomena with unprecedented catalytic selectivity, durability, and efficiency under a fluctuating solar resource, using pure or impure feedstocks.

B-O-8: Center for Closing the Carbon Cycle

[EFRC - 4C] Jenny Yang[1] (Director), Christopher Hahn[2], Charles McCrory[3], Joshua Spurgeon[4], John Gregoire[5], Joel Haber[5], Robert Sacci[6], Gabriel Veith[6], Aaron Appel[7], Vy Dong[1], Robert Nielsen[1], Chantal Stieber[8], Burcu Gurkan[9], Bijandra Kumar[10], Jesús Velázquez[11], Louise Berben[11], Anastassia Alexandrova[12], Carlos Morales-Guio[12], Michael Findlater[13], Marsha Massey[14], Wilson Smith[15], Michael Janik[16]

[1]University of California, Irvine; [2]Lawrence Livermore National Laboratory; [3]University of Michigan; [4]University of Louisville; [5]California Institute of Technology; [6]Oak Ridge National Laboratory; [7]Pacific Northwest National Laboratory; [8]California State Polytechnic University, Pomona; [9]Case Western Reserve University; [10]Elizabeth City State University; [11]University of California, Davis; [12]University of California, Los Angeles; [13]University of California, Merced; [14]University of Central Arkansas; [15]University of Colorado Boulder; [16]The Pennsylvania State University

4C aims to advance the foundational science and define key integration parameters for synergistic CO2 capture and conversion, or reactive capture of CO2.

B-O-9: Exascale Catalytic Chemistry Project

[CCS - ECC] Judit Zádor[1] (Director), Habib N. Najm[1], Khachik Sargsyan[1], C. Franklin Goldsmith[2], Richard H. West[3], Eric J. Bylaska[4], David H. Bross[5], Branko Ruscic[5]

[1]Sandia National Laboratories, Livermore; [2]Brown University; [3]Northeastern University; [4]Pacific Northwest National Laboratory; [5]Argonne National Laboratory

Our goal is to build predictive models for gas/solid heterogeneous catalytic systems. We want to go beyond many of the approximations routinely used in simulating such systems. Specifically, we want to:

- Improve the accuracy of both enthalpic and entropic contributions in thermodynamic functions of adsorbates at minima and first-order saddle points.

- Advance the state of the art in modeling the kinetics of catalytic reaction systems by creating automated frameworks with more realistic physical representations.

- Develop methods applicable to metals and their alloys.

- Create and extend exascale-ready computational tools that can achieve our scientific goals and help others to adopt our approaches.

B-O-10: Catalyst Design for Decarbonization Center

[EFRC - CD4DC] Laura Gagliardi[1] (Director), Joseph Hupp[2], Chibueze Amanchukwu[1], John Anderson[1], Karena W. Chapman[3], Juan de Pablo[1], Massimiliano Delferro[4], Omar Farha[2], Andrew Ferguson[1], Ian Foster[1], Rachel Getman[5], Ksenija Glusac[6], Jian Zhi Hu[7], Eliu Huerta[4], Matthew Neurock[8], Justin Notestein[2], Donald Truhlar[8], Anna Wuttig[1]

[1]University of Chicago (lead institution); [2]Northwestern University; [3]Stony Brook University; [4]Argonne National Laboratory; [5]The Ohio State University; [6]University of Illinois at Chicago; [7]Pacific Northwest National Laboratory; [8]University of Minnesota

CD4DC aims to identify promising pathways for the addition and removal of hydrogen in carbon-based energy carriers. To support this goal, we employ both experimental and theoretical approaches to uncover the underlying mechanisms of key chemical reactions, providing essential insights to guide the rational design and development of effective catalysts. A central focus is on the discovery and engineering of reticular metal-organic framework (MOF) materials, which offer unique structural and chemical properties that make them particularly well-suited as catalysts for low-temperature hydrogenation and dehydrogenation processes, as well as for facilitating carbon–carbon bond transformations.

B-O-11: Center for Electrochemical Dynamics and Reactions on Surfaces

[EFRC - CEDARS] Dhananjay Kumar[1] (Director), Tanja Cuk[2], Jin Suntivich[3], Ethan Crumlin[4], Geoffroy Hautier[5], Ismaila Dabo[6], Bishnu Bastakoti[1], Shyam Aravamudhan[1], Kristen Rhinehardt[1], Junko Yano[4], David Jonas[2], Darrell Schlom[3], William McMahon[7], Yang Shao-Horn[8]
[1]North Carolina A&T State University; [2]University of Colorado Boulder; [3]Cornell University; [4]Lawrence Berkeley National Laboratory; [5]Dartmouth College; [6]Carnegie Mellon University; [7]National Renewable Energy Laboratory; [8]Massachusetts Institute of Technology

The mission of CEDARS is to reveal step-by-step the formation of the transient intermediates of oxygen evolution reaction (OER) and hydrogen evolution reaction (HER), and what causes the O-O and H-H bond to form, how the catalyst evolves before, during, and after catalysis, as a function of time and reaction conditions. In doing so, we will provide the next-generation workforce with a unique skillset by which they could drive the hydrogen effort at terawatt scales through fundamental research.

D. Energy Storage

D-O-1: Center for Hybrid Approaches in Solar Energy to Liquid Fuels (CHASE)

[Hub - CHASE] Gerald Meyer[1] (Director), Jillian Dempsey[1], Jessica Anna[2], Joanna Atkin[1], James Cahoon[1], Felix Castellano[3], Javier Concepcion[4], Mehmed Zahid Ertem[4], Karen Goldberg[5], David Grills[4], Sharon Hammes-Schiffer[6], Nilay Hazari[7], Elena Jakubikova[2], Yosuke Kanai[1], Tianquan Lian[8], Matthew Lockett[1], Rene Lopez[1], Paul Maggard[9], Tom Mallouk[5], Gerald Manbeck[4], James Mayer[7], Alexander Miller[1], Greg Parsons[3], Dmitry Polyansky[4], José Rodriguez[4], Eric Stach[5], Hailiang Wang[7]
[1]University of North Carolina at Chapel Hill; [2]University of Pittsburgh; [3]North Carolina State University; [4]Brookhaven National Laboratory; [5]University of Pennsylvania; [6]Princeton University; [7]Yale University; [8]Emory University; [9]Baylor University

The CHASE mission is to develop hybrid photoelectrodes for cooperative sunlight-driven generation of liquid fuels from CO2 and water.

D-O-2: Energy Storage Research Alliance (ESRA)

[Hub - ESRA] Y. Shirley Meng[1,2] (Director), Bryan McCloskey[3,4] (Deputy Director), Wei Wang[5] (Deputy Director), James Burrow[1,2] (Deputy Assistant Director), Yang Shao-Horn[6], Dan Steingart[7], Brett Helms[3], Yan Yao[8], Paul Fenter[1], Vijay Murugesan[5], Gerbrand Ceder[3,4], Maria Chan[1], Ethan Crumlin[3], Kamila Wiaderek[1], Kelsey Hatzell[9], Venkat Srinivasan[1], Neil Dasgupta[10]

[1]Argonne National Laboratory (lead institution); [2]University of Chicago; [3]Lawrence Berkeley National Laboratory; [4]University of California, Berkeley; [5]Pacific Northwest National Laboratory; [6]Massachusetts Institute of Technology; [7]Columbia University; [8]University of Houston; [9]Princeton University; [10]University of Michigan

ESRA is an Energy Innovation Hub funded by the U.S. Department of Energy (DOE) focused on energy storage and next-generation battery discovery. ESRA aims to enable transformative discoveries in materials chemistry, gain a fundamental understanding of electrochemical phenomena at the atomic scale, lay the scientific foundations for breakthroughs in energy storage technologies, and train the next-generation battery workforce to ensure U.S. scientific and economic leadership.

D-O-3: Mechano-chemical Understanding of Solid Ion Conductors (MUSIC)

[EFRC - MUSIC] Jeff Sakamoto[1,2], Neil Dasgupta[1], Matt McDowell[3], Partha Mukherjee[4], David Kwabi[5], Kelsey Hatzell[6], Miaofang Chi[7], Donald Siegel[8], David Mitlin[8], Bart Bartlett[1], Yet-Ming Chiang[9], Sossina Haile[10], Nicola Perry[11], Katsuyo Thornton[1], Michael Thouless[1], Bilge Yildiz[9], Raphaele Clement[2]

[1]University of Michigan; [2]University of California, Santa Barbara; [3]Georgia Institute of Technology; [4]Purdue University; [5]Yale University; [6]Princeton University; [7]Oak Ridge National Laboratory; [8]University of Texas at Austin; [9]Massachusetts Institute of Technology; [10]Northwestern University; [11]University of Illinois Urban-Champaign

MUSIC Integrate the fields of materials science, electrochemistry, and solid-state mechanics to understand the mechano-electrochemical phenomena underlying the manufacturing and operation of ceramics for advanced electrochemical technologies.

D-O-4: Center for Mesoscale Transport Properties

[EFRC - m2M#s] Amy Marschilok[1,2] (Director), Esther Takeuchi[1,2] (Founding Director), Kenneth Takeuchi[1,2] (Deputy Director), Shan Yan[2] (Center Operations Officer), Lynden Archer[3], Carlos Colosqui[1], Marca Doeff[4], Ping Liu[2], Lamar Meda[5], Elsa Reichmanis[6], Alan West[7], Stanislaus Wong[1], Guihua Yu[8], Yimei Zhu[2]

[1]Stony Brook University (lead institution); [2]Brookhaven National Laboratory; [3]Cornell University; [4]Lawrence Berkeley National Laboratory; [5]Xavier University of Louisiana; [6]Lehigh University; [7]Columbia University; [8]University of Texas at Austin

To understand and harness disorder and entropy to build the science foundation for new design
spaces that enable sustainable, long cycle life electrochemical energy storage.

D-O-5: Breakthrough Electrolytes for Energy Storage Systems (BEES2)

[EFRC - BEES2] Burcu Gurkan[1] (Director), Robert Savinell[1] (Deputy Director), Joshua Sangoro[2], Emily Pentzer[3], Thomas Zawodzinski[4], Jesse Wainright[1], Robert Warburton[1], Rohan Akolkar[1], Clemens Burda[1], Steve Greenbaum[5], Mark Tuckerman[6], Edward Maginn[7], Yong Zhang[7], Juaquin Rodríguez-López[8], David Powers[3], Mark Dadmun[4], Emmanouil Doxastakis[4]

[1]Case Western Reserve University (lead institution); [2]The Ohio State University; [3]Texas A&M University; [4]University of Tennessee-Knoxville; [5]Hunter College; [6]New York University; [7]University of Notre Dame; [8]University of Illinois Urbana-Champaign

MISSION: To uncover the transport mechanisms of ions, protons, redox species, and electrons in nano to meso scale structured electrolytes in the bulk and at the electrode-electrolyte interfaces to achieve high energy and power density in next generation energy storage systems.

D-O-6: Fast and Cooperative Ion Transport in Polymer Based Materials

[EFRC - FaCT] Valentino R. Cooper[1] (Director), Susan B. Sinnott[2], Jodie L. Lutkenhaus[3], Michael A. Hickner[4], Rajeev Kumar[1], Alexei P. Sokolov[1], Xi Chelsea Chen[1], Wesley F. Reinhart[2], Tomonori Saito[1], Albina Y. Borisevich[1], Raphaële J. Clément[5], Ralph H. Colby[2], Sheng Dai[1], Tageshi Egami[6], Catalin Gainaru[1], Kenneth S. Schweizer[7], Yuya Shinohara[1], Gangli Wang[8], Tao Wang[1], Thomas Zac Ward[1]

[1]Oak Ridge National Laboratory (lead institution); [2]The Pennsylvania State University; [3]Texas A&M University; [4]Michigan State University; [5]University of California, Santa Barbara; [6]University of Tennessee-Knoxville; [7]University of Illinois Urbana-Champaign; [7]Georgia State University

To understand and control fast, correlated ion and proton transport at multiple length and time scales in polymer-based electrolytes to overcome the current limitations of energy storage and conversion technologies.

D-O-7: Geo-processes in mineral carbon storage

[EFRC - GMCS] E. Detournay[1], Z. Bazant[2], G. Buscarnera[2], B. Guzina[1], L. Hansen[1], H. Huang[3], J. Hyman[4], P. Kang[1], Q. Kang[4], J. Labuz[1], J. Le[1], J. Matter[5], S. Mogilevskaya[1], C. Wren Neil[4], J. Rudnicki[2], G. Srinivasan[4], H. Viswanathan[4], V. Voller[1]
[1]University of Minnesota, [2]Northwestern University, [3]Georgia Institute of Technology, [4]Los Alamos National Laboratory, [5]University of Southampton

Geologic mineralization of carbon offers a route towards the permanent storage of CO2, and GMCS has made notable advances in the science needed to quantify the potential of this process. Critical insights, fundamental understanding, and practical tools have provided: (i) an identification of damage and fracture mechanisms for the creation of new pathways and surface area in low permeable rocks; (ii) experiments and theory that illuminate the flow and mixing process in fracture networks; and (iii) large scale computations of mineralization operations explicitly linked to detailed geologic data collected from an active field scale project.

D-O-8: Center for Scalable Predictive Methods for Excitations and Correlated Phenomena

[CCS - SPEC] Sotiris S. Xantheas[1,2] (Director), Karol Kowalski[1,2], Niri Govind[1,2], Edo Apra[1], Daniel Mejia-Rodriguez[1], Ajay Panyala[1], Bo Peng[1], Erdal Mutlu[1], Fernando Vila[2], John Rehr[2], Xiaosong Li[2], Wibe de Jong[3], Chao Yang[3], David Williams-Young[3], So Hirata[4], Dominika Zgid[5], Jiri Brabec[6], Libor Veis[6], Ors Legeza[7]
[1]Pacific Northwest National Laboratory (lead institution); [2]University of Washington; [3]Lawrence Berkeley National Laboratory; [4]University of Illinois Urbana-Champaign; [5]University of Michigan; [6]J. Heyrovsky Institute of Physical Chemistry; [7]Wigner Institute

The Center for "Scalable Predictive methods for Excitations and Correlated phenomena" (SPEC) develops open-source, scalable software libraries of high-level electronic structure methods for excited states that run efficiently on hardware architectures in Leadership Computing Facilities (LCFs). These theoretical and computational capabilities will enable transformational scientific discoveries in areas such as light-harvesting systems, artificial photosynthesis, carbon-based materials, solvation chemistry, catalysis, geochemistry, and novel ultrafast femtosecond techniques. SPEC is implementing novel scalable programming models and libraries for coupled cluster, multireference, and Green's function electronic structure methods in conjunction with novel computational tools to enable their efficient deployment on existing and forthcoming DOE LCF systems. These libraries will be interoperable with existing codes and will simulate excited states and processes with unprecedented predictive power and orders-of-magnitude greater computational performance than current methods.

F. Energy-Water

F-O-1: FLOSIC: Efficient density functional calculations without self-interaction

[CCS - FLOSIC] Koblar Jackson[1] (Director), Juan Peralta[1], Mark R. Pederson[2], Tunna Baruah[2], Rajendra Zope[2], J. Karl Johnson[3], John P. Perdew[4], Adrienn Ruzsinszky[4], George Christou[5]
[1]Central Michigan University (lead institution); [2]University of Texas at El Paso; [3]University of Pittsburgh; [4]Tulane University; [5]University of Florida

The mission of the FLOSIC Center is to develop and test an efficient and accurate method for removing the effects of unphysical electron self-interaction from the results of density functional theory calculations. The method will be implemented and made available in open source software.

F-O-2: The Center for Enhanced Nanofluidic Transport—Phase 2 (CENT2)

[EFRC - CENT2] Michael Strano[1] (Director), Cody Ritt[1], Zuzanna Siwy[2], Narayana Aluru[3], Menachem Elimelech[4], Tuan Anh Pham[5], Heather Kulik[1], YuHuang Wang[6], Amir Haji-Akbari[4], Martin Bazant[1], Daniel Blankschtein[1], John Cumings[6], John Fourkas[6]6, Arun Majumdar[7], Aleksandr Noy[5], Javier Sanchez-Yamagishi[2]
[1]Massachusetts Institute of Technology; [2]University of California, Irvine; [3]University of Texas at Austin; [4]Yale University; [5]Lawrence Livermore National Laboratory; [6]University of Maryland; [7]Stanford University

Phase 2 of the Center for Enhanced Nanofluidic Transport (CENT2) will continue to address emerging and compelling knowledge gaps (KGs) for fluid flow and molecular transport in SDNs to establish the scientific foundation for developing transformative molecular separation technologies impacting the Water–Energy Nexus and other sectors of the US economy. Leveraging our newfound insights, this vision encompasses vastly more precise and energy efficient separations, such as self-pumping membranes, pores with tunable selectivity, and feedback control to modulate the transport medium.

F-O-3: Advanced Materials for Energy-Water Systems

[EFRC - AMEWS] Chibueze Amanchukwu[1], Seth B. Darling[1,2] (Director), Juan J. de Pablo[1,2], Jeffrey W. Elam[1,2], Paul Fenter[2], Giulia Galli[1,2], Kelsey B. Hatzell[3], Chong Liu[1], Alex B.F. Martinson[2], Karen Mulfort[2], Paul F. Nealey[1,2], Nicholas H.C. Lewis[1], Pietro Papa Lopes[2], George Schatz[4], Dmitri Talapin[1], Matthew V. Tirrell[1], Andrei Tokmakoff[1], Christopher Wolverton[4]

[1]University of Chicago; [2]Argonne National Laboratory (lead institution); [3]Princeton University; [4]Northwestern University

Our mission is to revolutionize our understanding of aqueous solutes in confined and electrified environments at interfaces, by integrating new experimental, theoretical, and modeling capabilities.

F-O-4: Center for Materials for Water and Energy Systems

[EFRC - M-WET] Christopher Bates[2], Raphaële Clément[2], Phillip Christopher[2], Ethan Crumlin[3], Berkin Dortdivanlioglu[1], Glenn Fredrickson[2], Benny Freeman[1] (Director), Venkat Ganesan[1], Craig Hawker[2], Graeme Henkelman[1], Lynn E. Katz[1] (Associate director), Manish Kumar[1], Gabriel Sanoja Lopez[1], Nathaniel Lynd[1], Dylan McReynolds[1], Zachariah Page[1], Rachel Segalman[2] (Associate director), Scott Shell[2], Todd Squires[2], Gregory Su[3]

[1]University of Texas at Austin (lead institution); [2]University of California, Santa Barbara; [3]Lawrence Berkeley National Laboratory

The mission of the Center for Materials for Water and Energy Systems (M-WET) is to discover and understand fundamental science to design new membrane materials, develop tools and knowledge to predict new materials' interactions with targeted solutes, inspired by the need to provide fit for purpose water from low quality water sources and recover valuable solutes with less energy.

G. Hydrogen

G-O-1: Hydrogen in Energy and Information Sciences

[EFRC - HEISs] Sossina Haile[1] (Director), Michael Bedzyk[1], Lin Chen[1,2], Vinayak Dravid[1], Yan-Yan Hu[3,9], Ju Li[4], Ryan O'Hayre[5], Katharine Page[6,7], Nicola Perry[8], James Rondinelli[1], Chris Wolverton[1], Bilge Yildiz[4]

[1]Northwestern University (lead institution); [2]Argonne National Laboratory; [3]Florida State University; [4]Massachusetts Institute of Technology; [5]Colorado School of Mines; [6]Oak Ridge National Laboratory; [7]University of Tennessee-Knoxville; [8]University of Illinois Urbana-Champaign; [9]Center of Interdisciplinary Magnetic Resonance, National High Magnetic Field Laboratory

HEISs aims to advance the fundamental understanding and discovery of multihued hydrogen transport in inorganic solids of earth-abundant elements, and of its transfer along and across interfaces within such materials, where ‘hydrogen’ includes all charge states of H: H^+ (proton), H^0 (atom), and H^- (hydride ion).

G-O-2: Center for Alkaline Based Energy Solutions; CABES: Center Mission, Progress and Synergies

[EFRC - CABES] Hector Abruña[1] (Director), David Muller[1], Andrej Singer[1], Brett Fors[1], Richard Robinson[1], Geoff Coates[1], Robert DiStasio[1], Emmanuel Giannelis[1], Jin Suntivich[1], Joel Brock[1], Tomas Arias[1], Peter Frazier[1], Bryan Pivovar[2], Piotr Zelenay[3], Sharon Hammes-Schiffer[4], Emmanouil Mavrakakis[5], Carlos Cabrera[6], Tom Mallouk[7], Ray Schaak[8], Kevin Noonan[9]

[1]Cornell University (lead institution); [2]National Renewable Energy Laboratory; [3]Los Alamos National Laboratory; [4]Princeton University; [5]University of Wisconsin-Madison; [6]University of Texas at El Paso; [7]University of Pennsylvania; [8]The Pennsylvania State University; [9]Carnegie Mellon University

CABES mission to advance the scientific understanding of the fundamental factors governing electrocatalysis and electrochemical energy conversion in alkaline media by focusing on the three science drivers 1.What factors govern electrocatalysis in alkaline media? 2.How do we understand and control transport in alkaline media? 3.What makes energy materials durable in alkaline media?

G-O-3: Photoelectrochemical Formation of Strategic Fuels Using Soft (Molecular Semiconductor) Materials – The Center for Soft PhotoElectroChemical Systems (SPECS)

[EFRC - SPECS] Neal R. Armstrong[1] (Director), Erin L. Ratcliff[2], Elisa Miller[3], Chad Risko[4], Natalie Stingelin[2], Tim Lian[5], Seth Marder[6], Steve Barlow[6], Jean-Luc Bredas[1], Andrew Ferguson[3], Ann Greenaway[3], Obadiah Reid[6], Alberto Salleo[7], Michael Toney[6]

[1]University of Arizona (lead institution); [2]Georgia Institute of Technology; [3]National Renewable Energy Laboratory; [4]University of Kentucky; [5]Emory University; [6]University of Colorado Boulder; [7]Stanford University

SPECS' mission is to understand the factors controlling charge and matter transport processes that underpin emerging energy conversion (i.e. catalysis) and energy storage technologies at conductive polymer/electrolyte interfaces across spatiotemporal scales to guide durable soft material development and optimization.

G-O-4: Understanding & Controlling Accelerated and Gradual Evolution of Materials for Energy

[EFRC - UNCAGE-ME] Ryan Lively[1] (Director), Jonas Baltrusaitis[2], Coray Colina[3], David Dixon[4], David Flaherty[1], K. Leslie Gilliard-AbdulAziz[5], Christopher Jones[1], Matthew McDowell[1], Sankar Nair[1], Tina Nenoff[6], Eranda Nikolla[7], Rampi Ramprasasd[1], Srinivas Rangarajan[2], Jessica Rimsza[6], Janani Sampath[3], David Sholl[8], Israel Wachs[2], Krista Walton[1], Juliane Weber[8], Zili Wu[8]
[1]Georgia Institute of Technology; [2]Lehigh University; [3]University of Florida; [4]University of Alabama; [5]University of Southern California; [6]Sandia National Laboratories; [7]University of Michigan; [8]Oak Ridge National Laboratory

To develop a deep knowledge base in the characterization, prediction, and control of materials evolution in the presence of realistic contaminants, processes, and mixtures to accelerate materials discovery for sustainable production and utilization of H_2 and CO_2.

H. Microelectronics

H-O-1: Three Dimensional Ferroelectric Microelectronics Manufacturing

[EFRC - 3DFeM2] Susan Trolier-McKinstry[1] (Director), Vijaykrishnan Narayanan[1], Elizabeth Dickey[2], Betul Akkopru-Akgun[1], Suman Datta[3], Lauren Garten[3], Venkatraman Gopalan[1], M. David Henry[4], Patrick Hopkins[5], Jon Ihlefeld[5], Thomas N. Jackson[1], Sergei Kalinin[6], Kyle Kelley[7], Asif Khan[3], A. Gilad Kusne[8], Ying Liu[1], Jon-Paul Maria[1], Kai Ni[9], Darren Pagan[1], Andrew Rappe[10], Clive Randall[1], Ichiro Takeuchi[8], Adri van Duin[1], Rama Vasudevan[7], Judith Yang[11]
[1]The Pennsylvania State University; [2]Carnegie Mellon University; [3]Georgia Institute of Technology; [4]Sandia National Laboratories; [5]University of Virginia; [6]University of Tennessee-Knoxville; [7]Oak Ridge National Laboratory; [8]University of Maryland; [9]The University of Notre Dame; [10]University of Pennsylvania; [11]Brookhaven National Laboratory

The 3DFeM2 mission is to integrate ferroelectric films at the required scale and reliability for 3D memory using next-generation manufacturing practices. We will implement digitalized processing instruments to generate large data sets, use physics-based ML to reduce experimental dimensionality, identify descriptors that can be monitored to assess properties in real time, establish autonomous experiments to expedite optimization, and develop digital twins that multiply predictive power.

H-O-2: A Holistic Approach to High-Precision Patterning Science

[EFRC - CHiPPS] Ricardo Ruiz[1] (Director), Bruno La Fontaine[1], Brett Helms[1], Christopher Ober[2], Stacey Bent[3], Rachel Segalman[4], Paul Nealey[5], Frances Houle[1], Samuel Blau[1], Oleg Kostko[1], Dahyun Oh[6], Cheng Wang[1], Weilun Chao[1]
[1]Lawrence Berkeley National Laboratory (lead institution); [2]Cornell University; [3]Stanford University; [4]University of California, Santa Barbara; [5]Argonne National Laboratory; [6]San Jose State University

The mission of CHiPPS is to create fundamental understanding and control of materials and processes for atomic precision, energy-efficient, large-area patterning, thereby enabling at-scale advanced manufacturing of future-generation electronics such as quantum computing, spin-based memory and logic devices.

H-O-3: Center for Hybrid Organic Inorganic Semiconductors for Energy

[EFRC - CHOISE] Matthew C. Beard[1] (Director), Joseph J. Berry[1,2], Jeffrey L. Blackburn[1], Volker Blum[3], Jinsong Huang[4], Joseph M. Luther[1], Seth Marder[2], David B. Mitzi[3], Yuan Ping[5], Peter Sercel[6], Adrienne Stiff-Roberts[3], Dali Sun[7], Michael F. Toney[2], Z. Valy Vardeny[8], Yanfa Yan[9], Yong Yan[10], Kai Zhu[1]

[1]National Renewable Energy Laboratory (lead institution); [2]University of Colorado Boulder; [3]Duke University; [4]University of North Carolina at Chapel Hill; [5]University of Wisconsin-Madison; [6]Center for Hybrid Organic Inorganic Semiconductors for Energy; [7]North Carolina State University; [8]University of Utah; [9]University of Toledo; [10]San Diego State University

Demonstrate unprecedented control over spin, charge, phonon and light properties through synthesis and characterization of crystalline Hybrid Organic Inorganic Semiconductors.

H-O-4: Center for Energy Efficient Magnonics (CEEMag)

[EFRC - CEEMag] Yuri Suzuki[1,2] (Director), Ramesh Budhani[3], Georgi Dakovski[1], Michael Flatté[4], Gregory Fuchs[5], Matthias Hoffmann[1], Harold Hwang[1,2], Roland Kawakami[6], Pedram Khalili[7], Wei-Sheng Lee[1], Elaine Li[8], Alexander Reid[1], Dan Ralph[5], Durga Paudyal[4], Clare Yu[9]

[1]SLAC National Accelerator Laboratory; [2]Stanford University; [3]Morgan State University; [4]University of Iowa; [5] Cornell University; [6]The Ohio State University; [7]Northwestern University; [8]University of Texas at Austin; [9]University of California, Irvine

The scientific mission of the "Center for Energy Efficient Magnonics" EFRC is to advance the basic scientific understanding of magnon excitation, propagation, transduction, and control that is motivated by an end use of magnon-based interconnects and their integration into microelectronics.

