Science for our Nation's Energy Future

Energy Frontier Research Centers
Principal Investigators' Meeting

July 29-30, 2019
Washington, D.C.

Washington Marriott
Wardman Park

U.S. DEPARTMENT OF ENERGY | Office of Science

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Pre-Meeting

Sunday, July 28, 2019

4:00 – 6:00 PM **Early Registration**

Agenda Day 1

Monday, July 29, 2019
8:30 AM – 6:30 PM

7:00 – 8:30 AM **Registration and Continental Breakfast**

Plenary Session

Thurgood Marshall Ballroom
Moderator: Harriet Kung, *Associate Director, Basic Energy Sciences*

8:30 – 9:00 AM **Welcome and Announcement of "EFRC Ten at Ten" Winners**
The Honorable Paul M. Dabbar
DOE Under Secretary for Science

9:00 – 9:20 AM **The EFRC Program at Ten: Looking Back, Moving Forward**
Andy Schwartz
Senior Technical Advisor for EFRCs

9:20 – 10:00 AM **Energy: Past Lessons and Future Opportunities**
Norman Augustine
Lockheed Martin Corporation

10:00 – 10:30 AM **Break**

Plenary Session (con't)

Moderator: Andy Schwartz

10:30 – 11:10 AM **Skew Lines: The Challenge of Meaningful Intersection**
Esther Takeuchi
Distinguished Professor of Chemistry, Stony Brook University

11:10 – 11:50 AM **America Leading the World in Science and Technology**
Kelvin Droegemeier
Director, White House Office of Science and Technology Policy

11:50 – 12:10 PM **Winners of the "Life at the Frontiers of Energy Research Video Contest"**

12:10 – 1:40 PM **Lunch (buffet lunch provided)**
12:30 – 1:30 PM **ECN Event: Diversity in Energy Science Lunch (all welcome) –** *Lincoln 2/3/4*

1:40 – 2:40 PM	**Science to Technology Transition: Perspectives from DOE Technology Offices** Moderator: Linda Horton, DOE Basic Energy Sciences *Panelists:* *Peter Faguy, Vehicle Technologies Office* *Eric Hsieh, Office of Electricity* *Mike McKittrick, Advanced Manufacturing Office* *Eric Miller, Fuel Cell Technologies Office* *Sven Mumme, Building Technologies Office* *Avi Shultz, Solar Energy Technologies Office*
2:40 – 3:30 PM	**Panel Discussion: EFRC Impact on Science and Technology** Moderator: Marc Kastner, Science Philanthropy Alliance *Panelists:* *Daniel Cosgrove, Penn State University* *Paul Dauenhauer, University of Minnesota* *Hunter McDaniel, UbiQD, Inc.* *Krista Walton, Georgia Tech University*
3:30 – 4:00 PM	**Break**
4:00 – 4:50 PM	**Panel Discussion: EFRC Impact on the Energy Workforce** Moderator: Michelle Buchanan, Oak Ridge National Laboratory *Panelists:* *Karena Chapman, Stony Brook University* *Brandi Cossairt, University of Washington* *Cary Hayner, NanoGraf, Inc.* *Liam Palmer, Northwestern University*
4:50 – 5:00 PM	**Recognition of EFRC Newsletter and Early Career Network Participants** **Announcement of Student & Postdoc Team Science Finalists** Andy Schwartz
5:00 – 6:30 PM	**Poster Session – Center Overviews (refreshments provided)** *Exhibition Hall C*
6:30 PM	**Adjourn**
7:00 PM – late	**ECN Event: Social Evening at Duke's Counter (early career scientists)**

*** ECN Event** – These activities are planned by the Early Career Network (ECN), a group of early career scientists from current EFRCs.