H-O-5: QuestC: Hierarchical, Scalable Green's Function Modeling of Chemistry at Interfaces

[CCS - QuestC] Mark van Schilfgaarde[1], Swagata Acharya[1], Dimitar Pashov[2]

[1]National Renewable Energy Laboratory; [2]King's College London

This project has three overall aims: first, it will adapt Questaal to the chemistry environment. Questaal is a Green's function based electronic structure method with a self-consistent low-order diagrammatic theory at its core, called the Quasiparticle Self-Consistent GW approximation. Second, it will build on recent new developments to significantly advance our ability to address complex chemical processes with high fidelity. It is hoped that the new advances will enable it to approximate the fidelity of the best quantum chemical approaches while scaling much better with system size, and also providing a natural route to make response functions. Finally it will apply the enhanced theory to two-dimensional excitonic systems, and photoexcitations in nanoscale particles used in catalysis.

H-O-6: Quantum Materials for Energy Efficient Neuromorphic Computing (Q-MEEN-C)

[EFRC - Q-MEEN-C] Alex Frano[1], Andrew D. Kent[2], Axel Hoffmann[3], Duygu Kuzum[1], Eric E. Fullerton[1], Giulia Galli[4], Ivan K. Schuller[1] (Director), Jonathan A. Schuller[5], Julie Grollier[6], Katie Schuman[7], Marcelo J. Rozenberg[1], Oleg G. Shpyrko[1], Robert C. Dynes[1], Shriram Ramanathan[8], Yayoi Takamura[9], Yimei Zhu[10]

[1]University of California, San Diego (lead institution); [2]New York University; [3]University of Illinois Urbana-Champaign; [4]The University of Chicago; [5]University of California, Santa Barbara; [6]Université Paris-Saclay, CNRS Laboratoire de Physique des Solides; [7]University of Tennessee-Knoxville; [8]Rutgers University; [9] University of California, Davis; [10]Brookhaven National Laboratory

To lay down the quantum-materials-based foundation for the development of an energy-efficient, fault-tolerant computer that is inspired and works like a brain ("neuromorphic").

Energy-efficient neuromorphic computing offers a potentially disruptive technological capability to process complex inputs and produce elegantly simple, useful outputs. The breakaway from the conventional technology Turing-von Neumann paradigm requires the development of new types of bio-inspired ("neuromorphic") devices with functionalities like artificial synapses, neurons, axons, and dendrites that can be used to construct machines with artificial intelligence capabilities. We aim to address these critical issues on two different platforms based on Charge- and Spin-related phenomena in quantum materials.

Technical Implementation: The Charge-based approach relies mainly on nanostructured quantum materials, which exhibit spectacular, unexpected changes in their electrical properties when subject to temperature, electric, and magnetic fields, strains, and light. Essential components of neuromorphic information processors will include artificial neurons, synapses, axons, and dendrites to mimic biological entities for transmission and processing of signals. These types of components will be realized in simple transition metal oxides or complex strongly correlated oxides, which exhibit metal-insulator transitions (MIT). In this fashion, we will aim to emulate typical neuronal activities, such as leaky-integrate-fire behavior, symmetric and asymmetric synaptic plasticity, and self-sustained oscillations. Eventually, several of these will be incorporated into complex circuits and architecture. Specific goals of these part of the EFRC are:

Identifying material platforms that can be controlled by non-thermal means such as electric fields, currents, strain, and light, Understanding ionic transport under highly non-equilibrium conditions, and Determining the ultimate limitations of MIT in these materials platforms.

The Spin-based approach relies on the implementation of neurons and synapses using heterostructured spin-torque oscillators, which utilize quantum-materials-based phenomena such as spin-orbit scattering. Neurons are emulated with magnetic oscillators, and the coupling between these oscillators mimics synapses. A charge current sent through these oscillators is converted into a spin current that can drive magnetization precession of nanoscale structures in a sustained and coherent way at room temperature. The underlying magnetization dynamics are highly non-linear, and tunable in phase, amplitude and frequency. Therefore, spintronic nano-oscillators can strongly modify their dynamics in response to small incoming signals resulting in outstanding phase locking and mutual synchronization properties. This is key for neural networks, where neurons should respond to external inputs, but also to signals coming from other neurons through synapses. Specific goals of these part of the EFRC are: 1) Design materials for efficient operation of oscillators, 2) Develop approaches that are best suited for reconfigurable coupling between oscillators and 3) Engineer large-scale oscillator networks that generate complex dynamics.

The scientific thrusts will be interconnected with cross-cutting methods spanning novel materials design, state-of-the-art characterization, and modern theory and computation.

H-O-7: Reconfigurable Electronic Materials Inspired by Nonlinear Neuron Dynamics (reMIND)

[EFRC - reMIND] R. Stanley Williams[1], Sarbajit Banerjee[1], Andrew J. Ferguson[2], Raymundo Arróyave[1], Perla B. Balbuena[1], Marcetta Y. Darensbourg[1], Kim R. Dunbar[1], Matt Pharr[1], Xiaofeng Qian[1], Patrick J. Shamberger[1], Jeffrey L. Blackburn[2], Katherine L. Jungjohann[2], Lance M. Wheeler[2], Suhas Kumar[3], A. Alec Talin[3], Jinghua Guo[4], Eli Rotenberg[4]

[1]Texas A&M University–Texas A&M Engineering Experiment Station (lead institution); [2]National Renewable Energy Laboratory; [3]Sandia National Laboratories, Livermore; [4]Lawrence Berkeley National Laboratory

reMIND's mission is to establish foundational scientific knowledge underpinning the function of reconfigurable materials, devices, and computing architectures that approach fundamental limits of energy efficiency and speed to enable emulation of specific neuronal and synaptic functions of the human brain.

H-O-8: A Center for Power Electronics Materials and Manufacturing Exploration (APEX)

[EFRC - APEX] Nancy M. Haegel[1] (Director), Michael Spencer[2], Kirstin Alberi[1], MVS Chandrashekhar[2], Patrick Hopkins[3], Stephan Lany[1], Jacob Leach[4], Jessica McChesney[5], Tyrel M. McQueen[6], John Simon[1], Heather Splawn[4], Steven Spurgeon[1], Vladan Stevanovic[7], M. Brooks Tellekamp[1], Andriy Zakutayev[1]

[1]National Renewable Energy Laboratory; [2]Morgan State University; [3]University of Virginia; [4]Kyma Technologies; [5]Argonne National Laboratory; [6]Johns Hopkins University; [7]Colorado School of Mines

APEX will enable a wider selection of materials and manufacturing methods built for speed and scale for next-generation power electronics. APEX seeks to understand chemical, physical, thermal, and electrical behavior and requirements at dissimilar interfaces. We are motivated by a co-design vision for "A on B," encompassing a range of materials and interfaces for power electronics—e.g., active layer on substrate, contact on active layer, dielectric on active layer, or device on heat sink.

H-O-9: Manipulation of Atomic Ordering for Manufacturing Semiconductors (μ-Atoms)

[EFRC - μ-ATOMS] Shui-Qing Yu[1] (Director), Jin Hu[1], Greg Salamo[1], Hugh Churchill[1], Hiro Nakamura[1], Tianshu Li[2], Jifeng Liu[3], Yong-Hang Zhang[4], Dragica Vasileska[4], Paul McIntyre[5], Andrew Minor[6], Damien West[7], Yuping Zeng[8], Ezra Bussmann[9], Tzu-Ming Lu[9], Shashank Misra[9], Michael Lilly[9], Mansour Mortazavi[10]

[1]University of Arkansas (lead institution); [2]George Washington University; [3]Dartmouth College; [4]Arizona State University; [5]Stanford University; [6]University of California, Berkeley; [7]Rensselaer Polytechnic Institute; [8]University of Delaware; [9]Sandia National Laboratories; [10]University of Arkansas at Pine Bluff

The overarching goal of the Manipulation of Atomic Ordering for Manufacturing Semiconductors (μ-ATOMS) Energy Frontier Research Center is to discover the underlying science principles determining the ordering of atoms in semiconductor alloys, enabling a breakthrough in synthesis for semiconductor properties and structures.

H-O-10: Ultra Materials for a Resilient, Smart Electricity Grid (ULTRA)

[EFRC – ULTRA] Robert Nemanich[1] (Director), Stephen Goodnick[1], Arunima Singh[1], David Smith[1], Fernando Ponce[1], Marco Saraniti[1], Houqiang Fu[1], Nidhin Kurian Kalarickal[1], Yuji Zhao[2], Martin Kuball[3], Grace Xing[4], Debdeep Jena[4], Timothy Grotjohn[5], Alexander Balandin[6], Richard Wilson[7], Jack Flicker[8], Robert Kaplar[8], Srabanti Chowdhury[9], Mary Ellen Zvanut[10], Michael Spencer[11], Hongping Zhao[1]

[1]Arizona State University; [2]Rice University; [3]University of Bristol; [4]Cornell University; [5]Michigan State University; [6]University of California, Los Angeles; [7]University of California, Riverside; [8]Sandia National Laboratories; [9]Standford University; [10]University of Alabama at Birmingham; [11]Morgan State University; [12]The Ohio State University

The mission of the Ultra Materials for a Resilient, Smart Electricity Grid (Ultra EFRC) is to understand fundamental phenomena in ultra-wide band gap (UWBG) materials – including synthesis, defect and impurity incorporation, electronic structure at interfaces, the interaction of electrons and phonons at high fields to achieve extreme electrical properties, and phonon phenomena that affect thermal transport. We will establish a Future Grid Co-Design Ecosystem enabling communication across all levels of the science and technology.

The need for higher power and higher switching frequency electronics is apparent as we move towards an electrified economy and more energy efficient interconnected society. The knowledge gained by the Ultra EFRC will provide the necessary scientific basis and a co-design ecosystem for a new power electronics economy with ultra high voltage and current capabilities, high frequency switching for highly efficient energy conversion, and efficient thermal transport. Together these advances will enable substantial downscaling in the size of energy conversion systems.

I. Nuclear

I-O-1: Center for Thermal Energy Transport under Irradiation

[EFRC - TETI] David H. Hurley[1] (Director), Marat Khafizov[2], Chris Marianetti[3], Miaomiao Jin[4], Amey Khanolkar[1], Michael Manley[5], James M. Mann[6], Farida Selim[7], Yongfeng Zhang[8], Elizabeth Sooby[9], Brelon May[1], Kaustubh Bawane[1], Linu Malakkal[1], Shuxiang Zhou[1], Zilong Hua[1], Chao Jiang[1], Boopathy Kombaiah[1], Krzysztof Gofryk[1]

[1]Idaho National Laboratory (lead institution); [2]The Ohio State University; [3]Columbia University; [4]The Pennsylvania State University; [5]Oak Ridge National Laboratory; [6]Air Force Research Laboratory; [7]Arizona State University; [8]University of Wisconsin-Madison; [9]University of Texas at San Antonio

To provide the foundational work necessary to accurately model and ultimately control electron- and phonon-mediated thermal transport in 5f-electron materials in extreme irradiation environments.

I-O-2: Fundamental Understanding of Transport Under Reactor Extremes

[EFRC - FUTURE] Blas Uberuaga[1] (Director), Mark Asta[2], Laurent Capolungo[1], Edward Holby[1], Peter Hosemann[2], Djamel Kaoumi[3], Tiffany Kaspar[4], Aaron Kohnert[1], Nan Li[1], Andy Minor[2], Raluca Scarlat[2], Dan Schreiber[4], John Scully[5], Farida Selim[6], Elizabeth Sooby[7], Sandra Taylor[4], Yongqiang Wang[1], Kayla Yano[4]

[1]Los Alamos National Laboratory (lead institution); [2]University of California, Berkeley; [3]North Carolina State University; [4]Pacific Northwest National Laboratory; [5]University of Virginia; [6]Arizona State University; [7]University of Texas at San Antonio

To understand how the coupled extremes of irradiation and corrosion work in concert to modify the evolution of materials by coupling experiments and modeling that target fundamental mechanisms.

I-O-3: Molten Salts in Extreme Environments

[EFRC - MSEE] James Wishart[1] (Director), Simerjeet Gill[1], Benjamin Ocko[1], Anatoly Frenkel[1,2], Yu-chen Karen Chen-Wiegart[1,2], Shannon Mahurin[3], Alex Ivanov[3], Vyacheslav Bryantsev[3], Santanu Roy[3], Sheng Dai[3,4], Claudio Margulis[5], Ruchi Gakhar[6], Gregory Holmbeck[6], Kaustubh Bawane[6], Jacy Conrad[6], Jay LaVerne[7], Edward Maginn[7], Adrien Couet[8], Katusyo Thornton[9]

[1]Brookhaven National Laboratory (lead institution); [2]Stony Brook University; [3]Oak Ridge National Laboratory; [4]University of Tennessee-Knoxville; [5]The University of Iowa; [6]Idaho National Laboratory; [7]University of Notre Dame; [8]The University of Wisconsin-Madison; [9]The University of Michigan

MSEE's mission is to provide fundamental and predictive understanding of molten salt bulk and interfacial chemistry that will establish robust principles to guide the technologies needed to deploy molten salt nuclear reactors.

I-O-4: Ion Dynamics in Radioactive Environments and Materials

[EFRC - IDREAM] Carolyn Pearce[1] (Director), Jaehun Chun[1], James De Yoreo[1], Gregory Kimmel[1], Kevin Rosso[1], Gregory Schenter[1], Michael Spradling[1], Zheming Wang[1], Xin Zhang[1], Linda Young[2], Thomas Orlando[3], Lynn Francesconi[4], Lawrence Anovitz[5], Jay LaVerne[6], Aurora Clark[7], Xiaosong Li[8]

[1]Pacific Northwest National Laboratory (lead institution); [2]Argonne National Laboratory; [3]Georgia Institute of Technology; [4]Hunter College of the City University of New York; [5]Oak Ridge National Laboratory; [6]University of Notre Dame; [7]University of Utah; [8]University of Washington

The scientific mission of the Ion Dynamics in Radioactive Environments and Materials (IDREAM) Energy Frontier Research Center (EFRC) is to master the cascade of radiation chemistry that drives far from equilibrium speciation and reactivity in chemically complex environments, linking attosecond timescales to decadal processes.

J. Quantum Information Science

J-O-1: Center for the Advancement of Topological Semimetals

[EFRC - CATS] Rob McQueeney[1] (Director), Benjamin Ueland[1], Adam Kaminski[1], Paul Canfield[1], Linlin Wang[1], Anand Bhattacharya[2], Ivar Martin[2], Ross McDonald[3], Johanna Palmstrom[3], Ashvin Vishwanath[4], Suyang Xu[4], Pablo Jarillo-Herrero[5], Joe Checkelsky[5], Qiong Ma[6], Susanne Stemmer[7], Thomas Searles[8], Anton Burkov[9]

[1]Ames National Laboratory (lead institution); [2]Argonne National Laboratory; [3]Los Alamos National Laboratory; [4]Harvard University; [5]Massachusetts Institute of Technology; [6]Boston

College; [7]University of California, Santa Barbara; [8]University of Illinois Chicago; [9]University of Waterloo

The mission of the Center for the Advancement of Topological Semimetals (CATS) is to transform how we discover, understand, and harness new topological states of matter through a highly collaborative fundamental research program.

J-O-2: Center for Molecular Magnetic Quantum Materials

[EFRC - M2QM] George Christou[1] (Director), Garnet Chan[2], Hai-Ping Cheng[3], Arthur Hebard[1], Richard Hennig[1], Stephen Hill[4], Chunjing Jia[1], Mark Pederson[5], Michael Shatruk[4], Neil Sullivan[1], Sameul Trickey[1], Vivien Zapf[6], Xiaoguang Zhang[1], Xiao-Xiao Zhang[1]
[1]University of Florida (lead institution); [2]California Institute of Technology; [3]Northeastern University; [4]Florida State University; [5]University of Texas at El Paso; [6]Los Alamos National Laboratory

Our mission is to deepen the understanding of critical materials physics and chemistry to the point of making useful quantum materials from molecular magnets. The driving objective is to design and perfect the underlying materials science essential for future computers and electronics.

J-O-3: Midwest Center for Computational Materials

[CMS - MICCoM] Giulia Galli[1,2], Juan de Pablo[3], Maria K. Chan[1], Andrew Ferguson[2], Joseph Heremans[1], Marco Govoni[4], Jie Xu[1], Victor Yu[1], Jonathan Whitmer[5]
[1]Argonne National Laboratory; [2]University of Chicago; [3]New York University; [4]Univerista' di Modena e Reggio Emilia; [5]Notre Dame University

The Midwest Integrated Center for Computational Materials (MICCoM) develops and disseminates interoperable computational tools - open source software, data, simulation templates, and validation procedures - that enable simulations and predictions of properties of materials for low-power electronics and for quantum technologies. The distinctive features of the center are:

-- Development of interoperable codes for simulation of materials at multiple length and time scales
-- Focus on heterogeneous materials, inclusive of defects, interfaces, and building blocks
-- Focus on spectroscopic and coherence properties

J-O-4: Center for Computational Study of Excited-State Phenomena in Energy Materials

[CMS - C2SEPEM] Steven G. Louie[1,2] (Director), James R. Chelikowsky[3], Jack R. Deslippe[1], Naomi Ginsberg[1,2], Felipe H. da Jornada[4], Zhenglu Li[5], Jeffrey B. Neaton[1,2], Diana Y. Qiu[6], Feng Wang[1,2], Chao Yang[1]

[1]Lawrence Berkeley National Laboratory (lead institution); [2]University of California, Berkeley; [3]University of Texas at Austin; [4]Stanford University; [5]University of Southern California; [6]Yale University

The center C2SEPEM develops new theories, methods, algorithms, and community codes to explain and predict excited-state phenomena in materials. The research focuses on first-principles quantum many-body perturbation theory and advanced algorithms for equilibrium and non-equilibrium processes, as well as their experimental validation, to enable understanding of a range of phenomena for optoelectronic and energy applications.

J-O-5: Center for Molecular Quantum Transduction

[EFRC - CMQT] Michael Wasielewski[1] (Director), Mark Hersam[1], Matthew Krzyaniak[1], George Schatz[1], Nathaniel Stern[1], Roel Tempelaar[1], Michael Flatté[2], Danna Freedman[3], Gregory Fuchs[4], Randall Goldsmith[5], Ezekiel Johnston-Halperin[6], Nathalie de Leon[7], Jeffrey Long[8], Xuedan Ma[9], Peter Maurer[10], Joel Yuen-Zhou[11]

[1]Northwestern University; [2]University of Iowa; [3]Massachusetts Institute of Technology; [4]Cornell University; [5]University of Wisconsin-Madison; [6]The Ohio State University; [7]Princeton University; [8]University of California, Berkeley; [9]Rice University; [10]University of Chicago; [11]University of California, San Diego

The mission of CMQT is to develop the fundamental scientific understanding needed to conduct quantum-to-quantum transduction - the coherent exchange of information between quantum systems - through a bottom-up synthetic approach that imparts atomistic precision to quantum systems.

J-O-6: Programmable Quantum Materials

[EFRC - Pro-QM] Dmitri Basov[1] (Director), Ana Asenjo- Garcia[1], Valentina Bisogni[2], Jiun-Haw Chu[3], David Cobden[3], Cory Dean[1], Milan Delor[1], James Hone[1], Michael Lipson[1], Mengkun Liu[2], James Mclver[1], Andrew Millis[1], Abhay Pasupathy[1,2], Raquel Quieroz[1], Xavier Roy[1], James Schuck[1], Alexandra Velian[3], Di Xiao[3], Xiadong Xu[3], Matthew Yankowitz[3], Xiaoyang Zhu[1]

[1]Columbia University; [2]Brookhaven National Laboratory; [3]University of Washington

To discover, characterize and deploy new forms of quantum matter controllable by light, gating, magnetic proximity electromagnetic environment, and nano-mechanical manipulation, effectively programming their quantum properties.

J-O-7: Quantum Photonic Integrated Design Center

[EFRC - QuPIDC] Libai Huang[1] (Director), Alexandra Boltasseva[1], Hadiseh Alaeian[1], Sophia Economou[2], Jonathan Hood[1], Han Htoon[3], Alisa Javadi[4], Sabre Kais[5], Tongcang Li[1], Teri Odom[6], Jiwoong Park[7], Matthew Pelton[8], Vladimir Shalaev[1], Sergei Tretiak[3], Jelena Vuckovic[9], Valentin Walther[1]

[1]Purdue University (lead institution); [2]Virginia Polytechnic Institute and State University; [3]Los Alamos National Lab; [4]University of Oklahoma; [5]North Carolina State University; [6]Northwestern University; [7]University of Chicago; [8]University of Maryland Baltimore County; [9]Stanford University

QuPIDC's Mission

To discover, design, and realize robust many-body entangled photon and matter states through multi-scale co-designing strategies in heterogeneous solid-state photonic systems.

J-O-8: Quantum Sensing and Quantum Materials (QSQM)

[EFRC - QSQM] Peter Abbamonte[1] (Director), Tai-Chang Chiang[1], Benjamin Feldman[2], Philip Phillips[1], Zhi-Xun Shen[2]

[1]University of Illinois Urbana-Champaign (lead institution); [2]SLAC National Accelerator Laboratory

The mission of this final phase of QSQM is to employ advanced scattering and scanning probe spectroscopy techniques to measure fundamental charge excitations in cutting-edge quantum materials – including strange metals, charge density wave systems, and interacting topological phases – with a focus on quantifying quantum entanglement and information density. Our goal is to visualize and characterize fractionalized excitations, as well as to quantify wave function geometry and entanglement, thereby supporting and informing advanced theoretical frameworks of superconductivity and topology in strongly correlated electron systems. Here, we highlight some recent critical results, on conformal invariance in strange metals, edge states in fractional Chern insulators, and other topics.

J-O-9: Numerically-Exact Relativistic Many-Body Electronic Structure Theory

[CCS - NEREST] Edward Valeev[1], Robert Harrison[2], Deborah Penchoff[3]
[1]Virginia Polytechnic Institute and State University; [2]Stony Brook University; [3]University of Central Florida

CCS Center "Numerically-Exact Relativistic many-body Electronic Structure Theory" (NEREST) innovates novel numerical representations for simulating the many-body electronic structure with rigorous control of the numerical errors necessary for predictive description of structures, energetics, and spectra of heavy-element compounds.

L. AI/ML

L-O-1: Navigating the Design Space of Heterostructures: Advancing Functionality of Modeling for Two-Dimensional Materials and Transition Metal Oxides

[CMS - HeteroFAM] Eric J. Bylaska[1], Nicholas Bauman[1], Ting Cao[2], Niranjan Govind[1], Juan Carlos Idrobo[1,2], Jenna Pope[1], Peter Sushko[1], Di Xiao[1,2]
[1]Pacific Northwest National Laboratory; [2]University of Washington

This project aims to revolutionize materials design by developing computational tools that facilitate exploration of the extensive design space of heterostructures comprising two-dimensional materials and transition metal oxides. We develop new computational material science tools for Exascale computing, building on the advances in plane-wave density functional theory, many-body coupled cluster methods, and machine learning, and integrating them with web applications and materials databases. By enabling efficient exploration of the materials design space, this project will open new avenues for the development of next-generation information processing and energy technologies.

L-O-2: Accelerating the discovery and design of advanced functional materials using AI/ML and exascale computing

[CMS - MLAMD] Cai-Zhuang Wang[1], Ying Wai Li[2], Feng Zhang[1], Yongxin Yao[1], Vladimir Antropov[1], Ryan Richard[1], Zhuo Ye[1], Weiyi Xia[1], Maxim Moraru[2]
[1]Ames National Laboratory; [2]Los Alamos National Laboratory

The center MLAMD develops open-source materials simulation codes and workflows that are Machine Learning (ML) integrated and mid to exascale computing capable to enable efficient prediction of new materials and related synthesis pathways and substantially Accelerate the pace of Materials Discovery (AMD). The research focuses on discovery of novel magnetic and superconducting materials for energy applications.

L-O-3: Multiscale Computational Framework for Biomolecular Energy Transduction: From Electrons to the Mesoscale

[CCS - CMSET] Gregory Voth[1] (Director), Garnet K. L. Chan[2], Tamara Bidone[3], Andrew Ferguson[1]
[1]University of Chicago (lead institution); [2]California Institute of Technology; [3]University of Utah

The Center for Multiscale Simulation of Energy Transduction (CMSET) aims to accurately model biomolecular energy transduction across multiple scales in complex environments.

M. Research at the Exascale

M-O-1: Exascale Multireference Wave Function Theory Method for Transition Metal Catalysis

[CCS - ExaPUC] Laura Gagliardi[1], Cong Liu[2], Christopher Knight[2], Matthew Hermes[1]
[1]University of Chicago; [2]Argonne National Laboratory

The overarching goal of this program is to implement advanced multireference (MR) wave function theory (WFT) methods, starting from the localized active-space self-consistent field (LASSCF) method, into exascale computing infrastructure that will dramatically improve the fidelity and efficiency of predicting extended transition metal (TM) systems with strong MR character (i.e., strong non-dynamical electron correlation due to near-degenerate electronic states). Such development will enable accurate computational predictions (spin configuration, reaction pathway energetics) of multimetallic TM catalysts for reactions such as C-H activation and C-C bond formation that are critical for hydrocarbon cracking, reforming, and upgrading of abundant U.S. shale gas and polymer wastes.

M-O-2: COMMS: Computational Mesoscale Materials Science

[CMS - COMMS] Long-Qing Chen[1] (Director), Ismaila Dabo[2], Eugene. A. Eliseev[3], Venkat Gopalan[1], Wenrui Hao[1], Jiamian Hu[4], Anna. N. Morozovska[3]
[1]The Pennsylvania State University; [2]Carnegie-Mellon University; [3]Ukraine Academy of Sciences; [4]University of Wisconsin-Madison

COMMS advances the basic mesoscale science of quantum and functional materials and develops open-source software for simulating the formation and responses of mesostructures in these materials to external stimuli towards accelerating their insertion into devices.

M-O-3: EPW - Toward Exascale Computing of Electron-Phonon Couplings for Finite-Temperature Materials Design

[CMS - EPW] Feliciano Giustino[1] (Director), Roxana Margine[2], Emmanouil Kioupakis[3]
[1]University of Texas at Austin; [2]Binghamton University; [3]University of Michigan

We develop advanced methods and scalable open-source software for accurate, efficient, and reproducible ab initio calculations of electron-phonon interactions, enabling predictive materials design for semiconductors and quantum technologies. Building on foundational work in many-body physics, phonon-assisted quantum processes, and transport phenomena, our project pushes the frontiers of first-principles calculations of advanced materials properties, including in the areas of topological quantum matter, high-power electronics, and neuromorphic computing. By optimizing the EPW code for leadership-class supercomputers and by refactoring this code for performance portability on GPU-based DOE Exascale systems, we are accelerating the discovery of next-generation semiconductors and quantum materials through cutting-edge theory, algorithms, and software.

M-O-4: Ab-initio Density-matrix Exascale-Parallelized Dynamics and Transport for Selectivity (ADEPTs)

[CCS - ADEPTs] Yuan Ping[1] (Director), Ravishankar Sundararaman[2]

[1]University of Wisconsin-Madison (lead institution); [2]Rensselaer Polytechnic Institute

Ab-initio Density-matrix Exascale-Parallelized Transport for Spin-Selectivity (ADEPTS) is a DOE Computational Chemical Sciences center, aiming at developing first-principles quantum dynamics and transport softwares with exascale computing capabilities and a focus on spin-related phenomena in solids.

M-O-5: Center for Predictive Simulations of Functional Materials

[CMS - CPSFM] P. Kent[1], R. Clay[2], P. Doak[1], P. Ganesh[1], J. Krogel[1], Y. Luo[3], C. Melton[2], L. Mitas[4], B. Rubenstein[5], K. Saritas[1], H. Shin[3]

[1]Oak Ridge National Laboratory; [2]Sandia National Laboratories; [3]Argonne National Laboratory; [4]North Carolina State University; [5]Brown University

The Center for Predictive Simulation of Functional Materials develops, applies, validates, and distributes external-parameter-free methods and open-source codes to accurately predict and understand the properties of functional and quantum materials. These materials have strong electronic correlations, van der Waals interactions, and spin-orbit interactions, which challenges conventional methods such as density functional theory. The Center develops the highly accurate Quantum Monte Carlo techniques and the open source QMCPACK code, and related datasets and workflows to achieve these goals. The latest release of QMCPACK runs performantly at exascale on GPUs from AMD, Intel, and NVIDIA, from a common codebase. Besides direct application to the prediction and understanding of individual materials systems and phenomena, we envisage a growing role for these methods in the computational materials databases that are of critical importance for machine learning and artificial intelligence-based techniques.

M-O-6: Center for MAny-Body Methods, Spectroscopies, and Dynamics for Molecular POLaritonic Systems (MAPOL)

[CCS - MAPOL] Niranjan "Niri" Govind[1] (Director), Jonathan J. Foley, IV[2], Karol Kowalski[1], Xiaosong Li[3]

[1]Pacific Northwest National Laboratory (lead institution); [2]University of North Carolina; [3]University of Washington

Light when nanoconfined in cavities and made to interact strongly with molecules results in hybrid light–matter states or polaritons, which can be used to modify and manipulate ground and excited-state potential energy surfaces and thus alter the reactivity and energy flow profoundly in molecular systems. The development of predictive theories for molecular polaritons requires combining electronic degrees of freedom, as provided by quantum chemistry methods, with quantum electrodynamics (QED) treatments of the photonic degrees of freedom.

Our vision is to develop a suite of theoretical frameworks, spanning low-order to high-level many-body methods, that will provide unprecedented ability to capture the structure and dynamics of molecular polaritonic systems and deliver scalable software source code and libraries that can harness leadership-class computational facilities (LCFs).

Objective 1: Develop a Gaussian basis set–based suite of methods spanning low-order to high-level ab initio many-body approaches for modeling and simulation of molecular polaritonic systems.
Objective 2: Implement polaritonic many-body methods to fully utilize modern heterogeneous (CPU/GPU) high-performance computing platforms at DOE's LCFs.
Objective 3: Apply developed methods to molecular polaritonic systems to validate, benchmark, and assess our developments with reference systems, progressing to advanced applications to complement experiments to enhance fundamental understanding of polaritonic chemistry.

M-O-7: Nonperturbative Studies of Functional Materials Under Nonequilibrium Conditions

[CMS - NPNEQ] Tadashi Ogitsu[1] (Director), Xavier Andrade[1], Alfredo Correa[1], Felipe Jornada[2,3], Aaron Lindenberg[2,3], Liang Tan[4], David Prendergast[4], Jacopo Simoni[5], Yuan Ping[5]

[1]Lawrence Livermore National Laboratory (lead institution); [2]SLAC National Accelerator Laboratory; [3]Stanford University; [4]Lawrence Berkeley National Laboratory; [5]University of Wisconsin-Madison

NPNEQ develops open source software suites, including real-time time-dependent density functional theory, for quantum mechanical time evolution of spins, electrons and ions relevant to a wide range of applications, including switching, memory, and optoelectronic devices, as well as new materials processing methods. The community software supports ab initio, non-perturbative studies far from equilibrium

M-O-8: QMC-HAMM: High accuracy multiscale models from quantum Monte Carlo

[CMS - QMC-HAMM] David Ceperley, Yueqing Chang, Elif Ertekin, Shubhang Goswami, Kevin Kleiner, Kitthithat Krongchon, Harley Johnson, Tawfiqur Rakib, Lucas Wagner
University of Illinois Urbana-Champaign

The QMC-HAMM project is focused on using high accuracy ab initio simulations to develop multiscale models with unprecedented accuracy. Our collaboration focuses on using quantum Monte Carlo. As our project is part of Computational Materials Sciences, we generate software and data products that enable these advances.

Our current focus includes quantum Monte Carlo (QMC) offers a way forward to learn more accurate potential energy surfaces with applications to the phase diagram of hydrogen, graphene-boron nitride, and battery materials, in which we find that the ion pathways computed by DFT are inaccurate. We also develop QMC to address excited states, which allows us to evaluate interacting coarse-grained electronic models, which enable detailed study of many systems, including strongly correlated light-emitting defects.

M-O-9: From Wave Functions to Exchange Correlation for Large-Scale Electronic Structure

[CCS - WFT2XC] Vikram Gavini, Paul Zimmerman
University of Michigan

This CCS project aims to advance wavefunction and density functional theories to reach high-accuracy quantum chemical simulations on large-scale materials systems.

POSTER SESSION I

A. Advanced Manufacturing

A-P1-1: Accelerating the Discovery of Sustainable Thermosets: High Throughput Testing and Data Management

[EFRC - REMAT] Ignacio Arretche[1], Javier Balta[1], Pengfei Cai[2], Pranav Krishnan[1], Tanver Hossain[1], Ramdas Tiwari[1], Qibang Liu[1], Donald Bistri[1], Connor D. Armstrong[1], Michael Zakoworotny[1], Arunachalam T. Kanaksabai[1], Jacob J. Lessard[1], Ben Galewsky[1], Nancy R. Sottos[1], Philippe H. Geubelle[1], Jeffey S. Moore[1], Rafael Gomez-Bombarelli[2], Randy H. Ewoldt[1], Sameh H. Tawfick[1]

[1]University of Illinois Urbana-Champaign; [2]Massachusetts Institute of Technology

A-P1-2: AI Enabled Process Optimization for Injection Molding Using Multi-Fidelity Neural Network

[EFRC - AIM] Dhanashree Shinde[1], Elham Kiyani[2], Chung-Yin Lin[3], Sai Aditya Pradeep[1], George Karniadakis[2], Lih-Sheng Turng[3], Srikanth Pilla[1]

[1]University of Delaware; [2]Brown University; [3]University of Wisconsin-Madison

A-P1-3: AI-Driven Materials Discovery and Analysis: Active Learning for Automated Experiment via Physics-Based Deep Image and Spectrum Segmentation

[EFRC - CSSAS] Kamyar Barakati[1], Mengqi Sun[2], Huat Thart Chiang[2], Kiran Vaddi[2], Aditya Raghavan[1], Mani Valleti[1], Hanson Chen[2], Muammer Yaman[2], Zachary M. Sherman[2], David Ginger[2], Sergei V. Kalinin[1], Lilo Pozzo[2]

[1]University of Tennessee-Knoxville; [2]University of Washington

A-P1-4: Using Chemical Inhibitors to Improve FROMP: From Stable Resins to Predictive Modeling Using Data Science Tools

[EFRC - REMAT] Pranav Krishnan[1], Samantha E. Sloane[2], Po-wen Wang[1], Elli Lu[1], Ren H. Bean[3], Matthew R. Creighton[4], Olivia Lucas[2], Lydia Dawson McDaniel[2], Jeffrey S. Moore[1], Nancy R. Sottos[1], Matthew S. Sigman[2], Leah N. Appelhans[3], Samuel C. Leguizamon[3], Jennifer A. Lewis[4]

[1]University of Illinois Urbana-Champaign; [2]University of Utah; [3]Sandia National Laboratories; [4]Harvard University

A-P1-5: Nozzle-free 3D Printing of Carbon-fiber Reinforced Composites

[EFRC - AIM] Yunxia Chen[1], Chuanshen Zhou[1], Yiwen Wu[1], Elijah C Baluyot[1], Konnor G. Hole[1], Jacob J. Bethke[1], Ali T. Shams[1], Benjamin J. Ryder[1], Gang Li[2], Srikanth Pilla[3], Yong Huang[1]

[1]University of Florida; [2]Clemson University; [3]University of Delaware

A-P1-6: From Force-Field Parameters to Programmable Nanostructures: Integrated Simulation, Active Learning, and Experiment for Peptoid-Based Hierarchical Materials

[EFRC - CSSAS] Alex Berlaga[1], Renyu Zheng[2], Kaylyn Torkelson[2], Xin Qi[2], Christopher D. Lowe[2], Helen Larson[2], Zeqian Zhang[2], Brandi M. Cossairt[2], Jim Pfaendtner[3], Chun-Long Chen[2,4], Andrew L. Ferguson[1]

[1]University of Chicago; [2]University of Washington; [3]North Carolina State University; [4]Pacific Northwest National Laboratory

A-P1-7: Multigenerational Additive Manufacturing of pDCPD Thermosets

[EFRC - REMAT] Edgar B. Mejia[1], Xuyi Luo[2], Hayden E. Fowler[3], Yasmeen S. Alfaraj[4], MJ Lee[1], Yong Min Kim[2], Amanda Rosario[1], Erick Ayala[1], Rohil Bose[1], Niharika Devaraju[1], Zhang Zhang[1], Andrew Lum[1], Ignacio Arretche[1], Mohammad T. Hossain[1], Ramdas Tiwari[1], Julian Cooper[1], Jeffrey S. Moore[1], Randy H. Ewoldt[1], Sameh Tawfick[1], Samuel C. Leguizamon[3], Leah Appelhans[3], Jeff W. Baur[1], Jeremiah A. Johnson[4], Yan Xia[2], Nancy R. Sottos[1]

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B. Catalysis

B-P1-1: Combining Chemistry and Biology to Convert Plastics Waste as a Valuable Feedstock for Manufacturing

[EFRC - CPI] Célestin Bourgery[1], Madan R. Gopal[2], Ali Kamali[2], Pedro Reis Moura[2], Roman M. Dickey[2], Sampanna V. Mhatre[2], Thomas H. Epps III[2], LaShanda T. J. Korley[2], Dionisios G. Vlachos[2], Aditya M. Kunjapur[2], Dongxia Liu[2], Joshua Michener[1]

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B-P1-2: Processive Polyolefin Deconstruction with Ultra-low Methane by a Microporous Catalyst

[EFRC - iCOUP] Frédéric A. Perras[1,2], Chao Meng[1,2], Simin Sun[1,2], Jiankai Ge[3], Shilin Cui[4], Xuchun Wang[5], Minda Chen[6], Jiayi Xu[5], Yi-Yu Wang[1,2], Minghui Niu[1,2], Anne M. LaPointe[4], Cong Liu[5], Byeongdu Lee[5], Geoffrey W. Coates[4], Baron Peters[3], Aaron D. Sadow[1,2], Wenyu Huang[1,2]

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B-P1-3: Transforming the Manufacturing Landscape of Polyurethanes and Polyureas: Depolymerization and Regeneration of Isocyanates

[EFRC - CPI] Sampanna Mhatre, Robert O'Dea, Mridula Nandi, Genevieve Kroll, Jackie Arnold, Yiqiu Qian, Grigorios Tatsis, Zhifei Yuliu, Marianthi Ierapetritou, LaShanda T. J. Korley, and Thomas Epps, III

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B-P1-4: Waste Polymer Functionalization Through Reactive Intermediates

[EFRC - iCOUP] Samuel Hunt[1], Xuchun Wang[1], Allen Román[1], Jenesis Pérez[1], Frédéric Perras[2], Byeongdu Lee[1], Jie Xu[1], Jessica Lamb[1], Maria Vocia[3], Sergio Tosoni[3], Martina Morrello[1], Jeremy Kropf[1], David Kaphan[1], Massimiliano Delferro[1]

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B-P1-5: Reactive Carbon Capture to C_2+ Products: Using Electrogenerated CO_2 Radical Anions for C-C Coupling Reactions

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B-P1-6: Confinement By Design: In Vitro Assembly as an Enabling Technology for Engineered Bacterial Microcompartment Shells

[EFRC - CCBC] Kyleigh L. Range[1,4], Samuel N. Snyder[3], Timothy K. Chiang[4], Nicholas M. Teft[2], Arinita Pramanik[4], Joel F. Landa[2], Yali Wang[2], Nina S. Ponomarenko[3], Xiaobing Zuo[3], Alexander Jussupow[2], Neetu Yadav[1], Michael Feig[2], Josh V. Vermaas[1,2], Eric L. Hegg[2], Lisa M. Utschig[3], Robert P. Hausinger[2], David M. Tiede[3], Michaela A. TerAvest[2], Markus Sutter[1,4], Cheryl A. Kerfeld[1,2,4]

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B-P1-7: Reactivity and Catalysis on Surfaces and Porous Materials

[EFRC - CD4DC] Špela Kunstelj[1], Linh Le[1], Andrea Darù[1], Hilal Daglar[1], Ningxin Jiang[1], Arturo Sauza-de la Vega[1], Mukunda Mandal[1], Haomiao Xie[3], Jan Hofmann[2], Simon M. Vornholt[2], Karena W. Chapman[2], Anna Wuttig[1], Omar Farha[3], John S. Anderson[1], Laura Gagliardi[1]

[1]University of Chicago; [2]Stony Brook University; [3]Northwestern University

B-P1-8: Insights into electrode processes for CO_2 electrolysis in solid oxide cells

[EFRC - UNCAGE-ME] Jina Cho[1], Neelesh Kumar[2], Musa Najimu[3], Kandis Leslie Gilliard-AbdulAziz[3], Israel E Wachs[2], Eranda Nikolla[1]

[1]University of Michigan; [2]Lehigh University; [3]University of Southern California

B-P1-9: Pulsed photochemical CO methanation on Pt: role of dynamic thermal and photochemical influences

[EFRC - CPEC] Silvia Marino, Samji Samira, Ryan Berry, Michael Gordon, Phillip Christopher

University of California, Santa Barbara

B-P1-10: Detecting oxygen evolution reaction intermediates on Titanium Oxide Facets by polarized transient optical spectroscopy

[EFRC - CEDARS] Cassius Boyd[1], David Jonas[1], Shay McBride[2], Sheila Cherono[3], Moritz Lang[1], Luka Mitrovic[4], Jennifer Sormberger[1], Y. Shao-Horn[5], Darrel Schlom[4], Dhananjay Kumar[3], Geoffery Hautier[2], Tanja Cuk[1]

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B-P1-11: Molecular approaches to understanding the mechanism of CO_2 reduction to methanol by CoPc/CNT

[Hub - LiSA] Emile E. DeLuca[1,2], Cheolwoo Park[1,3], Hao Chen[1,3], Mori J. Taylor[1,2], Lydia R. Weddle[1,2], Pooja Basera[1,3], Michal Bajdich[1,3], Amy A. Cordones[1,3], Clifford P. Kubiak[1,2]

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B-P1-12: Evaluation of Partition Functions for Adsorbed Reactive Intermediates and First Order Saddle Points with Multiple Anharmonic Configurations

[CCS - ECC] Kirk D. Badger[1], Branko Ruscic[2], David H. Bross[2], Khachik Sargsyan[3], C. Franklin Goldsmith[1]

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B-P1-13: Connecting encapsulated bacterial microcompartment reactions via intershell electron shuttle mechanisms

[EFRC - CCBC] Samuel Snyder[1], Joel Landa[2], Nicholas Tefft[2], Eric Hegg[2], Markus Sutter[2,3], Karen Mulfort[1], Paul Ashby[3], Michaela TerAvest[2], Lisa Utschig[1]

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B-P1-14: Engineering High-Capacitance Catalytic Condensers and Spectroscopic investigation of the Metal-Dielectric Interface

[EFRC - CPEC] Rachita Rana, Mostapha Dakhchoune, Katelyn Groenhout, Yuriy Roman-Leshkov
Massachusetts Institute of Technology

B-P1-15: Understanding the Effects of Sorbent and Catalyst Speciation for Electrocatalytic Reactive Carbon Capture in Amines

[EFRC - 4C] Jounghwan Choi[1], Avishek Banerjee[1], Shawn Chiu[1], Dominic Ross[2], Yulan Han[1], Ab Mir[3], Piyush Verma[4], Jenna Ynzunza[5], Cocoro Nagasaka[5], Robert Lavroff[1], Zisheng Zhang[1], Ferdawss Ihiri[1], Feven Gebresilassie[3], Hui-Yun Jeong[2], Aditya Prajapati[2], Chantal Stieber[7], Robert Sacci[7], Gabriel Veith[7], Jesús Velázquez[5], Charles McCrory[4], Jenny Yang[3], Christopher Hahn[2], Anastassia Alexandrova[1], Carlos Morales-Guio[1]
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B-P1-16: Probing Surface/Bulk Structural Chemistry of Materials for Solid Oxide Cells with Operando Spectroscopy

[EFRC - UNCAGE-ME] Neelesh Kumara[1], Musa O. Najimu[2], Yoon Jin Cho[3], Kandis Leslie Gilliard-AbdulAziz[2], Eranda Nikolla[3], Zili Wu[4], Israel E. Wachs[1]
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B-P1-17: Alkaline Electrocatalysis for Fuel Cells and Electrolyzers for the New Energy Frontier

[EFRC - CABES] David Muller, Tomas Arias
Cornell University

B-P1-18: Structure Characterization of Bacterial Microcompartments via X-ray Scattering: Measuring Extents of Cargo Capture and Time-Resolved Assembly

[EFRC - CCBC] Adam K. Nijhawan[1], Alex Gao[1], Nina S. Ponomarenko[1], Timothy K. Chiang[2], Kyleigh L. Range[2,3], Yali Wang[3], Robert Hausinger[3], Nicholas Tefft[8], Michaela TerAvest[3], Alex Jussupow[3], Neetu Yadav[3], Josh Vermaas[3], Michael Feig[3], Markus Sutter[2,3], Cheryl A. Kerfeld[2,3], Xiaobing Zuo[1], David M. Tiede[2]
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D. Energy Storage

D-P1-1: Experimental and Theoretical Techniques for Studies of Redox Kinetics in Structured Electrolytes

[EFRC - BEES2] Robert Warburton[1], Zeynep Bagbudar[1], Saransh Gupta[1], Vaishnavi Sree Jeganthan[1], Rohan Akolkar[1], Zeru Syum Hidaru[1], Jesse Wainright[1], Armando Santiago Carboney[2], Peisen Qian[2], Joaquín Rodríguez-López[2], Zulqarnain Arif[3], Thomas Zawodzinski[3]

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D-P1-2: Development and Improvement of a Catalytic Cascade for the Conversion of Carbon Dioxide to Methanol via a Formate Intermediate

[Hub - CHASE] Sergio Fernández[1], Young Hyun Hong[2], Xiaofan Jia[2], Eleanor Stewart-Jones[2], Pablo Fernandez[1], Amanda Arnoff[3], Abhishek Kumar[2], Eric Assaf[1], Shahbaz Ahmad[4], Benjamin Travis[1], Marisé García-Batlle[1], Julia Curley[2], Charlotte Montgomery[1], Justin Wedal[2], Jose Alvarez-Hernandez[2], Albert Gang[2], Noah Gibson[2], Madison Houck[2], Sungho Jeon[3], Jongbeom Kim[3], Hyeongjun Koh[3], Brandon Mercado[2], Hannah Nedzbala[2], Nicole Piekut[2], Christine Quist[2], Yihui Zhang[3], Colton Sheehan[3], Shi He[1], Carrie L. Donley[1], Eric Stach[3], James M. Mayer[2], Jillian Dempsey[1], Thomas Mallouk[3], Mehmed Ertem[4], Alexander Miller[1], Gregory Parsons[5], James Cahoon[1], René Lopez[1], Nilay Hazari[2]

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D-P1-3: Solvation control for reaction control: rethinking the opportunities and challenges of the metal air battery

[Hub - ESRA] Yang Shao-Horn[1], Dan Steingart[2], Chibueze Amanchukwu[3], Rajeev Assary[4], Jordi Cabana[4,5], Ethan Crumlin[6], Neil Dasgupta[7], Betar Gallant[1], Rafael Gómez-Bombarelli[1], Kelsey Hatzell[8], Brett Helms[6], Yiyang Li[7], Chen Liao[4], Di-Jia Liu[4], Lauren Marbella[2], Bryan McCloskey[6], Tod Pascal[9], Wu Xu[10], Y. Shirley Meng[3,4]

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D-P1-4: From Molecular Design to Electrochemical Performance: Exploring Structure-Property Relationships in Deep Eutectic Solvent Electrolytes

[EFRC - BEES2] Desiree Mae Prado[1], Robert Savinell[1], Zeru Hidaru[1], Nicholas Sinclair[1], Dinis Abranches[2], Clemens Burda[1], Edward Maginn[2], Jesse Wainright[1]

[1]Case Western Reserve University; [2]University of Notre Dame

D-P1-5: Methanol Production Via CO Intermediate Mediated by Recyclable Proton/Electron Mediators

[Hub - CHASE] Andressa Müller[1], Hannah Nedzbala[2], Rebecca Powers[3], Irene Barba-Nieto[1], Shahbaz Ahmad[1], Jake Sirlin[3], Dalaney Westbroek[2], Hannah Margavio[4], Hyuenwoo Yang[4], Hyunho Noh[2], Samantha Magpantay[2], Amar Kumbhar[3], Charles Titus[1], Dominik Wierzbicki[1], Cherno Jaye[1], Sai Desai[1], Chiara Cappuccino[1], Annie Knapp[2], Ryan Gentile[3], Pierpaolo Vecchi[3], John Dickenson[3], Kenneth Chua[3], Paul Griffin[3], Carrie Donley[3], Megan Jackson[3], Renato Sampaio[3], José Rodriguez[1], Alexander Miller[3], Gregory Parsons[4], James Mayer[2], James Cahoon[3], Mehmed Ertem[1], Dmitry Polyansky[1], David Grills[1], Gerald Meyer[3], Javier Concepcion[1], Jillian Dempsey[3]

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D-P1-6: Hydro-chemo-mechanical modeling of hydration reactions and the implication on reaction induced cracking

[EFRC - GMCS] Tiansheng Zhang[1], Haiying Huang[1], Emmanuel Detournay[2], Vaughan Voller[2]

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D-P1-7: Effects of Multipolar Interactions on Structures, Dynamics and Dielectric Responses in Polyzwitterion Melts

[EFRC - FaCT] Qinyu Zhu[1], Hongwei Li[2], Autumn Kudlack[2], Jodie L. Lutkenhaus[2], Rajeev Kumar[1]

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D-P1-8: Electronic and Structural Properties of the Polymer–Electrolyte Interphase in Electrochemically Doped Polymers

[EFRC - SPECS] Megan Brown[1], Shuya Li[2], Jonathan Thurston[3], William Kopcha[2], Joel Bombile[1], Sa Suo[4], Bo Dong[4], Zhiting Chen[5], Dennis Norlund[6], Luis Iglesias[3], Collin Sindt[3], Santosh Kumar[7], David Grinter[7], Arianna Magni[8], Obadiah Reid[2,3], Andrew

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D-P1-9: Factors Controlling Activation Barriers for Charge Transport in Single Ion Conducting Polymers

[EFRC - FaCT] Harmandeep Singh[1], Ivan Popov[2], Michelle L. Lehmann[3], Md Anisur Rahman[3], Kenneth S. Schweizer[4], Rajeev Kumar[3], Tomonori Saito[1,3], Alexei P. Sokolov[1,3], Catalin Gainaru[3]

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D-P1-10: Compositionally Complex Spinel Oxides as Conversion Anodes

[EFRC - m2M#s] Ki-Hun Nam[1], Zhongling Wang[2], Jessica Luo[2], Juhyeon Ahn[1], Zachary Mansley[3], Armando Rodriguez-Campos[2], Cynthia Huang[2], Marie Millares[2], Alexis Pace[2], Yimei Zhu[3], Esther Takeuchi[2,3], Amy Marschilok[2,3], Shan Yan[3], Kenneth Takeuchi[2,3], Marca Doeff[1]

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D-P1-11: Advanced Cathodes

[EFRC - MUSIC] Partha Mukherjee[1], Bairav Sabarish[1], Kelsey Hatzell[2], Ana Claus[2], Shae Hagler[3]

[1]Purdue University; [2]Princeton University; [3]University of Michigan

D-P1-12: Coupled fracture mechanics-geochemical model of reaction-driven cracking

[EFRC - GMCS] Rui Feng[1], Pouyan Asem[2], John Rudnicki[1], Emmanuel Detournay[2]

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G. Hydrogen

G-P1-1: Interfacial chemistry and H transfer kinetics in composite heterostructures

[EFRC - HEISs] Paul Chery[1], Elizabeth Griffin[1], Yong-Yun Hsiau[3], Bernadette Cladek[2], Chang-Ti Chou[1], Gabriel T. dos Santos[1], Sara C. Sand[1], Sean Drewry[2], Roberto dos Reis[1], Chris M. Wolverton[1], Katharine Page[2,4], Vinayak P. Dravid[1], Sossina M. Haile[1], Nicola H. Perry[3]

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G-P1-2: Co-design of charge transport superhighways to connect catalytic sites in soft photoelectrochemical systems

[EFRC - SPECS] Zhiting Chen[1], Hong Li[1], Eui Hyun Suh[2], Bo Dong[3], Shuya Li[4], Ann Greenaway[4], Yael Tsarfati[5,6], Alberto Salleo[5, 6], Jean-Luc Bredas[1], Erin Ratcliff[2], Neal Armstrong[1]

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G-P1-3: $ATiO_3$-xHy Perovskite Oxyhydrides: Understanding the Role of Structure and Cation Chemistry with Neutron Scattering

[EFRC - HEISs] Megan Burrill[1], Kennedy Agyekum[2], Bernadette Cladek[2], Danilo Puggioni[1], Luke Daemen[3], Katharine Page[2,3], James Rondinelli[1], Sossina Haile[1]

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G-P1-4: Identifying Efficiency-Limiting Mechanisms in Charge Separation Within a Donor-Acceptor Photoelectrode Across Multiple Time Scales

[EFRC - SPECS] Bo Dong[1], William Kopcha[2], A. Abhisek Mohapatra[3], Eui Hyun Suh[4], Sa Suo[1], Casey Davis[3], Jonathan Thurston[3], Chamikara Karunasena[5], Megan Brown[6], Joshua Carr[2], Ann Greenaway[2], Chad Risko[6], Jean-Luc Bredas[5], Veaceslav Coropceanu[5], Michael Toney[3], Stephen Barlow[2,3], Seth Marder[2,3], Melissa Gish[2], Andrew Ferguson[2], Erin Ratcliff[4], Obadiah Reid[2,3], Tianquan Lian[1]

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G-P1-5: Investigating effect of symmetry and lattice dynamics on hydrogenation and proton migration in ternary oxides

[EFRC - HEISs] Heejung Chung[1], Zhen Jiang[2], Jie Song[2], James Rondinelli[2], Christopher Wolverton[2], Sossina Haile[2], Bilge Yildiz[1]

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H. Microelectronics

H-P1-1: How to characterize “latent images” in EUV resists before development?

[EFRC - CHiPPS] Qi Zhang[1], Kas Andrle[1], Padraic O’Reilly[2], Beihang Yu[1], Weilun Chao[1], Warren Holcomb[1], Areza Sumitro[1], Lauren McQuade[3], Maireyee Bhattachary[4], Sonia Castellanos[4], Ryan Miyakawa[1], Patrick Naulleau[1], Sung Park[2], Bruno La Fontaine[1], Ricardo Ruiz[1], Cheng Wang[1]

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H-P1-2: Dense and Reliable 3D Ferroelectric Capacitor-Based Memory

[EFRC - 3DFeM2] Prasanna Venkat Ravindan[1], Salma M. Soliman[1], Shan Deng[2], Rudra Biswas[3], Vijaykrishnan Narayanan[3], Kai Ni[2], Asif Khan[1]

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H-P1-3: The effect of short range order on electrical and thermal properties in Group IV alloys

[EFRC - µ-ATOMS] Sungjae Hong[1], Manish Sharma[2], Troy Alexander Hutchins-Delgado[1], Siddhant Gangwal[3], Adelaide Maria Bradicich[1], Priyanka Petluru[1], Shui-Qing Yu[2], Michael Lilly[1], Dragica Vasileska[3], Jin Hu[2], Tzu-Ming Lu[1]

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H-P1-4: Electronic Properties of AlGaN/TaC Interfaces for High Power Electronics

[EFRC - APEX] Daniel Harrison[1], Sharad Mahatara[2], Kishak Cinfwat[1], Nancy M. Haegel[2], Stephan Lany[2], M. Brooks Tellekamp[2], Michael Spencer[1], MVS Chandrashekhar[1]

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H-P1-5: Ab Initio Studies of Dopable Extreme-Gap Semiconductors and Phonon-Mediated Nonlinear Optical Processes

[CMS - EPW] Sieun Chae[1,2], Nocona Sanders[1], Kelsey A. Mengle[1]1, Amanda Wang[1], Xiao Zhang[1], Jon Lafuente Bartolome[3,4], Kaifa Luo[3], Yen-Chun Huang[2], Feliciano Giustino[3], John T. Heron[1], Emmanouil Kioupakis[1]

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H-P1-6: Enabling Next-Gen Computing with Wurtzite Ferroelectrics: Synthesis, Defect Control, and Switching Behavior

[EFRC - 3DFeM2] Drew Behrendt[1], Ian Mercer[2], Benjamin Aronson[3], Bogdan Dryzhakov[4], Ece Gunay[5], Sebastian Calderon[5], Betul Akkopru-Akgun[2], Erdem Ozdemir[2], Jack Eckstein[4], Albert Suceava[2], Venkatraman Gopalan[2], Susan Trolier-McKinstry[2], Elizabeth Dickey[5], Kyle Kelley[4], Jon Ihlefeld[3], Jon-Paul Maria[2], Andrew Rappe[1]

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H-P1-7: Electrochemically Stabilized Phase Coexistence for Reconfigurable Processing of Information

[EFRC - reMIND] Sangheon Oh[1], Timothy D. Brown[1], Saul Perez Beltran[2], Hao-En Lai[2], Sean R. Bishop[3], Kyung Seok Woo[1], R. Stanley Williams[2], Elliot J. Fuller[1], Suhas Kumar[1], Perla B. Balbuena[2], A. Alec Talin[1]

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H-P1-8: Stochastic Coupled Neural Networks Implementations and Evaluations

[EFRC - Q-MEEN-C] Seoyoung An[1], George Evans[1], Erbin Qiu[2], Duygu Kuzum[2], Ivan Schuller[2], Catherine Schuman[1]

[1]University of Tennessee; [2]University of California, San Diego

H-P1-9: In situ and operando studies of imaging chemistry in extreme UV photoresist materials

[EFRC - CHiPPS] Frances Houle[1], Oleg Kostko[1], Honggu Im[1], Bernhard Luttgenau[1], Areza Sumitro[1], Jacob Milton[1], Maximillian Mueller[2], Alex Aguilar Oliveros[2], Cuc Ngan Tran[2], Dahyun Oh[2], Caleb Arata[3], Laura McHale[3], Chris Rella[3], John Hoffnagle[3]

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H-P1-10: Materials Selection and Circuit Design for Electro-Thermal Oscillator-Based Neuromorphic Primitives

[EFRC - reMIND] Fatme Jardali[1], Timothy D Brown[2], Jenny L Chong[1], Yeonju Yu[1], Alan Zhang[2], Elena Salagre Rubio[2], Raymundo Arroyave[1], Elliot Fuller[2], Suhas Kumar[2], R. Stanley Williams[1], Patrick J. Shamberger[1]

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H-P1-11: A new material for energy-efficient magnonics

[EFRC - CEEMag] Katya Mikhailova[1,2], Junwei Tong[3], Xiangcheng Liu[3], Shrishti Pal[4], Christopher Parzyck[1], Lerato Takana[2], Herve Carruzo[5], Durga Paudyal[6], Xiaoqin Elaine Li[3], Gregory Fuchs[4], Clare Yu[5], Georgi Dakovski[1], Wei-Sheng Lee[1], Yuri Suzuki[1,2]

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H-P1-12: Photodoped Metal-to-Insulator Switching in Moiré Devices

[EFRC - Pro-QM] Yiliu Li, Esteban Rojas-Gatjens, Yinjie Guo, Birui Yang, Dihao Sun, Luke Holtzman, Cory R. Dean, James C. Hone, Eric A. Arsenault, Xiaoyang Zhu

Columbia University

H-P1-13: Applications of QuestC/Questaal

[CCS - QuestC] Mai-anh Ha[1], Swagata Acharya[1], Dimitar Pashov[2], Mark van Schilfgaarde[1]

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H-P1-14: Chiral excitons and optical activity in hybrid organic-inorganic semiconductors

[EFRC - CHOISE] Peter C. Sercel[1], Matthew P. Hautzinger[2], Alan J. Phillips[2,3], Ruyi Song[4], Md Azimul Haque[2], Liang Yan[5], Yi Xie[6], Qiutong Ge[2], Rebecca A. Scheidt[2], Heshan Hewa Walpitage[7], David B. Mitzi[4], Wei You[5], Valy Vardeny[6], Jeffrey L. Blackburn[2], Volker Blum[4], Matthew C. Beard[2]

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H-P1-15: High Radiation Tolerance Due to Superlattice Structures

[EFRC - TETI] Farida A. Selim[1], Thai hang Chung[1], Ella K. Pek[2], Kevin Vallejo[2], Anshul Kamboj[2], Kaustubh Bawane[2], Amey R. Khanolkar[2], Boopathy Kombiah[2], David Hurley[2]
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I. Nuclear

I-P1-1: Revealing molten salt-induced structural heterogeneity in metal solutes using a multi-modal approach

[EFRC - MSEE] Nirmalendu Patra[1], Alejandro Ramos-Ballesteros[2], Santanu Roy[3], Ellie Kim[4], Nicholas Marcella[5], Shuxiang Zhou[2], Anna Smith[6], Ruchi Gakhar[2], Vyacheslav Bryantsev[3], Sheng Dai[3,4], James F. Wishart[1], Anatoly I. Frenkel[1,5], Simerjeet K. Gill[1]
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I-P1-2: A Multiscale Perspective of Ion Network Reactivity, Structure, and Dynamics

[EFRC - IDREAM] Yihui Wei[1], Trent Graham[2], Robert Felsted[2], Maxime Pouvreau[2], Abdullah Ozkanlar[1], Eric Walter[2], Hemanth Haridas[1], Simantini Paul[1], Jacob Morton[2], Emily Nienhuis[2], Sebastian Mergelsberg[2], Aurora Clark[1], Gregory Kimmel[2]
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I-P1-3: Decoding Bulk and Interfacial Structure in Molten Salts: Insights from Polarizable MD and Synchrotron X-ray Measurements

[EFRC - MSEE] Matthew S. Emerson[1,2], Bichitra Borah[2], Leighanne C. Gallington[3], Patra Nirmalendu[1], Andreas Kuhlmann[4], Hans-Georg Steinrück[4], John J. Ferrari[5], Karena W. Chapman[5], Ellie Kim[6], Phillip Halstenberg[6,7], Harald Reichert[8], Bobby Layne[1], Kazuhiro Iwamatsu[1], Diwash Dhakal[1], Simerjeet Gill[1], Sheng Dai[6,7], Santanu Roy[7], Claudio J. Margulis[2], Benjamin M. Ocko[1], James F. Wishart[1]
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I-P1-4: Effect of Cation Traps on Solvation Dynamics and Structure with Ultrafast Probes

[EFRC - IDREAM] Shuai Li[1], Aodong Liu[2], Ryan Beck[2], Eleftherios Lambros[2], Emily Nienhuis[3], Douglas Garratt[4], Robin Santra[5], Jay LaVerne[6], Brant Jones[7], Thomas Orlando[7], Yihui Wei[8], Aurora Clark[8], Linda Young[1], Xiaosong Li[2]
[1]Argonne National Laboratory; [2]University of Washington; [3]Pacific Northwest National Laboratory; [4]SLAC National Accelerator Laboratory; [5]Deutsches Elektronen-Synchrotron (DESY); [6] University of Notre Dame; [7]Georgia Institute of Technology; [8]University of Utah

I-P1-5: Dealloying of Post-Irradiated Model Ni20Cr (wt.%) Alloy in Molten FLiNaK Salts

[EFRC - FUTURE] Harjot Singh[1], Ho Lun Chan[1], Sean Mills[2], Matthew Chancey[3], Benjamin Derby[3], Elena Romanovskaia[1], Valentin Romanovski[1], Nathan Bieberdorf[2], Yongqiang Wang[3], Mark Asta[2], Andrew Minor[2], Peter Hosemann[2], John Scully[1]

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I-P1-6: Redox-Driven Interfacial Chemistry, Microstructure Evolution, and Corrosion Mechanisms of Metallic Materials in $EuCl_3$-Doped LiCl-KCl Molten Salts

[EFRC - MSEE] Aaron G. Penders[1], Kailee Buttice[2], Stephanie Castro Baldivieso[1], Bonita Goh[2], Ellie M. Kim[3], Phillip W. Halstenberg[3], Alejandro Ramos Ballesteros[1], William Phillips[2], Isabelle Baggenstoss[2], Shea McCarthy[2], George Vukovic[2], Yuxiang Peng[4], Bruce Ravel[5], Bobby Layne[5], Sheng Dai[3,6], James F. Wishart[5], Karen Chen-Wiegart[4,5], Ruchi Gakhar[1], Kaustubh Bawane[1], Adrien Couet[2]

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I-P1-7: Synthesis, Structure, and Transport Properties of Actinide Oxides and Nitrides

[EFRC - TETI] Kevin D. Vallejo[1], Brelon J. May[1], Mira Khair[2], Elizabeth Sooby[2], Sabin Regmi[1], Volodymyr Buturlim[1], Krzysztof Gofryk[1]

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I-P1-8: Effect of Ion Network Structure on Particle Aggregation in Concentrated Electrolytes Under Irradiation

[EFRC - IDREAM] Elias Nakouzi[1], Jaehun Chun[1], Micah Prange[1], Lili Liu[1], Xin Zhang[1], Lawrence Anovitz[2], Pravalika Butreddy[1], Nikhil Rampal[3], Andrew Stack[2], Jaeyoung Heo[1], Benjamin Legg[1], James De Yoreo[1], Kevin Rosso[1], Gregory Schenter[1]

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I-P1-9: Interfacial Effects on Defect Evolution and Transport in Oxides Under Irradiation

[EFRC - FUTURE] Jijo Christudasjustus[1], Ben Derby[2], Tiffany Kaspar[1], Hyosim Kim[2], Dongye Liu[3], Sean Mills[3], Andrew Minor[3], Elizabeth Peterson[2], Dan Schreiber[1], Farida Selim[4], Blas Uberuaga[2], Yongqiang Wong[2], Kayla Yano[1]

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I-P1-10: Decoding Thermal Conductivity: Experimental and Theoretical Insights into Lattice Anharmonicity and Defects in Fluoride Oxides

[EFRC - TETI] Linu Malakkal[1], Ella Kartika Pek[1], Saqeeb Adnan[2], M. Minaruzzaman[2], James Mathew Mann[3], Zilong Hua[1], Shuxiang Zhou[1], Amey Khanolkar[1], Chris Marianetti[4], Marat Khafizov[2], David Hurley[1]

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J. Quantum Information Science

J-P1-1: Generation and Characterization of Entanglement from Solid-State Quantum Emitters

[EFRC - QuPIDC] Arshag Danageozian[1], Souvik Biswas[2], Sophia Economou[1], Jelena Vuckovic[2], Tongcang Li[3]

[1]Virginia Polytechnic Institute and State University; [2]Stanford University; [3]Purdue University

J-P1-2: Interplay between chirality, spin and charge in chiral semiconductors: from steady-state to terahertz timescales

[EFRC - CHOISE] Aeron McConnell[1], Pius M. Theiler[2], Yifan Dong[2,3], Md Azimul Haque[2], Shripathi Ramakrishnan[2,4], Matthew P. Hautzinger[2], Andrew H. Comstock[1], Joseph M. Luther[2], Peter C. Sercel[5], Matthew C. Beard[2], Dali Sun[1]

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J-P1-3: Chemical functionalization of 2D materials for readout of quantum states

[EFRC - CMQT] S. Carin Gavin[1], Riddhi Ananth[1], M. Iqbal Bakti Utama[1], Anushka Dasgupta[1], Rafael Lopez-Arteaga[1], Tumpa Sadhukhan[1], Hongfei Zeng[1], Hsun-Jen Chuang[3], Moumita Kar[1], David D. Xu[1], Albert F. Vong[1], Seok Daniel Namgung[1], Yi Liang[1], Alina Bennett[1], Fateme Mahdikhany[1], Hong Youl Park[1], Brendan P. Kerwin[1], Xi Wan[1], Dana E. Kachman[1], Dmitry Lebedev[1], Jia-Shiang Chen[2], Wei Wang[2], Sung-Joon Lee[4], Xiangzhi Li[4], Kenji Watanabe[5], Takashi Taniguchi[5], Vinod K. Sangwan[1], Chad A. Mirkin[1], Berend T. Jonker[3], Emily A. Weiss[1], Tobin J. Marks[1], Xuedan Ma[2,6], George C. Schatz[1], Mark C. Hersam[1], Nathaniel P. Stern,

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J-P1-4: Coupling Quantum Emitters with Nanophotonic Structures

[EFRC - QuPIDC] Emma Daggett[1], Artem Kryvobok[1], Souvik Biswas[2], Jon Hood[1], Alexandra Boltasseva[1], Vladimir Shalaev[1], Jelena Vuckovic[2]

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J-P1-5: Engineering Clock Transitions in Lanthanide Complexes as Potential Molecular Spin Qubits

[EFRC - M2QM] Miguel Gakiya-Teruya[1], Shuanglong Liu[2], Ferdous Ara[3], Dibya Jyoti Mondal[1], Hai-Ping Cheng[2], Stephen Hill[1,3], Michael Shatruk[1]

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J-P1-6: Molecular Lithography on Moiré Heterostructures

[EFRC - Pro-QM] Michael Riehs[1], Daniel Rizzo[2], Hang Liu[3], Dongbin Shin[3,4], Igor Vasilevskiy[5], Takashi Taniguchi[6], Kenji Watanabe[7], Tobias Stauber[5], Angel Rubio[3,8,9], Dmitri Basov[2], Alexandra Velian[1]

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J-P1-7: A Surface Molecular Qubit Scaffolded by hBN

[EFRC - CMQT] Tian-Xing Zheng[1], M. Iqbal Bakti Utama[2], Moumita Kar[2], Sungsu Kang[1], Tengyang Ruan[1], Hanyan Cai[1], Guanming Lao[1], Uri Zvi[1], David Ovtasky[1], Omri Raz[1], Yuxin Wang[3], Magdalena H. Czyz[2], Sanskriti Chitrash[1], Grant Smith[1], Leah Weiss[1], Alex Fairhall[4], Randall Goldsmith[4], David D. Awschalom[1], Paul Alivisatos[1], George Schatz[2], Mark Hersam[2], Peter C. Maurer[1]

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J-P1-8: Quantum Properties of 166 Kagome Metals

[EFRC - CATS] Tyler Slade[1], Joanna Bławat[2], Tianxiong Han[1], Lin-Lin Wang[1], Junho Seo[3], John Singleton[4], Ben Ueland[1], Rob McQueeney[1], Philip Moll[3], Ross McDonald[2], Paul C. Canfield[1]

[1]Ames National Laboratory; [2]Los Alamos National Laboratory; [3]Max Planck Institute for the Structure and Dynamics of Matter; [4]National High Magnetic Field Laboratory

J-P1-9: Covalently-linked Metalloporphyrin Dimers and their Magnetic and Spectroscopic Properties

[EFRC - M2QM] Alexander Diodati[1], Shuanglong Liu[2], Zain Becerra[1], Hai-Ping Cheng[2], Alexander Angerhofer[1], George Christou[1]
[1]University of Florida; [2]Northeastern University

J-P1-10: Momentum-resolved EELS study of lattice excitations in 1T-TaS_2

[EFRC - QSQM] Farzaneh Hoveyda-Marashi[1], Xuefei Guo[1], Caitlin Kengle[1,3], Dipanjan Chaudhuri[1], Jin Chen[1], Peter Abbamonte[1]
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J-P1-11: A New Topological and Correlated Insulator

[EFRC - CATS] Jian Tang[1], Thomas Ding[1], Su-Yang Xu[2], Qiong Ma[1]
[1]Boston College; [2]Harvard University

J-P1-12: Adaptive control of numerical error in all-electron simulation of periodic solids

[CCS - NEREST] Jonathon Misiewicz[1], Robert Harrison[2], Edward Valeev[1]
[1]Virginia Polytechnic Institute and State University; [2]Stony Brook University

M. Research at the Exascale

M-P1-1: Scaling the Random Phase Approximation for beyond-DFT electrochemistry

[CCS - BEAST] Daniel Weinberg[1], Jacob Clary[2], Olivia Hull[2], Ravishankar Sundararaman[3], Derek Vigil-Fowler[2], Mauro Del Ben[1]
[1]Lawrence Berkeley National Laboratory; [2]National Renewable Energy Laboratory; [3]Rensselaer Polytechnic Institute

M-P1-2: Enabling Multireference Calculations on Multimetallic Systems with Graphic Processing Units

[CCS - ExaPUC] Valay Agarawal[1], Rishu Khurana[1,2], Cong Liu[2], Matthew R. Hermes[1], Christopher Knight[2], Laura Gagliardi[1]
[1]University of Chicago; [2]Argonne National Laboratory

M-P1-3: A performance-portable GPU implementation of electron-phonon interaction interpolation in EPW

[CMS - EPW] Tae Yun Kim[1], Zhe Liu[2], Elena Roxana Margine[2], Feliciano Giustino[1]
[1]The University of Texas at Austin; [2]Binghamton University-SUNY

M-P1-4: Spatio-temporal spin and charge transport from first principles density-matrix dynamics

[CCS - ADEPTs] Mayada Fadel[2], Mayank Gupta[1], Joshua Quinton[2], Mani Chandra[2], Jacopo Simoni[1], Yuan Ping[1], and Ravishankar Sundararaman[2]

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M-P1-5: Insights into Correlated Solids Using Quantum Monte Carlo

[CMS - CPSFM] P. Ganesh[1], H. Shin[2], A. Dumi[3], A. Lopez[4], B. Rubenstein[4], K. Saritas[1], J. Krogel[1], P. Kent[1]

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M-P1-6: Non-Equilibrium Quantum Dynamics Theory and Implementation in the INQ Code

[CMS - NPNEQ] Jacopo Simoni[1], Xavier Andrade[2], Andrew Grieder[1], Emma Simmerman[3,4], Sangeeta Rajpurohit[2,5], Wuzhang Fang[1], Chris Ciccarino[3,4], Jonah Haber[3,4], Alfredo Correa[2], David Prendergast[5], Felipe Jornada[3,4], Liang Tan[5], Yuan Ping[1], Tadashi Ogitsu[2]

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POSTER SESSION II

A. Advanced Manufacturing

A-P2-1: Interfacing Proteins with Inorganic Materials

[EFRC - CSSAS] Ying Xia[1], Zhiyin Zhang[2], Chenyang Shi[3], Hao Shen[1], Charlotte Zhao[4], Timothy Moore[4], Sharon Glotzer[4], David Baker[1], Shuai Zhang[1,3], F. Akif Tezcan[2], Christopher J. Mundy[1,3], James J. De Yoreo[1,3]

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A-P2-2: Morphogenic Growth 3D Printing

[EFRC - REMAT] Yun Seong Kim[1], Brandon R. Clarke[2], Minjiang Zhu[1], Mohammad T. Hossain[1], Derrick Sanders[1], Nancy R. Sottos[1], Jeffrey S. Moore[1], Randy H. Ewoldt[1], Phillipe H. Geubelle[1], Jennifer A. Lewis[2], Sameh H. Tawfick[1]

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A-P2-3: Microstructure-Informed Mesoscale Modeling to Predict Mechanical Behavior of Additively Manufactured Polymer Composites

[EFRC - AIM] Mostafa Elnaggar[1], Koorosh Delavari[1], Amit M. Deshpande[2], Taejoon Park[1], Gang Li[3], Srikanth Pilla[2], Farhang Pourboghrat[1]

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A-P2-4: Protein- and Peptide-Directed Inorganic Nucleation

[EFRC - CSSAS] Emily Saccuzzo Close[1], William Wixson[2], Harley Pyles[2], Aditya Sonpal[3], Paul Kwon[2], Tracy Yu[2], Marlo Zorman[2], Jim Pfaendtner[3], Wendy Shaw[1], Christopher J. Mundy[1,2], David Baker[2], James J. De Yoreo[1,2], François Baneyx[2]

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A-P2-5: Experimental Investigation and Modeling of Effect of Cooling Rates on the Mechanical Properties of Thermoformed Fiber Reinforced Thermoplastic Composites

[EFRC - AIM] Amit M. Deshpande[1], Tatiana Stepanova[2], Mostafa Elnaggar[3], Dhanashree Shinde[1], Taejoon Park[3], Sai Aditya Pradeep[1], Gang Li[2], Farhang Pourboghrat[3], Srikanth Pilla[1]

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A-P2-6: Morphogenic Patterning of Polymers by Frontal Polymerization

[EFRC - REMAT] Anna C. Cramblitt[1], Philippe H. Geubelle[1], Leah A. Appelhans[2], Ignacio Arretche[1], Donald Bistri[1], Amyra A. Black[1], Lauren Chua[3], Reid Cope[1], Ethan Curran[1], Dan Darby[2], Rafael Gómez-Bombarelli[3], Andrew Greenlee[1,2], Melissa Kirby[1], Samuel Leguizamon[2], Mya G. Mills[1], Jeffrey S. Moore[1], Luis E. Rodríguez Koett[1], Nancy R. Sottos[1], Michael Zakoworotny[1], Conan Zhang[1]

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A-P2-7: Transforming Biomolecular Systems through Physical and Molecular Stimuli

[EFRC - CSSAS] Daphne Shen[1], Iris Zhang[2], Progyateg Chakma[3], Huat Thart Chiang[4], Yifeng Cai[4], Lilo Pozzo[4], François Baneyx[4], Chun-Long Chen[3,4], Oleg Gang[1], F. Akif Tezcan[2]

[1]Columbia University; [2]University of California, San Diego; [3]Pacific Northwest National Laboratory; [4]University of Washington

A-P2-8: Synthesis of Circular-by-Design Polyolefin-like Materials

[EFRC - CPI] Sam Marsden[1], Isabella Vettese[1], Amelia Seropian[1], Heyi Liang[2], Maria Ley Flores[2], Andrew Qin[2], Juan de Pablo[2], Stuart Rowan[1]

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B. Catalysis

B-P2-1: Revealing the Role of Crystal Morphology and Surface Terminations on Water Oxidation Activity of Single $BiVO_4$ Microparticles

[EFRC - EPN] Avishek Banik[1], Kevin Dunn[2], Javier Fajardo, Jr.[3], Thomas Chen[3], Hiroaki Maekawa[4], Mahdi Hesari[5], Akihiko Kudo[6], Nien-Hui Ge[4], A. Alec Talin[3], Daniel V. Esposito[2], Justin B. Sambur[1]

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B-P2-2: Understanding Ionic Liquid Mediated Reactive Capture and Electrochemical Conversion of CO_2

[EFRC - 4C] Francois Nkurunziza[1], Saudagar Dongare[2], Soumya Chatterjee[3], Bhavi Shah[1], Manu Gautam[1], Baleeswaraiah Muchharla[4], Bijandra Kumar[4], Michael J. Janik[3], Burcu Gurkan[2], Robert L. Sacci[5], and Joshua M. Spurgeon[1]

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B-P2-3: Designing Single Atom Sites in Semiconductor Perovskite Oxides for Programmable Catalysis

[EFRC - CPEC] Junhao Huang[1], Silvia Marino[2], Ryan Berry[2], Michael Gordon[2], Philip Christopher[2], Eranda Nikolla[1]

[1]University of Michigan, Ann Arbor; [2]University of California, Santa Barbara

B-P2-4: Preparation of Highly Reactive Photocatalysts via Ionic Bond Photolysis in Low Dielectric Solvents

[EFRC - BioLec] Justin L. Ratkovec[1], Justin D. Earley[1], Max Kudisch[2], William P Kopcha[2], Eve Yuanwei Xu[3], Robert R. Knowles[3], Garry Rumbles[1,2], Obadiah G. Reid[1,2]

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B-P2-5: Re-imagining the solar cell architecture for diurnal durability of photoelectrodes for solar fuels production

[Hub - LiSA] Darci Collins[1,2], Zebulon G. Schichtl[1,2], Ann L. Greenaway[1,2], Emily L. Warren[1,2]

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B-P2-6: Molecular Control of Charge-Separated-State Lifetimes in Nanocrystal–Molecule Hybrids

[EFRC - EPN] Olivia F. Bird[1], Faith A. Flinkingshelt[2], Sophia M. Click[1], Madison Jilek[1], Della Hagemann[3], Kenneth M. Drbohlav[3], Evan K. Gowdy[3], Hyuna Kwon[4], Yisrael M. L. Lamb[3], Tadashi Ogitsu[4], Jenny Y. Yang[2], Kenneth A. Miller[3], Gordana Dukovic[1]

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B-P2-7: Frontiers in Probing Bacterial Microcompartments as Nanoreactors for Catalysis in Confinement

[EFRC - CCBC] Nina Ponomarenko[1], Samuel Snyder[1], Timothy Chiang[2], Neetu Yadav[3], Paul Ashby[2], Markus Sutter[2,3], Cheryl Kerfeld[2,3], Karen Mulfort[1], Josh Vermaas[3], Lisa Utschig[1], David Tiede[1], Oleg Poluektov[1]

[1]Argonne National Laboratory; [2]Lawrence Berkeley National Laboratory; [3]Michigan State University

B-P2-8: Development of ZnTe and ZnGa2Te$_4$ as photocathode materials for CO$_2$ reduction reaction

[Hub - LiSA] Andriy Zakutayev[1,2], Shaham Quadir[1,2], Christopher P. Muzzillo[1,2], Yungchieh Lai[1].[3], Sage R. Bauers[1,2], Wayne Zhao[1,4], Kristin A. Persson[1,4], Joel A. Haber[1,3]

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B-P2-9: Clarifying the Influence that Inter-Absorber Photon Recycling and Interfacial Charge Trapping can have on Ensemble Photosynthetic Activity

[EFRC - EPN] Wentao Zhang[1], Honghao Liu[2], Danielle R. Lustig[3], Fangqi Chen[4], Olivia F. Bird[5], Javier Fajardo, Jr.[6], Justin T. Mulvey[2], Pushp Raj Prasad[2], Enes Buz[7], Kevin R. Kittilstved[7], Joseph P. Patterson[2], Gordana Dukovic[5], Shane Ardo[2], A. Alec Talin[6], Justin B. Sambur[3], Shu Hu[1], Rohini Bala Chandran[4]

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B-P2-10: Iron-Sulfur Based Materials for CO_2 Conversion

[EFRC - CD4DC] Andrea Darù[1], Hilal Daglar[1], Linh Le[1], Špela Kunstelj[1], Ningxin Jiang[1], Jianming Mao[1], Jan Hofmann[2], Simon M. Vornholt[2], Karena W. Chapman[2], Andrew L. Ferguson[1], Anna Wuttig[1], John S. Anderson[1], Laura Gagliardi[1]

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B-P2-11: Transport Mechanisms and Architectures in Alkaline Media

[EFRC - CABES] Brett Fors, Casandra Haynes

Cornell University

B-P2-12: Synthesis and Characterization of Photo(electro)catalytic Materials for Water Splitting

[EFRC - CEDARS] Sheilah Cherono[1], Luka Mitrovic[2], Swapnil Nalawade[1], Ikenna Chris-Okoro[1], Daniel Zheng[3], Haldrian Iriawan[3], Binod Raj KC[1], Mengxin Liu[1], Ghanashyam Gyawali[1], Bishnu Bastakoti[1], Yang Shao-Horn[3], Darrell Schlom[2], Jin Suntivich[2], Shyam Aravamudhan[1], Dhananjay Kumar[1]

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B-P2-13: Mechanistic Insights into Aromatic Hydrogenation in Protic Solvents for LOHCs Using Bifunctional Catalysts

[EFRC - CD4DC] Ciara Tyler[1], Huy Nguyen[1], Yinjie Ji[2], Seryeong Lee[3], Jacob Bryant[4], Maryam Mansoori[1], Donald Truhlar[1], Omar Farha[3], Max Delferro[4], Johannes Lercher[2], and Matthew Neurock[1]

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B-P2-14: Highly-Destabilized Ligand Field Excited States of Iron Carbene Complexes and Their Relation to Charge Transfer State Lifetimes

[EFRC - BioLEC] Reagan X. Hooper[1], Benjamin I. Poulter[1], Jesper Schwarz[2], Marwa Al Rammal[3], Mariam Barakat[3], Kristjan Kunnus[1], Kacie J. Nelson[1], Aleksandra Ilic[2], Clara Mateos[2], Jens Uhlig[2], Kenneth Wärnmark[2], Elena Jakubikova[3], Amy A. Cordones[1], and Kelly J. Gaffney[1]

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B-P2-15: Fermi-orbital descriptors, electron localization function and Born maxima: Chemical structure from self-interaction correction

[CCS - FLOSIC] Jerónimo Lira[1], Duyen B. Nguyen[1], John P. Perdew[2], Koblar A. Jackson[1], and Juan E. Peralta[1]

[1]Central Michigan University; [2]Tulane University

B-P2-16: Probing Material and Device Activity and Durability in Alkaline Media

[EFRC - CABES] Tom Mallouk[1], Wonil Jung[1], Bryan Pivovar[2]

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B-P2-17: Tunable Active Sites in Metal–Organic Frameworks for Selective Hydrogenation Catalysis

[EFRC - CD4DC] Seryeong Lee[1], Haomiao Xie[1], Milad Ahmadi Khoshooei[1], Dawson Grimes[1], Mukunda Mandal[3], Simon M. Vornholt[4], Jan Hofmann[4], Luke M. Tufaro[4], Kent O. Kirlikovali[1], Kira Fahy[1], KaiKai Ma[1], Yongwei Chen[1], Jenny G. Vitillo[5], John S. Anderson[3], Justin M. Notestein[1], Karena W. Chapman[4], Laura Gagliardi[3], Joseph Hupp[1], Massimiliano Delferro, Omar K. Farha[1,2]

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B-P2-18: Understand electrochemical and optical in-operando measurement on RuO_2 and TiO_2 thin film through ab-initio calculations

[EFRC - CEDARS] Lei Zhang[1], Simon Gelin[2], Shay McBride[1], Jan Kloppenburg[1], Chia-Yi Lin[3], Luka Mitrovic[3], Cassius Boyd[4], Michael Paolino[4], Moritz Lang[4], Tanja Cuk[4], Ismaila Dabo[2], Darrell G Schlom[3], Jin Suntivich[3], Geoffroy Hautier[1]

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D. Energy Storage

D-P2-1: First-Principles Investigation of Ionic Conductivity Mechanisms in Zwitterion-Based Electrolytes

[EFRC - FaCT] Yifan Liu[1], Zitan Huang[2], Ralph H. Colby[2], Valentino R. Cooper[1]
[1]Oak Ridge National Laboratory; [2]The Pennsylvania State University

D-P2-2: Quantum-Driven Proton Transfer in Concentrated Hydrogen-Bonded Electrolytes

[EFRC - BEES2] Miguel Muñoz[1], Giselle de Araujo Lima e Souza[2], Michael S. Chen[3], Kaylie Glynn[4], Benworth B. Hansen[4], Peisen Qian[5], Thomas Simunovic[6], Mrinlini Kolaprath[6], Mark Dadmun[6], Thomas Zawodzinski[6], Joaquín Rodríguez-López[5], Steve G. Greenbaum[2], Mark Tuckerman[3], Joshua R. Sangoro[4], and Burcu Gurkan[1]
[1]Case Western Reserve University; [2]Hunter College-CUNY; [3]New York University; [4]The Ohio State University; [5]University of Illinois Urbana-Champaign; [6]University of Tennessee-Knoxville

D-P2-3: Energy Storage Research Alliance: Soft Matter Omics

[Hub - ESRA] Brett Helms[1], Yan Yao[2], Rajeev Assary[3], Pieremanuele Canepa[2], Ying Chen[4], Ruozhu Feng[4], Rafael Gómez-Bombarelli[5], Jeremiah Johnson[5], Yiyang Li[6], Chen Liao[3], Lamartine Meda[7], Y. Shirley Meng[3,8], Tod Pascal[9], Shrayesh Patel[8], Joaquín Rodríguez-López[10], Mary Scott[1,11], Nirala Singh[6], Venkat Srinivasan[3], Wei Wang[4], Kamila Wiaderek[3]
[1]Lawrence Berkeley National Laboratory; [2]University of Houston; [3]Argonne National Laboratory; [4]Pacific Northwest National Laboratory; [5]Massachusetts Institute of Technology; [6]University of Michigan; [7]Xavier University of Louisiana; [8]University of Chicago; [9]University of California, San Diego; [10]University of Illinois Urbana-Champaign; [11]University of California, Berkeley

D-P2-4: Integrated Microscopic Theories of Structure, Polymer Dynamics, and Conductivity in Polymerized Ionic Liquids

[EFRC - FaCT] Ankita Das[1], Kenneth S Schweizer[1], Catalin Gainaru[2], Anisur Rahman[2], Michelle Lehmann[2], Rajeev Kumar[2], Alexei P Sokolov[2]
[1]University of Illinois Urbana-Champaign; [2]Oak Ridge National Laboratory

D-P2-5: pH-driven mixing-induced carbonate precipitation linking pore-scale microfluidics to subsurface mineralization

[EFRC - GMCS] David Kyungtae Kim, Peter K. Kang
University of Minnesota, Twin Cities

D-P2-6: Fluid interfaces and Flow cells

[EFRC - MUSIC] David Kwabi[1], Jeff Sakamoto[2,3], Miaofang Chi[4]
[1]Yale University; [2]University of Michigan; [3]University of California, Santa Barbara; [4]Oak Ridge National Laboratory

D-P2-7: Deciphering Unique Electrochemical Processes in Zinc-Aqueous Batteries

[EFRC - m2M#s] Jingxu Zheng[1], Xiaosi Gao[1], Yue Deng[1], Prayag Biswal[1], Regina Garcia-Mendez[1], Shuo Jin[1], Shifeng Hong[1], Keun-Il Kim[1], Tian Tang[1], Kenneth Takeuchi[2,3], Esther Takeuchi[2,3], Amy Marschilok[2,3], Lynden Archer[1].
[1]Cornell University; [2]Stony Brook University; [3]Brookhaven National Laboratory

D-P2-8: Tailoring Negolyte Design for Next Generation Redox Flow Batteries

[EFRC - BEES2] Emily Pentzer[1], Miguel Muñoz[2], Uddalak Sengupta[1], Ananya Banik[1], Sabhapathy Palani[2], Jesse Wainright[2], Burcu Gurkan[2], David Powers[1]
[1]Texas A&M University; [2]Case Western Reserve University

D-P2-9: Solar Methanol Production Using Molecular Cobalt Phthalocyanine Hybrid Photoelectrodes

[Hub - CHASE] Bo Shang[1], Fengyi Zhao[2], Sa Suo[2], Langqiu Xiao[3], Conor Rooney[1], Yuanzuo Gao[2], Colton Sheehan[3], Sungho Jeon[3], Jing Li[1], Oliver Leitner[1], Hanqing Fan[1], Menachem Elimelech[1], Leizhi Wang[1], David J. Gallagher[1], Bernie Wang[1], Andrey Krayev[5], Hadar Shema[6], Nia J. Harmon[1], Samuel R. Bottum[4], Elad Gross[6], Gerald Meyer[4], Eric Stach[3], Thomas Mallouk[3], Tianquan Lian[2], James F. Cahoon[4], Hailiang Wang[1]
[1]Yale University; [2]Emory University; [3]University of Pennsylvania; [4]University of North Carolina at Chapel Hill; [5]HORIBA Instruments; [6]Hebrew University of Jerusalem

D-P2-10: Enhancing Composite Electrode Electrochemistry via Control of Interfacial Interactions

[EFRC - m2M#s] Haoze Ren[1], Han Li[1], Zeyuan Sun[1], Donghee Gueon[1], Miguel Gonzalez[1], Meng Wang[1], Mengting Sun[1], Armando Rodriguez Campos[2], Alexis Pace[2], Esther Takeuchi[2,3], Amy Marschilok[2,3], Shan Yan[3], Kenneth Takeuchi[2,3], Elsa Reichmanis[1]
[1]Lehigh University; [2]Stony Brook University; [3]Brookhaven National Laboratory

D-P2-11: Reaction Processes at Metal-Ceramic Ion Conductor Interfaces

[EFRC - MUSIC] Mathew McDowell[1], Pinar Alsac[1], Donald Siegel[2]
[1]Georgia Institute of Technology; [2]University of Texas at Austin

D-P2-12: MECR-based viscoelastic characterization: a framework for the “constitutive MRI” of rocks

[EFRC - GMCS] Prasanna Salasiya, Ali Aminzadeh, Joseph F. Labuz, Bojan B. Guzina
University of Minnesota, Twin-Cities

F. Energy-Water

F-P2-1: Effect of Ion Pairing on Salt Transport in Ion Exchange Membranes (IEMs)

[EFRC - M-WET] Z. Rachel Huang[1], Meng Wang[1], Zahra Bajalan[1], Rahul Sujanani[1,2], Graeme Henkelman[1], Lynn Katz[1], Benny Freeman[1]
[1]The University of Texas at Austin; [2]University of California, Santa Barbara

F-P2-2: Degradation of PFAS by Reactive Metal-Mediated Electrochemical Reduction

[EFRC - AMEWS] Bidushi Sarkar[1], Rameshwar L. Kumawat[2], Peiyuan Ma[1], Ke-Hsin Wang[1], Matin Mohebi[1], George C. Schatz[2], Chibueze V. Amanchukwu[1]
[1]University of Chicago; [2]Northwestern University

F-P2-3: Exploring Structure-Selectivity Relationships in Hindered Ion Transport Through Molecular Simulations and Advanced Sampling Methods

[EFRC - CENT2] Omar Khalifa[1], Camille Violet[1], Akash Ball[2], Heather Kulik[2], Menachem Elimelech[3], Amir Haji-Akbari[1]
[1]Yale University; [2]Massachusetts Institute of Technology; [3]Rice University

F-P2-4: The Role of Hydration on Ion Transport in Polyether Electrolytes

[EFRC - M-WET] Nico Marioni[1], Liam Warlick[2], Tokio Mimura[2], Rahul Sujanani[2], Venkat Ganesan[1], Rachel Segalman[2], Benny Freeman[1]
[1]University of Texas at Austin; [2]University of California, Santa Barbara

F-P2-5: Precise ion transport through single-crystal MOF membranes for aqueous resource recovery

[EFRC - CENT2] Camille Violet[1,2], Alex T. Hall[3], Zuzanna Siwy[4], John Cumings[3], Menachem Elimelech[5]
[1]Yale University; [2]Lawrence Livermore National Laboratory; [3]University of Maryland, College Park; [4]University of California, Irvine; [5]Rice University

F-P2-6: Exploring the Ultimate Limits of Nanoscale Solute Separation

[EFRC - AMEWS] Feng Gao[1], Wen Chen[1,2], Jamila G. Eatman[1,2], Paul F. Nealey[1,2], Seth B. Darling[1,2]
[1]Argonne National Laboratory; [2]University of Chicago

F-P2-7: Integrating Universal Membrane Chemistry and Model Fluid Platforms with Synchrotron Characterization Techniques to Accelerate Membrane Innovation

[EFRC - M-WET] Jose Carlos Diaz[1,2], Matthew R. Landsman[1,2], Mostafa Nassr[1], Noah Wamble[1], Louise Kuehster[1], Cameron McKay[1], Suzana Invandic[1], Connor Coolidge[1], Meng Wang[1], Lynn E. Katz[1], Nathaniel Lynd[1], Benny Freeman[1], Joan Brennecke[1], Gregory Su[2]
[1]University of Texas at Austin; [2]Lawrence Berkeley National Laboratory

H. Microelectronics

H-P2-1: Hafnia/Zirconia Materials Innovation for Ferroelectric Microelectronics: Enhancing Growth, Defect control, and Switching

[EFRC - 3DFeM2] Ece Gunay[1], Songsong Zhou[2], Benjamin Aronson[3], Shihan Qin[2], Sebastian Calderon[1], Jon Ihlefeld[3], Andrew M. Rappe[2], Elizabeth Dickey[1]
[1]Carnegie Mellon University; [2]University of Pennsylvania; [3]University of Virginia

H-P2-2: Precision synthesis, multimodal characterization, and implementation of high-resolution block copolymers for the fundamental understanding of molecular self-assembly for semiconductor manufacturing: EUV plus DSA

[EFRC - CHiPPS] Kyunghyeon Lee[1], Emma Vargo[2], Ki Hyun Kim[1], Christopher J. Eom[1], Whitney Loo[1], Ricardo Ruiz[2], Paul F. Nealey[1]
[1]Argonne National Laboratory; [2]Lawrence Berkeley National Laboratory

H-P2-3: Low Temperature Growth of AlGaN by Halide Vapor Phase Epitaxy

[EFRC - APEX] Jacob H. Leach[1], Connor Raines[1], Kevin Udwary[1], Heather Splawn[1], Kevin Schulte[2], Kirstin Alberi[2], John Simon[2]
[1]Kyma Technologies; [2]National Renewable Energy Laboratory

H-P2-4: Epitaxial Transfer for Fully Relaxed (Si)GeSn Direct Bandgap Compound Semiconductor Alloys

[EFRC - µ-ATOMS] Suho Park[1], Haochen Zhao[1], Shedrack Dafe[1], Jifeng Liu[2], Diandian Zhang[3], Yunsheng Qiu[3], Shui-Qing Yu[3], Yuping Zeng[1]
[1]University of Delaware; [2]Dartmouth College; [3]University of Arkansas

H-P2-5: Dynamic Film-Substrate Interactions: Asymmetric Substrate Strain Imprint and Feedback Mechanisms in Oxide Thin Films

[EFRC - Q-MEEN-C] Elliot Kisiel[1,2], Pavel Salev[1], Alexandre Pofelski[3], Spencer Reisbick[3], Chuhang Liu[3], Andreas Glatz[2,4], Ishwor Poudyal[2], Wei He[1], Rourav Basak[1], Kaan Alp Yay[5,6], Junjie Li[1], Zhan Zhang[2], Arndt Last[7], Yimei Zhu[3], Ivan Schuller[1], Zahir Islam[2], Alex Frano[1]

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H-P2-6: Chemical Tailoring and Characterization of $M_xV_2O_5$ Neuromorphic Materials

[EFRC - reMIND] John Ponis[1], Jialu Li[2], George Agbeworvi[1], Shruti Hariyani[1], Thanh Luan Phan[3], Kenna Ashen[1], Michelle A. Smeaton[3], Srikrishna Sagar[3], Katherine L. Jungjohann[3], Andrew J. Ferguson[3], Jeffrey L. Blackburn[3], Xiaofeng Qian[1], Matt Pharr[1], Sarbajit Banerjee[1], Jinghua Guo[2], Lance M. Wheeler[3]

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H-P2-7: Novel perspective on finite momentum exciton physics using high-resolution resonant inelastic X-ray scattering

[EFRC - Pro-QM] Connor Occhialini[1,2], Benjamin Zager[2], Taehun Kim[2], Yifeng Cao[2], Jonathan Pelliciari[2], Daniel Chica[1], Vinicius Avelar[1], Gillian Minarik[1], Taketa Handa[1], Eric Arsenault[1], Xavier Roy[1], Xiaoyang Zhu[1], Dmitri Basov[1], Valentina Bisogni[2]

[1]Columbia University; [2]Brookhaven National Laboratory

H-P2-8: Thin-Film Ferroelectric Field-Effect Transistors for High Density 3D Memory

[EFRC - 3DFeM2] Quyen T. Tran[1], Sharadindu Gopal Kirtania[2], Jiahui Duan[3], Kai Ni[3], Vijaykrishnan Narayanan[1], Suman Datta[2], Thomas Jackson[1]

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H-P2-9: Spin Crossover Neurons Based Upon Rare Earth Cobaltates

[EFRC - reMIND] Elena Salagre Rubio[1], Jialu Li[2], Byoung Ki Choi[2], Timothy D. Brown[1], Yeonju Yu[3], Fatima Jardali[3], Michelle A. Smeaton[4], Katherine L. Jungjohann[4], Eli Rotenberg[2], R. Stanley Williams[3], A. Alec Talin[1], Suhas Kumar[1], Patrick Shamberger[1], Jinghua Guo[2], Elliot J. Fuller[1]

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H-P2-10: Probing Structurally and Chemically Heterogeneous Epitaxial Interfaces

[EFRC - APEX] M. Brooks Tellekamp[1], Evan Crites[2], Satya Kushwaha[2], Ahamed Raihan[3], Dennice Roberts[1], Anthony Rice[1], Jordan Hachtel[4], Sharad Mahatara[1], Stephan Lany[1], Tyrel M. McQueen[2], MVS Chandrashekhar[3], Nancy M. Haegel[1]

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H-P2-11: Multimodal Characterization of Short-Range Order in Group IV Alloys with APT and 4D-STEM

[EFRC - μ-ATOMS] Xiaochen Jin[1], Sophia Lafia Arvin[2], Lilian Vogl[2], Shunda Chen[1], Peter Schweizer[2], Shang Liu[3], Jifeng Liu[3], Shui-Qing Yu[4], Tianshu Li[1], Andrew Minor[2]

[1]George Washington University; [2]University of California, Berkeley; [3]Dartmouth College; [4]University of Arkansas, Fayetteville

H-P2-12: Adding Functionality to Magnon Interconnects Using Spin-Orbit Torque

[EFRC - CEEMag] Orion Smedley[1], Kwangyul Hu[2], Thow Min Cham[1], Sanyum Channa[3], Anthony D'Addario[1], Minyong Han[3], Xiaoxi Huang[1], Kelly Luo[1], Daisy O'Mahoney[3], Wanyu (Tiffany) Zhao[1], Charles Zheng[3], Katja Nowack[1], Michael E. Flatté[2], Gregory D. Fuchs[1], Harold Y. Hwang[3], Daniel C. Ralph[1], Yuri Suzuki[3]

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H-P2-13: Integration of Chirality Induced Spin Selectivity with Conventional Optoelectronics

[EFRC - CHOISE] Matthew Hautzinger[1], Jiselle Y. Ye[1], Steven C. Hayden[1], Xin Pan[2], Z. Valy Vardeny[2], Joeseph J. Berry[1], Kirstin Alberi[1], Matthew C. Beard[1]

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H-P2-14: Current-induced modulation and enhanced antiferromagnetic tunnel readout for magnonics

[EFRC - CEEMag] Jaimin Kang[1], Anthony D'Addario[2], Shun Kong Cheung[1], Mohammad Hamdi[1], Eric Matt[1], Sevdenur Arpaci[1], Soho Shim[2], Wenyi Zhou[3], Yuqing Zhu[3], Roland Kawakami[3], Gregory Fuchs[2], Pedram Khalili[1]

[1]Northwestern University; [2]Cornell University; [3]The Ohio State University

J. Quantum Information Science

J-P2-1: First principles simulations of the optical cycle and coherence properties of spin defects

[CMS - MICCoM] Victor Yu[1], Siyuan Chen[2], Marco Govoni[1,2,3], François Gygi[4], Joseph Heremans[1], Benchen Huang[2], Yu Jin[2], Arpan Kundu[2], Jonah Nagura[2], Mykyta Onizhuk[2], Michael Toriyama[1], Jiawei Zhan[2], Cunzhi Zhang[2] Giulia Galli[1,2] (Director)
[1]Argonne National Laboratory; [2]University of Chicago; [3]University of Modena and Reggio Emilia; [4]University of California, Davis

J-P2-2: Excitation dynamics in out-of-equilibrium quantum materials

[CMS - NPNEQ] Xavier Andrade[1], Alfredo Correa[1], Tadashi Ogitsu[1], Jonah Haber[2,3], Chris Ciccarino[2,3], Felipe Jornada[2,3], Kevin Moseni[4], Sangeeta Rajpurohit[4], Revsen Karaalp[4], Liang Tan[4], David Prendergast[4], Andrew Grieder[5], Yuan Ping[5], Christian Jooss[6], Simone Techert[6,7], Peter E. Blochl[6,8], Marcos Calegari Andrade[1,9], Hiroyuki Takenaka[9]
[1]Lawrence Livermore National Lab; [2]SLAC National Accelerator Laboratory; [3]Stanford University; [4]Lawrence Berkeley National Laboratory; [5]University of Wisconsin-Madison; [6]Georg-August-Universität Göttingen; [7]Deutsches Elektronen-Synchrotron (DESY); [8]TU Clausthal; [9]University of California, Santa Cruz

J-P2-3: Crosscutting Theory and Machine-Learning Needs for Spin Manipulation in Magnetic-Molecule Arrays: Multi-Level Quantum Many-Body Hamiltonians and Ligand-Spin Optimization

[EFRC - M2QM] Mark Pederson[1], Chunjing Jia[2], Xiaoguang Zhang[2], Samuel Trickey[2], Richard Hennig[2], Hai-Ping Cheng[3], Garnet Chan[4]
[1]University of Texas at El Paso; [2]University of Florida; [3]Northeastern University; [4]California Institute of Technology

J-P2-4: Correlated and Topological Phases in Toy Lattice Systems in 2D and 3D

[EFRC - CATS] Caolan John, Joshua Wakefield, Paul Neves, Joseph Checkelsky
Massachusetts Institute of Technology

J-P2-5: Spin and orbital dynamics and chiral-optical properties from first-principles

[CCS - ADEPTs] Andrew Grieder[1], Joshua Quinton[2], Christian Multunas[2], Junting Yu[1], Kejun Li[1], Shihao Tu[1], Jacopo Simoni[1], Ravishankar Sundararaman[2], Yuan Ping[1]
[1]University of Wisconsin-Madison; [2]Rensselaer Polytechnic Institute

J-P2-6: Optimal Control of Numerical Errors in Relativistic Multiconfiguration Electronic Structure

[CCS - NEREST] Erica Mitchell[1], Robert Harrison[2], Edward Valeev[1]
[1]Virginia Polytechnic Institute and State University; [2]Stony Brook University

J-P2-7: Many-Body Excited-State Phenomena in Materials: Theory and Validation

[CMS - C2SEPEM] Steven G. Louie[1,2], James R. Chelikowsky[3], Jack R. Deslippe[1], Naomi Ginsberg[1,2], Felipe H. da Jornada[4], Zhenglu Li[5], Jeffrey B. Neaton[1,2], Diana Y. Qiu[6], Feng Wang[1,2], Chao Yang[1]
[1]Lawrence Berkeley National Laboratory; [2]University of California, Berkeley; [3]University of Texas at Austin; [4]Stanford University; [5]University of Southern California; [6]Yale University

J-P2-8: Ferroelectric Quantum Transducers: Materials Theory, Phase-Field Model, and Exascale Computing

[CMS - COMMS] Yujie Zhu[1], Aiden Ross[2], Saurav Shenoy[2], Anna N. Morozovska[3], Eugene A. Eliseev[3], Venkatraman Gopalan[2], Long-Qing Chen[2], Jiamian Hu[1]
[1]University of Wisconsin-Madison; [2]The Pennsylvania State University; [3]National Academy of Sciences of Ukraine

J-P2-9: Electronic Structure and Magnetism in Complex Quantum Materials

[EFRC - CATS] Andrew Eaton, Tyler Slade, Paul Canfield, Lin-Lin Wang, Benjamin Schrunk, Yevhen Kushnirenko, Tianxiong Han, Benjamin Ueland, Robert McQueeney, Adam Kaminski
Ames National Laboratory

J-P2-10: Quantum Correlations in Many-Body Systems

[EFRC - QuPIDC] Aanal Shah[1], Rahul Trivedi[2], Hadiseh Alaeian[1], Alisa Javadi[3]
[1]Purdue University; [2]Max Planck Institute of Quantum Optics; [3]University of Oklahoma

L. AI/ML

L-P2-1: Machine learning for the accurate modeling of electronic structure and reaction pathways in electrocatalysis

[CCS - BEAST] Nima Karimitari[1], Teerachote Pakornchote[1], Abdulaziz Alherz[2], Jacob Clary[3], Cooper Tezak[2], Derek Vigil-Fowler[3], Ravishankar Sundararaman[4], Charles Musgrave[2], Christopher Sutton[1]
[1]University of South Carolina; [2]University of Colorado Boulder; [3]National Renewable Energy Laboratory; [4]Rensselaer Polytechnic Institute

L-P2-2: Multiscale Modeling of Biomolecular Energy Transduction: Coarse-Graining, Machine Learning, and Mesoscopic Dynamics

[CCS - CMSET] Jiangbo Wu[1], Siva K. Dasetty[1], Tomasz Skora[2], Thomas Qu[1], Sahithya Sridharan Iyer[1], Tamara Bidone[2], Andrew Ferguson[1], Gregory Voth[1]

[1]University of Chicago; [2]University of Utah

L-P2-3: ChemFM: A Foundation Model for Chemical Design and Property Prediction

[EFRC - AIM] Feiyang Cai[1], Katelin Hanna[1], Tianyu Zhu[1], Tzuen-Rong Tzeng[1], Yongping Duan[2], Ling Liu[3], Srikanth Pilla[4], Gang Li[1], Feng Luo[1]

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L-P2-4: Autonomous materials discovery via ML-enabled scanning probe microscopy: from structure-property relationships to combinatorial libraries

[EFRC - 3DFeM2] Yu Liu[1], Ian Mercer[2], Kamyar Barakati[1], Aditya Raghavan[1], Ichiro Takeuchi[3], Jon-Paul Maria[2], Sergei V. Kalinin[1,4]

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L-P2-5: Web-Application Workflow for Simulations of Correlated and Magnetic Materials

[CMS - HeteroFAM] Jenna Pope[1], Henry Sprueill[1], Nicholas Bauman[1], Bhumika Jayee[1], Duo Song[1], Manh Nguyen[1], Peter Sushko[1], Ting Cao[2], Eugene Ilton[1], Eric Bylaska[1]

[1]Pacific Northwest National Laboratory; [2]University of Washington

L-P2-6: exa-AMD: A scalable ML-guided framework for rapid materials discovery and design

[CMS - MLAMD] Ying Wai Li[2], Weiyi Xia[1], Maxim Moraru[2], Feng Zhang[1], Yongxin Yao[1], Vladimir Antropov[1], Ryan Richard[1], Cai-Zhuang Wang[1]

[1]Ames National Laboratory; [2]Los Alamos National Laboratory

L-P2-7: Understanding the phase diagram of dense Hydrogen using Machine-Learning based Interatomic potentials trained on Quantum Monte-Carlo data

[CMS - QMC-HAMM] Kevin Kleiner[1], Sonali Joshi[1], Woncheol Lee[2], Alexander Hampel[3], Malte Rosner[4], Cyrus Dreyer[3,5], Lucas K. Wagner[1]

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M. Research at the Exascale

M-P2-1: A Meta-Generalized Gradient Approximation Exchange-Correlation Functional for Strongly Coupled Light-Matter Systems

[CCS - MAPOL] Daniel Mejia Rodriguez, Niranjan "Niri" Govind
Pacific Northwest National Laboratory

M-P2-2: exa-PD: A massively parallelizable computational scheme for multi-element phase diagram prediction

[CMS - MLAMD] Feng Zhang[1], Zhuo Ye[1], Weiyi Xia[1], Yongxin Yao[1], Ying Wai Li[2], Maxim Moraru[2], Ryan Richard[1], Cai-Zhuang Wang[1]
[1]Ames National Laboratory; [2]Los Alamos National Laboratory

M-P2-3: Many-Body Excited-State Phenomena in Materials: Methods and Software

[CMS - C2SEPEM] Steven G. Louie[1,2], James R. Chelikowsky[3], Jack R. Deslippe[1], Naomi Ginsberg[1,2], Felipe H. da Jornada[4], Zhenglu Li[5], Jeffrey B. Neaton[1,2], Diana Y. Qiu[6], Feng Wang[1,2], Chao Yang[1]
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M-P2-4: Quantum Monte Carlo Methodological Advances for Correlated Quantum Materials

[CMS - CPSFM] J. Krogel[1], C. Melton[2], R. Clay[2], B. Kincaid[3], L. Mitas[3], A. Lopez[4], B. Rubenstein[4], H. Shin[5], P. Kent[1]
[1]Oak Ridge National Laboratory; [2]Sandia National Laboratories; [3]North Carolina State University; [4]Brown University; [5]Argonne National Laboratory

M-P2-5: Quantum Electrodynamics Coupled-Cluster at Scale: High Performance Implementation for Complex Systems

[CCS - MAPOL] Himadri Pathak, Marcus Liebenthal, Nicholas Bauman, Ajay Panyala, Daniel Mejia Rodriguez, Niranjan "Niri" Govind, Karol Kowalski
Pacific Northwest National Laboratory

M-P2-6: Deploying Novel Computational Toolkit to Design Catalysts for Single-electron Reduction of CO_2

[CCS - ExaQC] George Baffour Pipim, Shaama Mallikarjun Sharada, Anna Krylov
University of Southern California

N. Operando Techniques

N-P2-1: Development of Operando X-ray spectroscopy methods for understanding the electronic structure of water oxidation catalysts

[EFRC - CEDARS] Aaron Kaufman[1], Johannes Mahl[1], Soyoung Kim[1], Mengxin Liu[2], Ikenna Chris-Okoro[2], Sheilah Cherono[2], Eric Jiahan Zhao[3], Yiming Ding[3], Lei Zhang[4], Geoffroy Hautier[4], Tanja Cuk[5], Jin Suntivich[3], Dhananjay Kumar[2], Ethan Crumlin[1], Junko Yano[1]

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N-P2-2: Synergizing Experimental and Kinetic Modeling Design to Understand Reactive Carbon Capture

[EFRC - 4C] Momoko Ishida[1], Jason Pfeilsticker[2], Robert Sacci[5], Gabriel Veith[5], Joel Haber[4], Christopher Hahn[3], Wilson Smith[2], Carlos G. Morales-Guio[1]

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N-P2-3: Exploring zero-gap electrochemical CO_2 reduction cell under simulated diurnal conditions

[Hub - LiSA] Sol A. Lee[1,2], Mason Jang[1,2], Zhiyuan Qi[2], Lily Shiau[1,2], Laura Paradis-Fortin[3], Dilworth Y. Parkinson[3], Walter S. Drisdell[3], Adam C. Nielander[1,4], Chengxiang Xiang[1,2], Harry A. Atwater[1,2]

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N-P2-4: In-Situ Characterization of Well-Defined Ruthenium Oxide Surfaces Using Non-Linear Spectroscopy

[EFRC - CEDARS] Brady Bruno[1], Austin Reese[1], Luka Mitrovic[1], Neha Wadehra[1], Simon Gelin[2], Lei Zhang[3], Eric Zhao[1], Jacob Som[1], Swapnil Nalawade[4], Shyam Aravamudhan[4], Ismaila Dabo[2], Geoffroy Hautier[3], Darrell Schlom[1], Jin Suntivich[1]

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N-P2-5: Understanding the Effects of Optically Excited Phonons on Proton Conductivity in Yttrium-doped Barium Zirconate

[EFRC - HEISs] Sara Sand[1], Jie Song[1], Madison Schwinn[1], Matthew Baldwin[1], Supriyo Majumder[1], James Rondinelli[1], Lin Chen[1,2], Sossina Haile[1]

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N-P2-6: Correlative Characterization Crosscut: Advancing a Multimodal Characterization Pipeline for Emerging Energy Storage Chemistries

[Hub - ESRA] Ethan Crumlin[1], Kamila Wiaderek[2], Nitash Balsara[1,3], James Burrow[2,4], Ying Chen[5], Miaofang Chi[6], Neil Dasgupta[7], Tim Fister[2], Betar Gallant[8], Kelsey Hatzell[9], Chong Liu[4], Di-Jia Liu[2], Lauren Marbella[10], Bryan McCloskey[1,3], Y. Shirley Meng[2,4], Mary Scott[1,3], Yuyan Shao[5], Oleg Shpyrko[11], Wei Wang[5]

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N-P2-7: Watching Soft Photoelectrodes in Action: Multiscale Probes of Polymer Structure–Function Dynamics

[EFRC - SPECS] Yael Tsarfati[1,2], Henry Kantrow[3], Arianna Magni[1], Jude Kpare[3], Casey Davis[4], Spencer Yeager[5], Megan Brown[6], William Kopcha[7], Aiswarya Abhisek Mohapatra[4], Sa Suo[8], Tim Lian[8], Michael Toney[4], Melissa Gish[7], Andrew Ferguson[7], Obadiah Reid[4,7], Chad Risko[6], Erin Ratcliff[3], Natalie Stingelin[3], Alberto Salleo[1,9]

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N-P2-8: H incorporation into triple conducting films: identifying surface reactions and kinetics with high-throughput structural, spectroscopic, and relaxation analysis

[EFRC - HEISs] Alexia Popescu[1], Supriyo Majumder[2], Zhen Jiang[2], Yong-Yun Hsiau[1], Sophia Chen[2], Guennadi A. Evmenenko[2], Paul A. Chery[2], Noah B. Welke[2], D. Bruce Buchholz[2], Christopher M. Wolverton[2], Sossina M. Haile[2], Nicola H. Perry[1], Michael J. Bedzyk[2]

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N-P2-9: Operando Characterization and Electrochemical Cell Engineering of Energy Materials and Devices

[EFRC - CABES] Andrej Singer, Saptarsi Das

Cornell University

N-P2-10: Nanoscale Characterization of Ultrafast Mott switching up to GHz Frequency Operation

[EFRC - Q-MEEN-C] Alexandre Pofelski[1], C. Liu[1], S. A. Reisbick[1], MG Han[1], L. Wu[1], H. Navarro[2], E. Qiu[2], T. D. Wang[2], D.J. Alspaugh[2], M. Rozenberg[2,3], S. Ramanathan[4], I.K. Schuller[2], and Y. Zhu[1]

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POSTER SESSION III

B. Catalysis

B-P3-1: Integrated Capture and Electrochemical Conversion of Imidazolium Carboxylates

[EFRC - 4C] Jared Stanley[1], Ciara Gillis[1], Hunter Pauker[1], Erin Kuker[1], Manu Gautam[2], Dominic Ross[3], Shawn Chiu[4], Tyler Kwak[4], Aaron Gaynes[5], Leila Filien[6], Chris Margolis[1], Ariel Rodriguez-Gutierrez[7], Vy Dong[1], Marsha Massey[7], Chantal Stieber[5], Robert Nielsen[1], Charles McCrory[6], Carlos Morales-Guio[4], Joshua Spurgeon[2], Anastassia Alexandrova[4], Christopher Hahn[3], Jenny Yang[1]

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B-P3-2: Multiscale Kinetic Modeling to Drive Rate Enhancement in Programmable Catalysis

[EFRC - CPEC] Rajat Daga, Jesse Canavan, Paul Dauenhauer, Matthew Neurock

University of Minnesota, Twin Cities

B-P3-3: Automated Generation of Microkinetic Models for Heterogeneous Catalysis

[CCS - ECC] Sevy Harris[1], Prosper Lekia[1], Azeez Akinyemi[1], Kirk D. Bager[2], Matthew S. Johnson[3], C. Franklin Goldsmith[2], Richard H. West[1]

[1]Northeastern University; [2]Brown University; [3]Sandia National Laboratories, Livermore

B-P3-4: Fundamental insights on electrodissolution from a density functional theory's point of view

[Hub - LiSA] Richard Kang[1,2,3], Yang Zhao[1,2,3], Catherine S. Wallace[1,2,3], Karnamohit Ranka[1,2], Frances A. Houle[1,2], Shannon W. Boettcher[1,2,3], Martin P. Head-Gordon[1,2,3]

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B-P3-5: Influence of Metal Ion Contaminants on Amine-Based Solid Sorbents

[EFRC - UNCAGE-ME] Botagoz Kuspangaliyeva, Christopher Jones, Ryan Lively

Georgia Institute of Technology

B-P3-6: Modeling the Kinetics and Co-polymer Microstructure Evolution in Hydrodechlorination of PVC to Polyethylene

[EFRC - iCOUP] Emmanuel Ejiogu[1], Tyeshia Sapp[2], Megan Fieser[2], Baron Peters[1]

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B-P3-7: Enabling the Chemical Deconstruction of Multilayer and Additive-Containing Polyolefin Waste into Valuable Chemicals via Catalyst Design

[EFRC - CPI] Christine M. Oberhausen, Ali Kamali, Jaqueline Ngu, Jessie Sun, Pedro Reis Moura, Esun Selvam, Zoé Schyns, Piaoping Yang, Keira Auchenbach, Alexander Bregvadze, Pavel Kots, Zachary Hinton, Sean Najmi, Brandon Vance, Caitlin Quinn, Weiqing Zheng, Thomas Epps, III, LaShanda T. J. Korley, Dongxia Liu, Dionisios Vlachos
University of Delaware

B-P3-8: Exascale Multireference Wave Function Theory Methods for Polymer Upcycling Catalysis

[CCS - ExaPUC] Rishu Khurana[1,2], Valay Agarawal[2], Matthew Hermes[2], Christopher Knight[1], Laura Gagliardi[2], Cong Liu[1,2]
[1]Argonne National Laboratory; [2]University of Chicago

B-P3-9: Polyethylene Upcycling via Acid-Catalyzed Olefin Formation and Alkylation Reactions

[EFRC - iCOUP] Alexandra Heuston[1], Rudan Feng[1], Danielle Burns[1], Jiankai Ge[1], Baron Peters[2], Andreas Heyden[3], Anne LaPointe[4], Mahdi Abu-Omar[1], Susannah Scott[1], Wenyu Huang[5], Simin Sun[5]
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B-P3-10: Enhanced gas solubility and additive-modulated contact angle in confined polymers

[EFRC - CPI] Kaiwen Wang[1], Joseph Tapia[2], Tian Ren[1], Peng Bai[2], John Vohs[1], Raymond Gorte[1], Daeyeon Lee[1]
[1]University of Pennsylvania; [2]University of Massachusetts Amherst

B-P3-11: Impact of SO_2 on NiFe Nanoparticle Exsolution and Dissolution from $LaFe_{0.9}Ni_{0.1}O_3$ Perovskite Oxides

[EFRC - UNCAGE-ME] Musa Najimu[1,2], Matthew Hurlock[3], Sahanaz Parvin[4], Courtney Brea[5], Neelesh Kumar[4], Yoon Jin Cho[6], Yiqing Wu[7], Guoxiang Hu[5], Zili Wu[7], Eranda Nikolla[6], Jonas Baltrusaitis[4], Tina Nenoff[8], Israel Wachs[4], Kandis Leslie Gilliard-AbdulAziz[1,2]
[1]University of Southern California; [2]University of California, Riverside; [3]Pacific Northwest National Laboratory; [4]Lehigh University, [5]Georgia Institute of Technology; [6]University of Michigan; [7]Oak Ridge National Laboratory; [8]Sandia National Laboratories

B-P3-12: Design of Multicomponent Interphase Coatings for Enhanced Nanoreactor Redox Selectivity

[EFRC - EPN] W. Wilson McNeary[1], Bradley W. Layne[2], William D. H. Stinson[3], Wenjie Zang[2], Moaz Waqar[2], Fikret Aydin[4], Yuichi Yamaguchi[5], Tuan Anh Pham[4], Akihiko Kudo[5], Shane Ardo[2], Young-Seok Shon[6], Oluwaseun I. Salako[7], Xiaoqing Pan[2], Tadashi Ogitsu[4], Daniel V. Esposito[3], Katherine E. Hurst[1]

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B-P3-13: Bacterial Microcompartment Assembly, Permeability, and Crowding through the Lens of a Computational Microscope

[EFRC - CCBC] Saad Raza, Neetu Yadav, Alexander Jussupow, Ananya Chakraborti, Michael Feig, Josh V. Vermaas

Michigan State University

B-P3-14: Influence of Surface Charge on Binding Energies, Activation Energies, and Scaling Relationships

[EFRC - CPEC] Rohit Punyapu[1], Dia Sahsah[2], Lars Grabow[2], Rachel B. Getman[1]

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B-P3-15: Polyethylene Hydrogenolysis with Ni/Co/Al2O$_3$ catalyst: High-Throughput Data-Driven Discovery to Valuable Products

[EFRC - iCOUP] Carly Byron[1], Katherine McCullough[1], Jacklyn Hall[1], Salai Ammal[2], Andreas Heyden[2], Jacob Bryant[1], Yi-Yu Wang[3,4], Kajol Tonk[3,4], Jianguo Wen[1], A. Jeremy Kropf[1], Wenyu Huang[3,4], Aaron D. Sadow[3,4], Massimiliano Delferro[1], Magali Ferrandon[1]

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B-P3-16: Free Energy and Surface Dynamics in Heterogeneous Catalysis via Machine Learning and Enhanced Sampling; Solution-Phase Uptake of LOHCs in Zr MOF-808

[EFRC - CD4DC] Yinan Xu[1], Yezhi Jin[1], Jireh S. Garcia[1], Jacob T. Bryant[2], Jan Hofmann[3], Magali Ferrandon[2], Karena W. Chapman[3], Massimiliano Delferro[2], Juan J. de Pablo[4]

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B-P3-17: Decoding Photocatalytic Function in Doped SrTiO$_3$ Nanoparticles using Multi-modal Electron Microscopy

[EFRC - EPN] Pushp Raj Prasad[1], Levi Brown[1], Levi Palmer[2], Bradley Layne[1], Zejie Chen[1], Brian Zutter[3], Akihiko Kudo[4], Shane Ardo[1], A. Alec Talin[3], Scott K. Cushing[2], Xiaoqing Pan[1], Joseph P. Patterson[1]

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D. Energy Storage

D-P3-1: Scaling Self-Interaction Correction in DFT: Theory and Applications

[CCS - FLOSIC] Rohan Maniar[1], Priyanka B Shukla[2], Chandra Shahi[1], Raj Sah[3], Jinliang Ning[1], J. Karl Johnson[2], Koblar A. Jackson[4], Juan E. Peralta[4], John P. Perdew[1]

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D-P3-2: Accelerating CoHBEs and Microemulsion Electrolyte Development: Coupling Active Learning with High-Throughput Experimentation and Modeling

[EFRC - BEES2] Eliandreina Cruz-Barrios[1], Emily Pentzer[1], Bryn Jenkins[1], Adam Imel[2], Yong Zhang[3], Edward Maginn[3], Thomas Zawodzinski[2]

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D-P3-3: Progress in Low Tg TFSI-Based Polyzwitterion/Polyanion Blends

[EFRC - FaCT] Autumn Kudlack[1], Hongwei Li[1], Yuya Shinohara[2], Zitan Huang[3], Michelle Lehmann[2], Tomonori Saito[2], Ralph Colby[3], Jodie Lutkenhaus[1]

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D-P3-4: Mechanistic Studies of p-Si Hybrid Photoelectrodes

[Hub - CHASE] Pierpaolo Vecchi[1], John Dickenson[1], Niklas Keller[1], Shi He[1], Bo Shang[2], Fengyi Zhao[3], Samuel Bottum[1], Ryan Gentile[1], Gabriella Bein[1], Rebecca Powers[1], Hannah Margavio[4], Oluwaseun Oyetade[1], Taylor Teitsworth[1], Samuel Shin[1], Sa Suo[3], Yuanzuo Gao[2], Colton Sheehan[5], Sungho Jeon[5], Jing Li[2], Conor Rooney[2], Oliver Leitner[2], Langqiu Xiao[5], Zihao Xu[3], Hanqing Fan[2], Menachem Elimelech[2], Leizhi Wang[2], Yunchangxiang Zheng[3], Jinhui Meng[3], Zhicheng Yang[3], David C. Grills[6], Jillian Dempsey[1], Alexander Miller[1], Renato Sampaio[1], Stephen Tereniak[1], Carrie Donley[1], Dmitry Polyansky[6], Matthew Lockett[1], Gregory Parsons[4], James Cahoon[1], Eric Stach[5], Thomas Mallouk[5], Hailiang Wang[2], Gerald Meyer[1], Tianquan Lian[3]

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D-P3-5: Unraveling the controls of rock permeability change during volatile-consuming reactions

[EFRC - GMCS] Hongwei Wu, Giuseppe Buscarnera
Northwestern University

D-P3-6: Electrochemically Driven Fracture Processes

[EFRC - MUSIC] Neil Dasgupta[1], Manoj Jangid[1], Cole Fincher[2]
[1]University of Michigan; [2]Massachusetts Institute of Technology

D-P3-7: Electrochemistry Beyond Solutions

[EFRC - m2M#s] David Arnot[1], Shan Yan[2], Alexis Pace[1], Esther Takeuchi[1,2], Amy Marschilok[1,2], Carlos Colosqui[1], Kenneth Takeuchi[1,2]
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D-P3-8: Energy Storage Research Alliance: Ion Choreography

[Hub - ESRA] Paul Fenter[1], Nitash Balsara[2,3], James Burrow[1,4], Jordi Cabana[1,5], Gerbrand Ceder[2,3], Maria Chan[1], Miaofang Chi[6], Ethan Crumlin[2], Timothy Fister[1], Kelsey Hatzell[7], Yiyang Li[8], Chong Liu[4], Y. Shirley Meng[1,4], Vijay Murugesan[9], Shrayesh Patel[1,4], Kristin Persson[2,3], Mary Scott[2,3], Oleg Shpyrko[10], Venkat Srinivasan[1]
[1]Argonne National Laboratory; [2]Lawrence Berkeley National Laboratory; [3]University of California, Berkeley; [4]University of Chicago; [5]University of Illinois at Chicago; [6]Duke University; [7]Princeton University; [8]University of Michigan; [9]Pacific Northwest National Laboratory; [10]University of California, San Diego

D-P3-9: Tuning Phase Morphology in a Model Ribbon-like Polymer Semiconductor & its Implications on Charge Transfer

[EFRC - SPECS] Jude Kpare[1], Spencer Yeager[2], Henry Kantrow[1], Arianna Magni[3], Thomas Spradley[1], Michel De Keersmaecker[1], Casey Davis[4], Ruipeng Li[5], Michael Toney[4], Alberto Salleo[3], Erin Ratcliff[1], Natalie Stingelin[1]
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D-P3-10: Inorganic and Polymeric Thin Films on Hybrid Photoelectrodes for Catalyst Stabilization and Reaction Product Control

[Hub - CHASE] Oluwaseun Oyetade[1], Hyuenwoo Yang[2], Ryan Gentile[1], Marisé Garcia-Batlle[1], Pablo Fernandez[1], John Dickenson[1], Samuel Bottom[1], Yuchen Liu[2], Bo Shang[3], Cole Hodges[2], Hannah Margavio[2], Carrie Donley[1], Renato Sampaio[1], Hailiang Wang[3], Gerald Meyer[1], Rene Lopez[1], James Cahoon[1]
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D-P3-11: Disorder from the Atomic to the Mesoscale: Elucidation of Point Defects, Short Range Order and Stacking Faults in High Entropy Oxides

[EFRC - m2M#s] Zachary Mansley[1], Jessica Luo[2], Cynthia Huang[2], Marie Millares[2], Patrick Barry[2], Zhongling Wang[2], Armando Rodriguez Campos[2], Esther Takeuchi[1,2], Amy Marschilok[1,2], Kenneth Takeuchi[1,2], Yimei Zhu[1]

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D-P3-12: MUSIC Cross-cutting Advanced Materials Characterization

[EFRC - MUSIC] Miaofang Chi[1], Kelsey Hatzell[2], Ana Claus[2]

[1]Oak Ridge National Laboratory; [2]Princeton University

F. Energy-Water

F-P3-1: Modeling Transport in Charged Nanopores: Nanoconfinement and Non-equilibrium Electrostatics

[EFRC - AMEWS] Joan M. Montes de Oca[1], Andres Cordoba[1], Wen Chen[1,2], Paul F. Nealey[1,2], Seth B. Darling[1,2], Juan J. de Pablo[1,2,3]

[1]University of Chicago; [2]Argonne National Laboratory; [3]New York University

F-P3-2: Formulation and Validation of a Nanoconfined Equation of State Using Thermally Driven Isobars Within Single Digit Nanopores

[EFRC - CENT2] Sanjay S. Garimella[1], Yu-Ming Tu[2], Rahul P. Misra[1], Lukas Arcuri[3], Samuel Faucher[1], Matthias Kuehne[4], Cody L. Ritt[1,5], Joshika Chakraverty[1], Xintong Xu[6], Hananeh Oliaei[7], Arun Majumdar[6], Narayan Aluru[7], Daniel Blankschtein[1], Michael S. Strano[1]

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F-P3-3: Elucidating Solute Thermodynamics and Kinetics in Membrane Materials with NMR and FTIR Spectroscopy

[EFRC - M-WET] Leo W. Gordon, Jonathan Aubuchon Ouimet, Rahul Sujanani, Phillip Christopher, Rachel A. Segalman, Raphaële J. Clément

University of California, Santa Barbara

F-P3-4: Quantitative Insights into Electrocatalyst Driven ROS Selectivity for Advanced Water Treatment

[EFRC - AMEWS] Igor Messias, Jacob Kupferberg, Caroline K. Williams, Ronnie Emmons, Ashley Bielinski, Alex Martinson, Pietro Papa Lopes

Argonne National Laboratory

F-P3-5: Leveraging Computational Chemistry to Unravel the Role of Confinement and Chemical Interactions on Water and Ion Transport Inside Metal-Organic Frameworks

[EFRC - CENT2] Akash Ball[1], Camille Violet[2], Omar Khalifa[2], Shuwen Yue[1], Amir Haji-Akbari[2], Menachem Elimelech[2], Heather Kulik[1]

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F-P3-6: Synthesis, Characterization, and Hydration Evaluation of Zwitterionic-based Membranes

[EFRC - M-WET] Suzana Ivandic[1], Harrison Landfield[2], Justin Yun[2], Craig Hawker[2], Chris Bates[2], Scott Shell[2], Rachel Segalman[2], Lynn E. Katz[1], Benny Freeman[1]

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F-P3-7: Vapor Phase Functionalization using Atomic Layer Deposition for Advanced Water Treatment

[EFRC - AMEWS] Bratin Sengupta[1,2], Vepa Rozyyev[1,3], Yining Liu[1,3], Noa Ram[4], Tamar Segal-Peretz[4], Seth B. Darling[1,3], Jeffrey W. Elam[1]

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F-P3-8: Physics-Based Modeling of Ion Transport in Electrically Gated MXene Membranes

[EFRC - CENT2] Arjun V. Yennemadi[1], Aaditya Pendse[2], Aleksandr Noy[2], Martin Z. Bazant[1]

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F-P3-9: Descriptors of Water's Local Structure from Computational X-ray Photoelectron Spectroscopy

[CCS - SPEC] Daniel Mejia-Rodriguez[1], Bo Peng[1], Ajay Panyala[1], Kristina M. Herman[2], Joseph P. Heindel[2], Edoardo Aprà[1], Niranjan Govind[1,2], Karol Kowalski[1,2], Sotiris S. Xantheas[1,2]

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H. Microelectronics

H-P3-1: Multiscale computations of organic mixed ionic-electronic conductors for neuromorphic devices

[CMS - MICCoM] Cesar Castro-Rubio[1,2], Yucheng Zhang[2], Jonathan K. Whitmer[3], Andrew Ferguson[4], Jie Xu[2,4], Juan de Pablo[1]

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H-P3-2: Integrating theory and experiments to predict materials for neuromorphic computing

[EFRC - Q-MEEN-C] Matthew Frame[1], Yongjin Shin[2], Shenli Zhang[2,3], Mingzhen Feng[1], Junjie Li[4], Alexandre Pofelski[5], Slavomir Nemsak[6], Christoph Klewe[6], Alpha N'Diaye[6], Dongwoo Kim[6], Gustavo Girotto[6], Maximilian Jaugstetter[6], Yimei Zhu[5], Ivan Schuller[4], Giulia Galli[2], Yayoi Takamura[1]

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H-P3-3: Understanding Conductance Switching in Transition Metal Coordination Complexes and Frameworks

[EFRC - reMIND] Alejandro Aviles[1], Saul Perez Beltran[1], Maryam Ghotbi[1], Donald Robinson[2], Jeffrey L. Blackburn[3], Dakota Jones[1], Kim Dunbar[1], Sarnali Sanfui[1], Akhil K. Singh[1], Marcetta Y. Darensbourg[1], A. Alec Talin[2], Andrew J. Ferguson[3], Perla B. Balbuena[1]

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H-P3-4: Precision Mapping of Short-Range Ordering Beyond Random Mixing

[EFRC - μ-ATOMS] Anis Attiaoui[1,2], Shunda Chen[3], Joseph C. Woicik[4], Tianshu Li[3], and Paul C. McIntyre[1,2]

[1]Stanford University; [2]SLAC National Accelerator Laboratory; [3]George Washington University; [4]National Institute of Standards and Technology

H-P3-5: Spin Oscillators Leveraging Complex Oxides and Magnetoelastic Coupling for Neuromorphic Computing

[EFRC - Q-MEEN-C] Padma Radhakrishnan[1], Robin Klause[2], Zhixin Zhang[2], Biswajit Sahoo[3], Katherine Matthews[3], Ahmet Koral Aykin[1], Juan Andres Hofer[3], Alex Frano[3], Ivan K. Schuller[3], Axel Hoffmann[2], Eric E. Fullerton[3], Andrew D. Kent[1]

[1]New York University; [2]University of Illinois Urbana-Champaign; [3]University of California, San Diego

H-P3-6: Excitons in 2D Magnets: quantitative and qualitative limitations of Tanabe-Sugano diagrams

[CCS - QuestC] Swagata Acharya[1], Dimitar Pashov[2], Mark van Schilfgaarde[1]

[1]National Renewable Energy Laboratory; [2]King's College London

H-P3-7: Selective Deposition through Growth-Promoter and Precursor Design Towards High-Precision Pattern Transfer

[EFRC - CHiPPS] Beihang Yu[1], Maggy Harake[2], Yujin Lee[2], Stacey F. Bent[2], Ricardo Ruiz[1]

[1]Lawrence Berkeley National Laboratory; [2]Stanford University

H-P3-8: Semiconductor properties of $NiGa_2O_4$ and $In_2Ge_2O_7$ materials at oxide power electronic interfaces

[EFRC - APEX] Krishna Acharya[1], Kingsley Egbo[2], Cheng-Wei Lee[1], Emily Garrity[1], Shivashree Shivamade[3], Ethan Scott[3], Patrick Hopkins[3], Michelle Smeaton[2], Steven Spurgeon[2], Vladan Stevanovic[1], Andriy Zakutayev[2]

[1]Colorado School of Mines; [2]National Renewable Energy Laboratory; [3]University of Virginia

H-P3-9: Semiconductor-Compatible Topological Digital Alloys

[EFRC - µ-ATOMS] Yunfan Liang[1], Adelaide Bradicich[2], Ram Joshi[3], Shunda Chen[4], Shengbai Zhang[1], Damien West[1], Ezra Bussmann[2], Hiro Nakamura[3], Tianshu Li[4], Shui-Qing Yu[5], Jifeng Liu[6]

[1]Rensselaer Polytechnic Institute; [2]Sandia National Laboratories; [3]University of Arkansas; [4]George Washington University; [5]University of Arkansas; [6]Dartmouth College

H-P3-10: Designing High-Performance Electro-Optic Materials Using the Phase-Field Method

[CMS - COMMS] Aiden Ross[1], Sankalpa Harza[1], Mohamed S. M. M. Ali[1,2], Albert Suceava[1], Akash Saha[1], Anya Kennedy Frazer[1,3], Ian Reed Philippi[1], Dylan Sotir[4], Rui Zu[1], Darrell G. Schlom[4], Ismaila Dabo[1,2], Venkatraman Gopalan[1], Long-Qing Chen[1]

[1]The Pennsylvania State University; [2]Carnegie Mellon University; [3]University of North Carolina; [4]Cornell University

H-P3-11: Thermal conductivity and interface resistances of UWBG materials and substrates for heterogeneous integration

[EFRC - APEX] Shivashree S. Gowda[1], Ethan Scott[1], Evan Crites[2], Tyrel M. McQueen[2], MVS Chandrashekhar[3], Michael Spencer[3], Andriy Zakutayev[4], Steven R. Spurgeon[4], Brooks Tellekamp[4], Jessica L. McChesney[5], Nancy M. Haegel[4], Patrick E. Hopkins[1]

[1]University of Virginia; [2]Johns Hopkins University; [3]Morgan State University; [4]National Renewable Energy Laboratory; [5]Argonne National Laboratory

H-P3-12: Sequence-defined polypeptoid photoresists for reducing material stochastics in photolithography

[EFRC - CHiPPS] Cameron P. Adams[1], Chenyun Yuan[2], Aung Paing[3], Oleg Kostko[4], Frances A. Houle[4], Christopher K. Ober[2], Rachel A. Segalman[1]

[1]University of California, Santa Barbara; [2]Cornell University; [3]San Jose State University; [4]Lawrence Berkeley National Laboratory

H-P3-13: Two-dimensional van der Waals magnets for magnonics

[EFRC - CEEMag] Rabindra Basnet[1], Mohammad Hamdi[2], Rakshit Jain[3], Jaimin Kang[2], Ziling Li[4], Yogendra Limbu[5], Hari Paudyal[5], Matthew Roddy[3], Wenyi Zhou[4], Yuqing Zhu[4], Pedram Khalili[2], Durga Paudyal[5], Daniel Ralph[3], Michael Flatté[5], Ramesh Budhani[1], Roland Kawakami[4]

[1]Morgan State University; [2]Northwestern University; [3]Cornell University; [4]The Ohio State University; [5]University of Iowa

H-P3-14: Remote Chirality Transfer and Spin Selectivity in Hybrid Metal Halide Semiconductors

[EFRC - CHOISE] Md Azimul Haque[1], Margherita Taddei[1], Andrew Grieder[2], Jiselle Y. Ye[1], Bennett Addison[1], Junxiang Zhang[3], Yi Xie[4], Matthew P. Hautzinger[1], Heshan Hewa Walpitage[5], Ian A. Leahy[1], Jeiwan Tan[1], Pius Markus Theiler[1], Aeron McConnell[6], Andrew H. Comstock[6], Yifan Dong[1], Kai Zhu[1], Kirstin Alberi[1], Jeffrey L. Blackburn[1], Zeev Valy Vardeny[5], David B. Mitzi[4], Joseph J. Berry[1,3], Laura Schelhas[1], Stephen Barlow[3], Seth R. Marder[1,3], Peter Sercel[7], Dali Sun[6], Yuan Ping[2], Joseph M. Luther[1,3], Matthew C. Beard[1,3]

[1]National Renewable Energy Laboratory; [2]University of Wisconsin-Madison; [3]University of Colorado Boulder; [4]Duke University; [5]University of Utah; [6]North Carolina State University; [7]Center for Hybrid Organic Inorganic Semiconductors for Energy

H-P3-15: Single-crystal freestanding magnetic membrane fabrication and characterization for magnonic applications

[EFRC - CEEMag] Alexander H. Reid[1], Ella R. Blake[1,2], Tiffany C. Wang[1,2], Jacob J. Wisser[2], Varun Harbola[1,2], Anthony D'Addario[3], Soho Shim[3], Mohammad Hamdi[4], Yogendra Limbu[5], Matthias Hoffmann[1], Pedram Khalili[4], Michael Flatté[5], Gregory D. Fuchs[3], Harold Hwang[1,2], Yuri Suzuki[1,2]

[1]SLAC National Accelerator Laboratory; [2]Stanford University; [3]Cornell University; [4]Northwestern University; [5]University of Iowa

H-P3-16: Chemical Vapor Deposition Growth of Cubic UWBG Semiconductors Including Diamond and Cubic Boron Nitride

[EFRC - ULTRA] Timothy Grotjohn[1], Robert Nemanich[2], Fernando Ponce[2], Mary Ellen Zvanut[3], Arunima Singh[2], David Smith[2], Srabanti Chowdhury[4], Richard Wilson[5], Alexander Balandin[5], Matthias Muehle[6], Aaron Hardy[6], Franz Koeck[2], Alec Fischer[2], Tathagata Biswas[2], Cody Milne[2], Saurabh Vishakarma[2], Shafiqul Mollik[3], Mohamadali Malakoutian[4], Kelly Woo[4], Frank Angeles[5], Erick Guzman[5], Fariborz Kargar[5]

[1]Michigan State University; [2]Arizona State University; [3]University of Alabama at Birmingham; [4]Stanford University; [5]University of California, Riverside; [6]Fraunhofer USA CMW

I. Nuclear

I-P3-1: Influence of He irradiation on microstructure and oxidation in Fe-Cr alloys

[EFRC - FUTURE] Jijo Christudasjustus[1], Mira Khair[2], Kayla Yano[1], Daniel Schreiber[1], Peter Hoseman[3], Elizabeth Sooby[2], Tiffany Kaspar[1]

[1]Pacific Northwest National Laboratory; [2]University of Texas at San Antonio; [3]University of California, Berkeley

I-P3-2: Mechanism of extended defect evolution in irradiated oxides and nitrides

[EFRC - TETI] Anshul Kamboj[1], Md Minaruzzaman[2], Lin-Chieh Yu[3], Kaustubh Bawane[1], Zilong Hua[1], Lin Shao[4], Marat Khafizov[2], Yongfeng Zhang[3], Miaomiao Jin[5], Jennifer Watkins[1], David Hurley[1], Boopathy Kombaiah[1],

[1]Idaho National Laboratory; [2]The Ohio State University; [3]University of Wisconsin; [4]Texas A&M University; [5]The Pennsylvania State University

I-P3-3: Validation of $ThCl_4$ Molten Salt Structures via Machine Learning and Computational Raman Spectroscopy

[EFRC - MSEE] Luke D. Gibson[1], Rajni Chahal[1], Raphael N. Ogbodo[2], Matthew Emerson[3], Santanu Roy[1], Claudio Margulis[2], Vyacheslav S. Bryantsev[1]

[1]Oak Ridge National Laboratory; [2]The University of Iowa; [3]Brookhaven National Laboratory

I-P3-4: Impurity Species Control Radiolytic Products in Chemically Complex Solutions and Solids

[EFRC - IDREAM] Hossam Elshendidi[1], Abhipsha Pandit[1], Ramsey Salcedo[2], Hemanth Haridas[3], Amita Bedar[4], Trent Graham[5], Xin Zhang[5], Carolyn Pearce[5], Donna McGregor[1], Benjamin Burton-Pye[1], Brant Jones[6], Thomas Orlando[6], Lynn Francesconi[2], Aurora Clark[3], Jay LaVerne[4]

[1]Lehman College of the City University of New York; [2]Hunter College of the City University of New York; [3]University of Utah; [4]University of Notre Dame; [5]Pacific Northwest National Laboratory; [6]Georgia Institute of Technology

I-P3-5: Solvated Electrons Have Multiple Personalities in Molten Salts

[EFRC - MSEE] Alejandro Ramos-Ballesteros[1], Hung H. Nguyen[2], Kazuhiro Iwamatsu[3,4], Santanu Roy[5], Vyacheslav Bryantsev[5], Michael E. Woods[1], Ruchi Gakhar[1], Phillip Halstenberg[6], Ellie Kim[6], Bobby Layne[3], Sheng Dai[5,6], Jay A. LaVerne[7], Claudio J. Margulis[2], James F. Wishart[3]

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I-P3-6: IDREAM Science Advances Radioactive Tank Waste Treatment

[EFRC - IDREAM] Jacob Reynolds[1], David Swanberg[2], Emily Nienhuis[3], Trent Graham[3], Xin Zhang[3], Xiaoxu Li[3], Kevin Rosso[3], Gregory Schenter[3], Aurora Clark[4], Jay LaVerne[5], Carolyn Pearce[3]

[1]Central Plateau Cleanup Company; [2]H2C: Hanford Tank Waste Operations & Closure; [3]Pacific Northwest National Laboratory; [4]University of Utah; [5]University of Notre Dame

I-P3-7: Isotopic Studies of Transport and Reactivity in Oxides

[EFRC - FUTURE] Kayla H. Yano[1], Sandra D. Taylor[1], Aaron A. Kohnert[2], Sten V. Lambeets[1], Matthew J. Olszta[1], Pauline G. Simonnin[1], Jijo Christudasjustus[1], Peter Hosemann[3], Yongqiang Wang[2], Tiffany C. Kaspar[1], Blas P. Uberuaga[2], Daniel K. Schreiber[1]

[1]Pacific Northwest National Laboratory; [2]Los Alamos National Laboratory; [3]University of California, Berkeley

I-P3-8: Phonon lifetimes in ordered and disordered nuclear materials: Neutron scattering and theory

[EFRC - TETI] Shaofei Wang[1], Ruining Zhang[2], Mark Mathis[2], J. Matthew Mann[3], Chris A. Marianetti[2], Michael E. Manley[1]

[1]Oak Ridge National Laboratory; [2]Columbia University; [3]Air Force Research Laboratory

I-P3-9: Grain Boundary Effects on Corrosion Morphologies in Molten Salts

[EFRC - FUTURE] Sean H. Mills[1,2], Ho Lun Chan[3], Nathan Bieberdorf[1,2], Elena Romanovskaia[3], Valentin Romanovski[3], Minh Tran[3], Laurent Capolungo[4], Mark Asta[1,2], John R. Scully[3], Andrew M. Minor[1,2], Peter Hosemann[1,2]

[1]University of California, Berkeley; [2]Lawrence Berkeley National Laboratory; [3]University of Virginia; [4]Los Alamos National Laboratory

J. Quantum Information Science

J-P3-1: Molecular color centers for quantum information science

[EFRC - CMQT] Rianna B. Greer[1], Arailym Kairalapova[2], Marquis M. McMillan[3], Noah Mendelson[3], Manoj V. H. Subramanya[4,5], Cindy Serena Ngompe Massado[1], Michael K. Wojnar[1], Benjamin S. Soloway[3], Majed S. Fataftah[6], Andrew Ozarowski[4], Sebastian M. Kopp[6], Shunta Nakamura[6], Yong Rui Poh[9], Kathryn R. Peinkofer[6], Brian T. Phelan[6], Stephen Hill[4,5], David. D. Awschalom[3,7], Timothy C. Berkelbach[2,8], Joel Yuen-Zhou[9], Matthew D. Krzyaniak[6], Danna E. Freedman[1], Michael R. Wasielewski[6]

[1]Massachusetts Institute of Technology; [2]Columbia University; [3]University of Chicago; [4]National High Magnetic Field Laboratory; [5]Florida State University; [6]Northwestern University; [7]Argonne National Laboratory; [8]Flatiron Institute; [9]University of California, San Diego

J-P3-2: Tunable Quantum Phases in 2D Systems: From Substrate-Controlled Naphthalocyanine Monolayers to Strain-Tuned Altermagnetism

[EFRC - M2QM] Chunjing Jia[1], Adrian Bahri[1], Shuyi Li[1], Yu Zhang[1], Xiao-Xiao Zhang[1], Shuanglong Liu[2], Hai-Ping Cheng[2]

[1]University of Florida; [2]Northeastern University

J-P3-3: Engineering Symmetry Breaking and Dimensionality in Organic-Inorganic Semiconductors by Molecular Design

[EFRC - CHOISE] Rayan Chakraborty[1], Yi Xie[1], Gabrielle Koknat[1], Jack Morgenstein[1], Peter C. Sercel[2], Kameron R. Hansen[3,4], Nicholas J. Weadock[5], Xixi Qin[1], Xiaoping Wang[6], Heshan Hewa-Walpitage[4], Carter M. Shirley[7], Purusharth Amrut[1], Daniel Nikiforov[4], Kathryn Bairley[5], Junxiang Zhang[5], Sasa Wang[1], Ruyi Song[1], Trigg Randall[7], Levi Homer[7], Garrett Davis[7], Stephen Barlow[5], Michael F. Toney[5], Seth R. Marder[5], Zeev Valy Vardeny[4], John S. Colton[7], Volker Blum[1], David B. Mitzi[1]

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J-P3-4: Localized 2D excitons as programmable quantum light sources

[EFRC - Pro-QM] Matthew C. Strasbourg[1], Emanuil S. Yanev[1], William P. Hayes[1], Thomas P. Darlington[1], Nicholas J. Borys[2], James C. Hone[1], P. James Schuck[1]

[1]Columbia University; [2]Montana State University

J-P3-5: Towards Scalable Generation of Coherent Quantum Emitters in the Solid State

[EFRC - QuPIDC] Artem Kryvobok[1], Zehra Naqvi[2], Alexandra Boltasseva[1], Vladimir Shalaev[1], Han Htoon[3], Jiwoong Park[2]

[1]Purdue University; [2]University of Chicago; [3]Los Alamos National Lab

J-P3-6: Van der Waals Waveguide Quantum Electrodynamics probed by Infrared Nano-Photoluminescence

[EFRC - Pro-QM] Samuel L. Moore[1], Hae Yeon Lee[2], Nicholas Rivera[3], Yuzuka Karube[1], Mark Ziffer[1], Emanuil Yanev[1], Thomas P. Darlington[1], Aaron J. Sternbach[4], Madisen Holbrook[1], Jordan Pack[1], Cory R. Dean[1], James Hone[1], Johnathan Owen[1], Xiaoyang Zhu[1], Xiaodong Xu[5], Milan Delor[4], P. James Schuck[1], Dmitri N. Basov[1]

[1]Columbia University; [2]Rice University; [3]Harvard University; [4]University of Maryland, College Park; [5]University of Washington

J-P3-7: Enabling Ambient Stability and Quantum Integration of Organometallic Magnonic Ferrimagnets via Atomic Layer Encapsulation

[EFRC - CMQT] Iqbal Utama[1], Robert Claassen[2], Srishti Pal[3], Hannah Christianson[4], Donley Cormode[2], Dmitry Lebedev[1], Subhajyoti Chaudhuri[1], Qin Xu[3], George Schatz[1], Jeffrey Long[4], Gregory Fuchs[3], Ezekiel Johnston-Halperin[2], Mark Hersam[1]

[1]Northwestern University; [2]The Ohio State University; [3]Cornell University; [4]University of California, Berkeley

J-P3-8: Quantum Control of Magnetic Molecules

[EFRC - M2QM] Andrew Cupo[1], Shuanglong Liu[1], Xiao Chen[1], Minseong Lee[2], James N. Fry[1], Xiaoguang Zhang[3], Vivien Zapf[2], Stephen Hill[4], Hai-Ping Cheng[1]

[1]Northeastern University; [2]Los Alamos National Laboratory; [3]University of Florida; [4]Florida State University

J-P3-9: Strong Photon Nonlinearity and Exciton Interactions

[EFRC - QuPIDC] Jonas Peterson[1], Zhaoyun Zheng[2], Zehra Naqvi[3], Shibalik Lahiri[1], Libai Huang[1], Valentin Walther[1], Teri Odom[2], Jiwoong Park[3], Matthew Pelton[4]

[1]Purdue University; [2]Northwestern University; [3]University of Chicago; [4]University of Maryland Baltimore County

J-P3-10: Electrodeposition of Porous Magnonic Materials

[EFRC - CMQT] Hannah Christianson[1], Robert Claassen[2], Matthew Dickson[1], Ryan A. Murphy[1,3], Kennedy C. McCone[1], Ellen Holmgren[2], Ezekiel Johnston-Halperin[2], Jeffrey R. Long[1,3]

[1]University of California, Berkeley; [2]The Ohio State University; [3]Lawrence Berkeley National Laboratory

J-P3-11: Magnetoresistance of the Surface States of Bi (111)

[EFRC - CATS] Eugene Ark[1], Siddhesh Ambhire[2], Michael Smith[1], Jagannath Jena[1], Hanu Arava[1], Jianguo Wen[1], Brandon Fisher[1], John Pearson[1], Jidong Jiang[1], Ivar Martin[1], Steven Zhang[2], Anand Bhattacharya[1]

[1]Argonne National Laboratory; [2]Case Western Reserve University

J-P3-12: Comparing the Dynamic Charge Response Measured with Transmission- and Reflection EELS

[EFRC - QSQM] Niels de Vries[1], Eric Hoglund[2], Dipanjan Chaudhuri[1], Sang Hyun Bae[1], Gillian Nolan[1], Jin Chen[1], Pinshane Huang[1], Jordan Hachtel[2], Peter Abbamonte[2]

[1]University of Illinois Urbana-Champaign; [2]Oak Ridge National Laboratory

L. AI/ML

L-P3-1: Machine Learning Workflows for Predictive Modeling of Moiré Superlattices in 2D Materials

[CMS - HeteroFAM] Yueyao Fan[1], Thomas Huang[1], Kaichen Xie[1], Eric J. Bylaska[2], Daniel Mejia Rodriguez[2], Niranjan Govind[2], Jenna Pope[2], Peter Sushko[2], Juan Carlos Idrobo[1,2], Di Xiao[1,2], Ting Cao[1]

[1]University of Washington; [2]Pacific Northwest National Laboratory

L-P3-2: Next Generation Molecular Dynamics: GPU Accelerated QM/MM With Machine Learning and Multiscale Reactive Molecular Dynamics

[CCS - CMSET] Chenghan Li[1], Hezhou Zhang[2], Scott Kaiser[2], Gregory A. Voth[2], Garnet K. L. Chan[1]

[1]California Institute of Technology; [2]University of Chicago

L-P3-3: Uncertainty quantification of machine learned interatomic potentials using quantum Monte Carlo references

[CMS - QMC-HAMM] Tawfiqur Rakib, Doruk Ucar, Young-Jae Choi, Jeonghwan Ahn, Lucas K. Wagner, David Ceperley, Harley Johnson, Elif Ertekin

University of Illinois Urbana-Champaign

L-P3-4: Energy Storage Research Alliance: Materials Acceleration Platform

[Hub - ESRA] Gerbrand Ceder[1,2], Maria Chan[3], Ruozhu Feng[4], Kristin Persson[1,2], Rajeev Assary[3], Rafa Gomez-Bombarelli[5], Wei Wang[4], Joaquín Rodríguez-López[6], Shyue Ping Ong[7], Tod Pascal[7], Brett Helms[1], Mary Scott[1,2], Jordi Cabana[3,8], Shrayesh Patel[9]
[1]Lawrence Berkeley National Laboratory; [2]University of California, Berkeley; [3]Argonne National Laboratory; [4]Pacific Northwest National Laboratory; [5]Massachusetts Institute of Technology; [6]University of Illinois Urbana-Champaign; [7]University of California, San Diego; [8]University of Illinois at Chicago; [9]University of Chicago

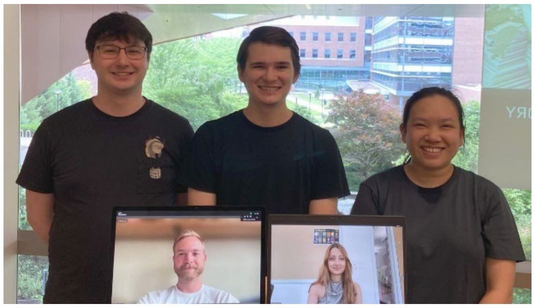
L-P3-5: Modeling Anion Exchange Membrane Degradation with Physics-Enforced Machine Learning

[EFRC - UNCAGE-ME] William Schertzer[1], Mohammed Al Otmi[2], Janani Sampath, Ryan P. Lively[1], Rampi Ramprasad[1]
[1]Georgia Institute of Technology; [2]University of Florida

L-P3-6: Smarter Chemistry, Better Energy: AI as the Catalyst for Breakthroughs in Alkaline Electrochemistry

[EFRC - CABES] Peter Frazier, Justin Tahmassebpur
Cornell University

GRADUATE STUDENT AND POSTDOCTORAL TEAM SCIENCE CONTEST



(Standing, from left) Albert Suceava, Ian Mercer, and Quyen Tran. (On screen, from left) Drew Behrendt and Ece Gunay

H-IV-3: Forging the Future of Ferroelectric Memory

[EFRC - 3DFeM2] Ece Gunay[1], Drew Behrendt[2]; Albert Suceava[3], Ian Mercer[3], Quyen Tran[3], Elizabeth C. Dickey[1], Thomas Jackson[3], Jon-Paul Maria[3], Venkatraman Gopalan[3], Andrew M. Rappe[2], Susan Trolier-McKinstry[3]

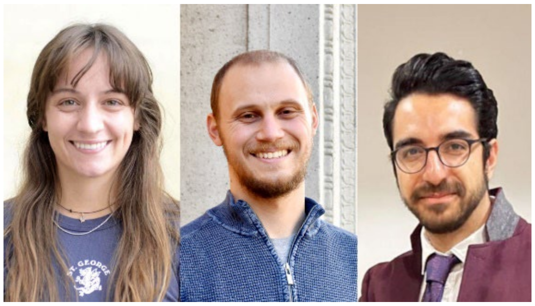
[1]Carnegie Mellon University; [2]University of Pennsylvania; [3]The Pennsylvania State University

(From left) Yaguang Zhu and Qinsi Xiong

F-II-3: More than a spectator: Critical Role of water in ion transport through 2D membranes

[EFRC - AMEWS] Yaguang Zhu[1], Qinsi Xiong[2], George C. Schatz[2], Kelsey B. Hatzell[1]

[1]Princeton University; [2]Northwestern University



(From left) Sophie Gerits, Daniel Weinberg and Nima Karimitari

C-III-1: Accurate Electrochemical Predictions with Many-Body and Machine-Learning Methods

[CCS - BEAST] Sophie Gerits[1], Daniel Weinberg[2], Nima Karimitari[3], Cooper Tezak[1], Jacob Clary[4], Taylor Aubry[4], Charles Musgrave[1], Mauro Del Ben[2], Christopher Sutton[3], Derek Vigil-Fowler[4], Ravishankar Sundararaman[5]

[1]University of Colorado Boulder; [2]Lawrence Berkeley National Laboratory; [3]University of South Carolina; [4]National Renewable Energy Laboratory; [5]Rensselaer Polytechnic Institute

(Top Row) Giselle de Araujo Lima e Souza, Benworth B. Hansen, Mrinlini Kolaprath (Middle Row) Miguel Muñoz and Thomas Simunovic (Bottom Row) Peisen Qian, Michael S. Chen, and Kaylie Glyn

D-IV-2: Quantum-Tuned Concentrated Hydrogen-Bonded Electrolytes for Enhanced Proton Transfer

[EFRC - BEES2] Miguel Muñoz[1], Giselle de Araujo Lima e Souza[2], Michael S. Chen[3], Kaylie Glynn[4], Benworth B. Hansen[4], Peisen Qian[5], Thomas Simunovic[6], Mrinlini Kolaprath[6], Mark Dadmun[6], Thomas Zawodzinski[6], Joaquín Rodríguez-López[5], Steve G. Greenbaum[2], Mark Tuckerman[3], Joshua R. Sangoro[4], and Burcu Gurkan[1]

[1]Case Western Reserve University; [2]Hunter College-CUNY; [3]New York University; [4]The Ohio State University; [5]University of Illinois Urbana-Champaign; [6]University of Tennessee-Knoxville

(Top row, from left) Luna Liu, Gurjyot Sethi, Jonah Haber (Bottom row, from left) Jinyuan Wu, Bowen Hou, Zhenfa Zheng

J-I-1: First-Principles Anatomy of Exciton Dynamics: From Dispersion to Quantum Transport

[CMS - C2SEPEM] Luna Liu[1], Gurjyot Sethi[2,3], Jonah Haber[4], Jinyuan Wu[1], Bowen Hou[1], Zhenfa Zheng[5], Jeffrey B. Neaton[2,3], Felipe H. da Jornada[4], Zhenglu Li[5], Diana Y. Qiu[1], Steven G. Louie[2,3]

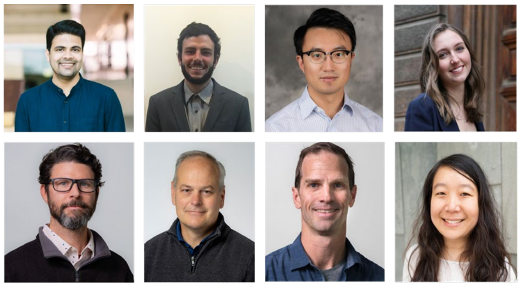
[1]Yale University; [2]Lawrence Berkeley National Laboratory; [3]University of California, Berkeley; [4]Stanford University; [5]University of Southern California

(From left) Sheilah Cherono, Cassius Boyd, Jennifer Sormberger, Shay McBride, Maritza Lang, Luka Mitrovic

C-II-4: PHOTO-ELECTROCHEMISTRY OF TITANIUM OXIDES: A PLATFORM FOR ASSIGNING VISIBLE SPECTRA TO OXYGEN EVOLUTION INTERMEDIATES

[EFRC - CEDARS] C. Boyd[1], S. McBride[2], S. Cherono[3], M. Lang[1], L. Mitrovic[4], J. Sormberger[1], D. Schlom[4], D. Jonas[1], D. Kumar[3], G. Hautier[2], T. Cuk[1]

[1]University of Colorado Boulder; [2]Dartmouth College; [3]North Carolina A&T State University; [4]Cornell University



(Top row, from left) Md Azimul Haque, Andrew Grieder, Yi Xie, Margherita Taddei

(Bottom row, from left) Joseph M. Luther, Matthew C. Beard, Jeffrey L. Blackburn, Yuan Ping

J-III-2: CHIRALITY TRANSFER AND SPIN SELECTIVITY IN HYBRID METAL HALIDE SEMICONDUCTORS

[EFRC – CHOISE] Md Azimul Haque[1], Andrew Grieder[2], Steven P. Harvey[1], Roman Brunecky[1], Jiselle Y. Ye[1], Bennett Addison[1], Junxiang Zhang[3], Yifan Dong[1], Yi Xie[4], Matthew P. Hautzinger[1], Heshan Hewa Walpitage[5], Ian A. Leahy[1], Jeiwan Tan[1], Margherita Taddei[1], Pius Markus Theiler[1], Aeron McConnell[6], Andrew H. Comstock[6], Kai Zhu[1], Kirstin Alberi[1], Jeffrey L. Blackburn[1], Zeev Valy Vardeny[5], David B. Mitzi[4], Joseph J. Berry[1,3], Seth R. Marder[1,3], Peter Sercel[7], Dali Sun[6], Joseph M. Luther[1], Yuan Ping[2], Matthew C. Beard[1]

[1]National Renewable Energy Laboratory; [2]University of Wisconsin-Madison; [3]University of Colorado Boulder; [4]Duke University; [5]University of Utah; [6]North Carolina State University; [7]Center for Hybrid Organic Inorganic Semiconductors for Energy

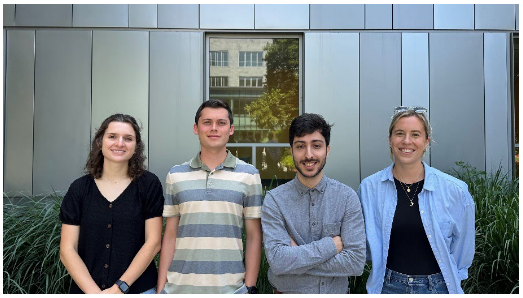
CMQT
CENTER FOR MOLECULAR QUANTUM TRANSDUCTION

(From left) Iqbal B. Utama, Robert Claassen, Srishti Pal, Hannah Christianson

J-III-1: ENABLING AMBIENT STABILITY AND QUANTUM INTEGRATION OF ORGANOMETALLIC MAGNONIC FERRIMAGNETS VIA ATOMIC LAYER ENCAPSULATION

[EFRC - CMQT] Iqbal B. Utama[1], Robert Claassen[2], Srishti Pal[3], Hannah Christianson[4], Donley S. Cormode[2], Dmitry Lebedev[1], Subhajyoti Chaudhuri[1], Qin Xu[3], George C. Schatz[1], Jeffrey R. Long[4], Gregory D. Fuchs[3], Ezekiel Johnston-Halperin[2], and Mark C. Hersam[1]

[1]Northwestern University; [2]The Ohio State University; [3]Cornell University; [4]University of California, Berkeley



(From left) Christine M. Oberhausen, Alex W. Hawkins, Pedro A. R. Moura, and Zoé O. G. Schyns

B-III-4: ENGINEERING SOLUTIONS FOR COMPLEX PLASTICS WASTE USING POLYMER SCIENCE AND CATALYSIS

[EFRC - CPI] Zoé O. G. Schyns, Pedro A. R. Moura, Christine M. Oberhausen, Alex W. Hawkins, Dionisios G. Vlachos, LaShanda T. J. Korley

University of Delaware

(From left) Alex Berlaga and Renyu Zheng

A-II-1: From Force-Field Parameters to Programmable Nanostructures: Integrated Simulation, Active Learning, and Experiment for Peptoid-Based Hierarchical Materials

[EFRC - CSSAS] Alex Berlaga[1], Renyu Zheng[2,3], Kaylyn Torkelson[2], Xin Qi[2], Christopher D. Lowe[4], Helen Larson[4], Brandi M. Cossairt[4], Jim Pfaendtner[5], Chun-Long Chen[2,3], Andrew L. Ferguson[1]

[1]University of Chicago; [2]University of Washington; [3]Pacific Northwest National Laboratory; [4]North Carolina State University

(From upper left) Olivia F. Bird, Faith A. Flinkingshelt, Sophia M. Click (From lower left) Della Hagemann, Hyuna Kwon, Kenneth M. Drbohlav, Evan K. Gowdy

B-II-5: EXTENDING CHARGE-SEPARATED-STATE LIFETIME IN NANOCRYSTAL–MOLECULE HYBRIDS VIA RATIONAL MOLECULAR DESIGN

[EFRC - EPN] Olivia F. Bird[1], Faith A. Flinkingshelt[2], Sophia M. Click[1], Hyuna Kwon[3], Della Hagemann[4], Kenneth M. Drbohlav[4], Evan K. Gowdy[4], Yisrael M. L. Lamb[4], Tadashi Ogitsu[3], Jenny Y. Yang[2], Kenneth A. Miller[4], Gordana Dukovic[1]

[1]University of Colorado Boulder; [2]University of California, Irvine; [3]Lawrence Livermore National Laboratory; [4]Fort Lewis College

ESRA
Energy Storage
Research Alliance

(From left) Alae Eddine Lakraychi, Harshan Reddy Gopidi, Jiaqi Wang, Zeqian (Francis) Zhang, Yu Chen

E-III-3: STRUCTURE–PROPERTY RELATIONSHIPS FOR MULTI-ELECTRON ORGANIC POSITIVE ELECTRODE MATERIALS

[Hub - ESRA] Alae Eddine Lakraychi[1], Harshan Reddy Gopidi[1], Jiaqi Wang[2], Zeqian Zhang[3], Yu Chen[4], Ying Chen[3], Kamila Magdalena Wiaderek[2], Mary C. Scott[4], Pieremanuele Canepa[1], Yan Yao[1]

[1]University of Houston; [2]Argonne National Laboratory; [3]Pacific Northwest National Laboratory; [4]Lawrence Berkeley National Laboratory

(From left): Ji-young Ock, Lauren B. Shepard, and Amit Bhattacharya

D-IV-1: Unlocking High Conductivity in Composite Electrolytes for Next Generation Energy Storage

[EFRC - FaCT] Ji-young Ock[1], Amit Bhattacharya[2], Lauren B. Shepard[3], Tao Wang[1], Miaofang Chi[1], Sheng Dai[1,4], Susan B. Sinnott[3], Alexei P. Sokolov[1,4], Raphaële J. Clément[2], Xi Chelsea Chen[1]

[1]Oak Ridge National Laboratory; [2]University of California, Santa Barbara; [3]The Pennsylvania State University; [4]University of Tennessee-Knoxville

(From left) Franziska Schmidt and Saikumaran Ayyappan

I-II-1: Metal Corrosion under Irradiation – Explaining in situ X-ray Spectroscopy with ex situ Microscopy and Atom Probe Tomography

[EFRC - FUTURE] Franziska Schmidt[1], Saikumaran Ayyappan[2], Kayla Yano[3], Matthew Chancey[1], Hyosim Kim[1], Djamel Kaoumi[2], Peter Hosemann[4], Blas Uberuaga[1], Yongqiang Wang[1]

[1]Los Alamos National Laboratory; [2]North Carolina State University; [3]Pacific Northwest National Laboratory; [4]University of California, Berkeley

(From left) Ryan Beck, Amita Bedar, Simantini Paul, and Robert Felsted

I-IV-5: Understanding how radiation uniquely transforms the physicochemical properties of electrolytes

[EFRC - IDREAM] Ryan Beck[1], Simantini Paul[2], Amita Bedar[3], Greg Felsted[4], Aodong Liu[1], Hemanth Haridas[2], Eleftherios Lambros[1], Maxime Pouvreau[4], Jacob Morton[4], Yifu Feng[4], Pravalika Butreddy[4], Ashley Kennedy[4], William Denman[5], Hossam Elshendidi[6], Shuai Li[7], Emily Nienhuis[4], Trent Graham[4], Xin Zhang[4]

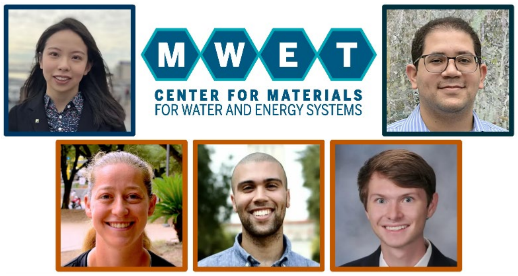
[1]University of Washington; [2]University of Utah; [3]Notre Dame University; [4]Pacific Northwest National Laboratory; [5]Georgia Institute of Technology; [6]Hunter College CUNY; [7]Argonne National Laboratory

(From left) Aisulu Aitbekova, Matthew Salazar, and Katherine Yan

B-II-4: A Solar-Driven Electrochemical/Photothermocatalytic Process for CO_2 conversion to C_6 oxygenates: An Assembly of Coupled Microenvironments

[Hub - LiSA] Matthew Salazar[1,2], Aisulu Aitbekova[1,2], Katherine Yan[1,3], Jonas C. Peters[1,2], Thomas F. Jaramillo[1,3], Harry A. Atwater[1,2], Theodor Agapie[1,2], Alexis T. Bell[1,4]

[1]Liquid Sunlight Alliance; [2]California Institute of Technology; [3]SLAC National Accelerator Laboratory; [4]Lawrence Berkeley National Lab



(Top row, from left) Chuqiao (Elise) Chen, José Carlos Diaz
(Bottom row, from left) Louise Kuehster, Adam Mann, Noah Wamble

F-I-4: Towards Rational Design of Tougher SNIPS Membranes for Water and Energy Systems

[EFRC - M-WET] Noah P. Wamble[1], Chuqiao Chen[2], José Carlos Díaz[1,3], Benjamin J. Pedretti[1], Adam N. Mann[1], Matthew R. Landsman[1,3], Louise Kuehster[1], Mostafa Nassr[1], Lynn E. Katz[1], Nathaniel A. Lynd[1], Glenn H. Fredrickson[2], Gregory M. Su[3], Gabriel E. Sanoja[1], Benny D. Freeman[1]

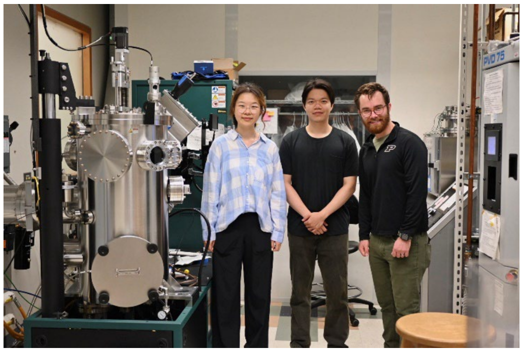
[1]University of Texas at Austin; [2]University of California, Santa Barbara; [3]Lawrence Berkeley National Laboratory

(From left) Elliot Kisiel, David Alspaugh, Pavel Salev

H-IV-5: Inhomogeneities of electrically triggered metal-insulator transitions in neuromorphic devices

[EFRC - Q-MEEN-C] Pavel Salev[1], Elliot Kisiel[1], David Alspaugh[1], Oleg Shpryko[1], Marcelo J. Rozenberg[1], Yayoi Takamura[2], Zahir Islam[3], Alex Frano[1], Ivan K. Schuller[1]

[1]University of California, San Diego; [2]University of California, Davis; [3]Argonne National Laboratory



(From left) Zhaoyun Zheng, Hanyu Hong and Jonas Mark Peterson

J-I-2: Strong Light–Matter Interaction in Plasmonic Arrays Enables Coherent Quantum Emission

[EFRC - QuPIDC] Zhaoyuan Zheng[1], Jonas Peterson[2], Hanyu Hong[3], Jiwoong Park[3], Libai Huang[2], and Teri Odom[1]

[1]Northwestern University; [2]Purdue University; [3]University of Chicago

(From left) Brandon R. Clarke, Pranav Krishnan, and Yun Seong Kim

A-II-2: Multi-Material 3D Printing with Frontally Polymerizable Resins

[EFRC - REMAT] Brandon R. Clarke[1], Pranav Krishnan[2], Connor D. Armstrong[2], Yun Seong Kim[2], Ignacio Arretche[2], Derrick Sanders[2], Jeffrey S. Moore[2], Sameh H. Tawfick[2], Nancy S. Sottos[2], Jennifer A. Lewis[1]

[1]Harvard University; [2]University of Illinois Urbana-Champaign

(From left) John Ponis, Kenna Ashen, Michelle Smeation, Jialu Li

H-IV-4: Mapping Atomistic Structure to Neuromorphic Function through Single-Crystal Neuronal Oscillators

[EFRC - reMIND] John Ponis[1], Kenna Ashen[1], Michelle Smeaton[2], Jialu Li[3], Fatme Jardali[1], George Agbeworvi[1], Jinghua Guo[3], Xiaofeng Qian[1], Katherine Jungjohann[2], Lance Wheeler[2], Patrick Shamberger[1], Sarbajit Banerjee[1]

[1]Texas A&M University; [2]National Renewable Energy Laboratory; [3]Lawrence Berkeley National Laboratory

(From left) Megan Brown, Spencer Yeager, Jude Kpare, Eui Hyun Suh, Henry Kantrow, Arianna Magni, and Yael Tsarfati

G-III-4: UNDERSTANDING AND MANIPULATING THE NANOENVIRONMENT OF RIBBON-LIKE (SOFT) POLYMER SEMICONDUCTORS TO ENABLE PHOTOELECTROCHEMISTRY

[EFRC - SPECS] Henry J. Kantrow[1], Yael Tsarfati[2,3], Spencer Yeager[4], Megan Brown[5], Arianna Magni[2], Eui Hyun Suh[1], Jude Kpare[1], Chad Risko[5], Alberto Salleo[2], Erin Ratcliff[1], Natalie Stingelin[1]

[1]Georgia Institute of Technology; [2]Stanford University; [3]Lawrence Berkeley National Laboratory; [4]University of Arizona; [5]University of Kentucky

ACRONYMS AND IDs

ENERGY FRONTIER RESEARCH CENTERS (EFRCs)

[EFRC – 3DFeM2] Center for 3D Ferroelectric Microelectronics Manufacturing
Susan Trolier-McKinstry, The Pennsylvania State University
Class: 2020 – 2028

[EFRC – 4C] Center for Closing the Carbon Cycle
Jenny Yang, University of California, Irvine
Class: 2022-2026

[EFRC – AIM] Artificially Intelligent Manufacturing Paradigm for Composites
Srikanth Pilla, Clemson University
Class: 2022-2026

[EFRC – AMEWS] Advanced Materials for Energy-Water Systems
Seth Darling, Argonne National Laboratory
Class: 2018 – 2026

[EFRC – APEX] A Center for Power Electronics Materials Manufacturing and Exploration
Nancy Haegel, National Renewable Energy Laboratory
Class: 2024-2028

[EFRC – BEES2] Breakthrough Electrolytes for Energy Storage Systems
Burcu Gurkan, Case Western Reserve University
Class: 2018 – 2026

[EFRC – BioLEC] Bioinspired Light-Escalated Chemistry
Gregory Scholes, Princeton University
Class: 2018 – 2026

[EFRC – CABES] Center for Alkaline-Based Energy Solutions
Héctor Abruña, Cornell University
Class: 2018 – 2026

[EFRC – CATS] Center for the Advancement of Topological Semimetals
Robert McQueeney, Ames National Laboratory
Class: 2018 – 2026

[EFRC – CCBC] The Center for Catalysis in Biomimetic Confinement
Cheryl Kerfeld, Michigan State University
Class: 2022-2026

[EFRC – CD4DC] Catalyst Design for Decarbonization Center
Laura Gagliardi, University of Chicago
Class: 2022-2026

[EFRC – CEDARS] Center for Electrochemical Dynamics and Reactions on Surfaces
Dhananjay Kumar, North Carolina A&T State University
Class: 2022-2026

[EFRC – CEEMag] Center for Energy Efficient Magnonics
Yuri Suzuki, SLAC National Accelerator Laboratory
Class: 2024-2028

[EFRC – CENT2] Center for Enhanced Nanofluidic Transport – Phase 2
Michael Strano, Massachusetts Institute of Technology
Class: 2018 – 2026

[EFRC – CHiPPS] Center for High Precision Patterning Science
Ricardo Ruiz, Lawrence Berkeley National Laboratory
Class: 2022-2026

[EFRC – CHOISE] Center for Hybrid Organic Inorganic Semiconductors for Energy
Matthew Beard, National Renewable Energy Laboratory
Class: 2018 – 2026

[EFRC – CHWM] Center for Hierarchical Waste Form Materials
Hanno zur Loye, University of South Carolina
Class: 2016 – 2025

[EFRC – CMQT] Center for Molecular Quantum Transduction
Michael Wasielewski, Northwestern University
Class: 2020 – 2028

[EFRC – CPEC] Center for Programmable Energy Catalysis
Paul Dauenhauer, University of Minnesota
Class: 2022-2026

[EFRC – CPI] Center for Plastics Innovation
LaShanda Korley, University of Delaware
Class: 2020 – 2028

[EFRC – CSSAS] Center for the Science of Synthesis Across Scales
François Baneyx, University of Washington
Class: 2018 – 2026

[EFRC – EPN] Ensembles of Photosynthetic Nanoreactors
Shane Ardo, University of California, Irvine
Class: 2022-2026

[EFRC – FaCT] Fast and Cooperative Ion Transport in Polymer-Based Electrolytes
Valentino Cooper, Oak Ridge National Laboratory
Class: 2022-2026

[EFRC – FUTURE] Fundamental Understanding of Transport Under Reactor Extremes
Blas Uberuaga, Los Alamos National Laboratory
Class: 2018 – 2026

[EFRC – GMCS] Center for Interacting Geo-processes in Mineral Carbon Storage
Emmanuel Detournay, University of Minnesota
Class: 2022-2026

[EFRC – HEISs] Hydrogen in Energy and Information Sciences
Sossina Haile, Northwestern University
Class: 2022-2026

[EFRC – iCOUP] Institute for Cooperative Upcycling of Plastics
Aaron Sadow, Ames National Laboratory
Class: 2020 – 2028

[EFRC – IDREAM] Interfacial Dynamics in Radioactive Environments and Materials
Carolyn Pearce, Pacific Northwest National Laboratory
Class: 2016 – 2028

[EFRC – m2M#S] Center for Mesoscale Transport Properties
Amy Marschilok, Stony Brook University
Class: 2014 – 2026

[EFRC – M2QM] Center for Molecular Magnetic Quantum Materials
Xiaoguang Zhang, University of Florida
Class: 2018 – 2026

[EFRC – MSEE] Molten Salts in Extreme Environments
James Wishart, Brookhaven National Laboratory
Class: 2018 – 2026
[EFRC – MUSIC] Mechano-Chemical Understanding of Solid Ion Conductors
Jeff Sakamoto, University of Michigan
Class: 2022-2026

[EFRC – M-WET] Center for Materials for Water and Energy Systems
Benny Freeman, University of Texas at Austin
Class: 2018 – 2026

[EFRC – Pro-QM] Programmable Quantum Materials
Dmitri Basov, Columbia University
Class: 2018 – 2026

[EFRC – Q-MEEN-C] Quantum Materials for Energy Efficient Neuromorphic Computing
Ivan Schuller, University of California, San Diego
Class: 2018 – 2026

[EFRC – QSQM] Quantum Sensing and Quantum Materials
Peter Abbamonte, University of Illinois Urbana-Champaign
Class: 2020 – 2026

[EFRC – QuPIDC] Quantum Photonic Integrated Design Center
Libai Huang, Purdue University
Class: 2024-2028

[EFRC –REMAT] Center for Regenerative Energy-Efficient Manufacturing of Thermoset Polymeric Materials
Nancy Sottos, University of Illinois Urbana-Champaign
Class: 2022-2026

[EFRC – REMIND] Reconfigurable Electronic Materials Inspired by Nonlinear Neuron Dynamics
R. Stanley Williams, Texas A&M Engineering Experiment Station
Class: 2022-2026

[EFRC – SPECS] Center for Soft PhotoElectroChemical Systems
Neal Armstrong, University of Arizona
Class: 2022-2026

[EFRC – TETI] Center for Thermal Energy Transport under Irradiation
David Hurley, Idaho National Laboratory
Class: 2018 – 2026

[EFRC – μ-ATOMS] Manipulation of Atomic Ordering for Manufacturing Semiconductors
Shui-Qing Yu, University of Arkansas
Class: 2022-2026

[EFRC – ULTRA] Ultra Materials for a Resilient, Smart Electricity Grid
Robert Nemanich, Arizona State University
Class: 2020 – 2026

[EFRC – UNCAGE-ME] Center for Understanding and Control of Acid Gas-induced Evolution of Materials for Energy
Ryan Lively, Georgia Institute of Technology
Class: 2014 – 2026

ENERGY INNOVATION HUBS (HUB)

[Hub – ABC] Aqueous Battery Consortium
Yi Cui, Stanford University
Started: 2024

[Hub – ESRA] Energy Storage Research Alliance
Y. Shirley Meng, Argonne National Laboratory
Started: 2024

**[Hub – CHASE] Center for Hybrid Approaches in
Solar Energy to Liquid Fuels**
Jerry Meyer, University of North Carolina at Chapel Hill
Started: 2020

[Hub – LiSA] Liquid Sunlight Alliance
Harry Atwater, California Institute of Technology
Started: 2020

COMPUTATIONAL MATERIALS SCIENCES (CMS)

[CMS – C2SEPEM] Center for Computational Study of Excited-State Phenomena in Energy Materials
Steven G. Louie, Lawrence Berkeley National Laboratory
Started: 2016

[CMS – COMMS] Computational Mesoscale Science and Open Software for Quantum Materials
Long-Qing Chen, The Pennsylvania State University
Started: 2019

[CMS – COMSCOPE] Center for Computational Material Spectroscopy and Design
Gabriel Kotliar, Brookhaven National Laboratory
Started: 2015
[CMS – CPSFM] Center for Predictive Simulation of Functional Materials
Paul Kent, Oak Ridge National Laboratory
Started: 2016

[CMS – EPW] Toward Exascale Computing of Electron-Phonon Couplings for Finite-Temperature Materials Design
Feliciano Giustino, University of Texas at Austin
Started: 2019

[CMS – HeteroFAM] Navigating the Design Space of Heterostructures - Heterostructures, Functionality, Advanced Modeling
Eric Bylaska, University of Washington
Started: 2024

[CMS – MICCoM] Midwest Integrated Center for Computational Materials
Giulia Galli, Argonne National Laboratory
Started: 2015

[CMS – MLAMD] Machine Learning Accelerated Materials Discovery Center
Cai-Zhuang Wang, Ames National Laboratory
Started: 2024

[CMS – NPNEQ] Center for Non-Perturbative Studies of Functional Materials under Non-Equilibrium Conditions
Tadashi Ogitsu, Lawrence Livermore National Laboratory
Started: 2019

[CMS – QMC-HAMM] From Accurate Correlated Quantum Simulations to Mesoscopic Scales

Lucas Wagner, University of Illinois Urbana-Champaign
Started: 2019

COMPUTATIONAL CHEMICAL SCIENCES (CCS)

[CCS – ADEPTS] Ab-initio Density-matrix Exascale-Parallelized Dynamics and Transport for Selectivity
Yuan Ping, University of Wisconsin-Madison
Started: 2022

[CCS – BEAST] Beyond-DFT Electrochemistry with Accelerated and Solvated Techniques
Ravishankar Sundararaman, Rensselaer Polytechnic Institute
Started: 2021

[CCS – CMSET] Center for Multiscale Simulation of Energy Transduction
Gregory Voth, University of Chicago
Started: 2022

[CCS – CSI] Chemistry in Solution and at Interfaces
Roberto Car, Princeton University
Started: 2018

[CCS – ECC] Exascale Catalytic Chemistry Project
Judi Zádor, Sandia National Laboratories
Started: 2017

[CCS – ExaQC] Novel Toolkit for Harnessing the Power of Exascale Computing for Catalyst Design
Anna Krylov, University of Southern California
Started: 2021

[CCS – ExaPUC] Exascale Multireference Wave Function Theory Method for Transition Metal Catalysis
Laura Gagliardi, University of Chicago
Started: 2022

[CCS – FLOSIC] Fermi-Lowdin Orbital Self-Interaction Correction Center
Koblar Alan Jackson, Central Michigan University
Started: 2017

[CCS – MAPOL] Center for MAny-Body Methods, Spectroscopies, and Dynamics for Molecular POLaritonic Systems
Niranjan Govind, Pacific Northwest National Laboratory
Started: 2022

[CCS – NEOQD] Multiscale Nuclear-Electronic Orbital Quantum Dynamics in Complex Environments
Hammes-Schiffer, Sharon, Princeton University
Started: 2022

[CCS – NEREST] Numerically-Exact Relativistic Many-Body Electronic Structure of Heavy Elements
Edward Valeev, Virginia Polytechnic Institute and State University
Started: 2021

[CCS – QuestC] Hierarchical Scalable Green's Function Modeling of Chemistry at Interfaces
Mark van Schilfgaarde, National Renewable Energy Laboratory
Started: 2021

[CCS – SPARC-X] SPARC: Simulation Package for Ab-initio Real-Space Calculations
Panish Suryanarayana, Georgia Tech

Started: 2018

[CCS – SPEC] Scalable Predictive Methods for Excitations and Correlated Penomena
Sotiris Xantheas, Pacific Northwest National Laboratory
Started: 2017

[CCS – WFT2XC] From Wave Functions to Exchange Correlation for Large-Scale Electronic Structure
Paul Zimmerman, University of Michigan
Started: 2021

U.S. NATIONAL LABORATORIES

AFRL - Air Force Research Laboratory
AMES - Ames National Laboratory
ANL - Argonne National Laboratory
BNL - Brookhaven National Laboratory
INL - Idaho National Laboratory
LBNL - Lawrence Berkeley National Laboratory
LLNL - Lawrence Livermore National Laboratory
LANL - Los Alamos National Laboratory
NHMFL - National High Magnetic Field Laboratory
NIST - National Institute of Standards and Technology
NREL - National Renewable Energy Laboratory
ORNL - Oak Ridge National Laboratory
PNNL - Pacific Northwest National Laboratory
SLAC - SLAC National Accelerator Laboratory
SNL - Sandia National Laboratories
SRNL - Savannah River National Laboratory