Agenda Day 2

Tuesday, July 30, 2019
8:00 AM – 5:15 PM

7:00 – 8:00 AM	**Registration and Continental Breakfast**
8:00 – 9:40 AM	**Parallel Talks Session I**
	A. Bio-inspired Science, *Lincoln 6*
	B. Catalysis I, *Lincoln 5*
	D. Energy Storage, *Thurgood Marshall East*
	F. Materials and Chemistry by Design, *Thurgood Marshall West*
	G. Nuclear Energy, *Thurgood Marshall South*
	H. Quantum Materials I, *Lincoln 3&4*
	J. Separation Science, *Thurgood Marshall North*
	K. Solar Energy, *Lincoln 2*
9:40 – 11:00 AM	**Poster Session I (refreshments provided)**
11:00 – 12:20 PM	**Parallel Talks Session II**
	B. Catalysis I, *Lincoln 5*
	D. Energy Storage, *Thurgood Marshall East*
	E. Energy - Water, *Thurgood Marshall North*
	F. Materials and Chemistry by Design, *Thurgood Marshall West*
	G. Nuclear Energy, *Thurgood Marshall South*
	H. Quantum Materials I, *Lincoln 3&4*
	L. Subsurface Science, *Lincoln 2*
	M. Synthesis Science, *Lincoln 6*
12:20 – 1:45 PM	**Lunch (buffet lunch provided)**
12:35 – 1:35 PM	**ECN Event: Elevator Pitches and Science Speed Dating (all welcome) –** *Lincoln 3&4*
1:45 – 3:45 PM	**Parallel Talks Session III**
	B. Catalysis I, *Lincoln 5*
	C. Catalysis II, *Lincoln 6*
	D. Energy Storage, *Thurgood Marshall East*
	E. Energy - Water, *Thurgood Marshall North*
	F. Materials and Chemistry by Design, *Thurgood Marshall West*
	G. Nuclear Energy, *Thurgood Marshall South*
	H. Quantum Materials I, *Lincoln 3&4*
	I. Quantum Materials II, *Lincoln 2*
3:45 – 5:15 PM	**Poster Session II (refreshments provided)**
4:30 PM	**Announce winners of the *Graduate Student and Postdoc Team Science Contest***
5:15 PM	**Adjourn**
7:00 PM – late	**ECN Event: Baseball Game at Nationals Park (all welcome)**

SPEAKER BIOGRAPHIES

PLENARY SPEAKERS

In order of appearance

Harriet Kung has served as the Associate Director of Science for Basic Energy Sciences (BES) since June 9, 2008. Under her leadership, BES has pursued new funding modalities in advancing the science for the energy research agenda, including the establishment of the Energy Frontier Research Centers program, the Fuels from Sunlight Energy Innovation Hub, and the Joint Center for Energy Storage Research Hub. From 2004 to 2008, she was the Director of the Materials Sciences and Engineering Division in BES. Before joining DOE in 2002 as a program manager in Materials Sciences and Engineering division, Dr. Kung was a technical staff member and a project leader in the Materials Science and Technology Division at Los Alamos National Laboratory (LANL).

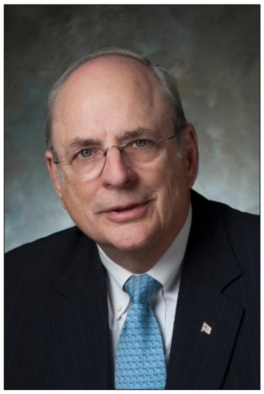
Paul M. Dabbar, Under Secretary for Science, serves as the Department's principal advisor on fundamental energy research, energy technologies, and science, driving this mission through programs including nuclear and high energy particle physics, basic energy, advanced computing, fusion, and biological and environmental research, and direct management over a majority of the Department's national labs and their world-leading user facilities. In addition, Mr. Dabbar manages the environmental and legacy management missions of the Department, addressing the U.S. legacy of nuclear weapons production and government-sponsored nuclear energy research. In addition, Mr. Dabbar is the lead for technology commercialization activities for the Department and its 17 national labs.

Prior to confirmation as Under Secretary for Science, Mr. Dabbar worked in operations, finance, and strategy roles in the energy sector. As a Managing Director at J.P. Morgan, leading various energy business areas, he has over $400 billion in investment experience across all energy sectors including solar, wind, geothermal, distributed-generation, utility, LNG, pipeline, oil & gas, trading, and energy technologies, and has also led the majority of all nuclear transactions. In addition, he had a senior leadership role for the company's commodity trading business, including power, oil and gas.

Before joining J.P. Morgan, Mr. Dabbar served as a nuclear submarine officer in Mare Island, California, and Pearl Harbor, Hawaii, including deploying to the North Pole where he conducted environmental research. He also served on the Department of Energy Environmental Management Advisory Board. He has been a lecturer at the U.S. Naval Academy, and conducted research at the Johns Hopkins Applied Physics Laboratory. He is also a member of the Council on Foreign Relations.

Mr. Dabbar received a B.S. degree from the U.S. Naval Academy, and a masters degree from Columbia University. Mr. Dabbar and his wife, Andrea, are the parents of two children.

Andrew Schwartz has served as Senior Technical Advisor for Energy Frontier Research Centers (EFRCs) since June 2013, leading the team of Basic Energy Sciences (BES) Program Managers and support staff that manages the EFRC program. From 2008 to 2013 Dr. Schwartz was the BES Program Manager for the Experimental Condensed Matter Physics (ECMP) program. Prior to joining BES, Dr. Schwartz spent seven years in industry leading a multi-disciplinary scientific and engineering team in the research and development of a new technology for semiconductor metrology.



Norman Augustine is the retired chairman and CEO of Lockheed Martin Corporation. He served as Under Secretary and Acting Secretary of the U.S. Army and as a lecturer with the rank of professor on the faculty of Princeton University. He has been a trustee of Princeton, Johns Hopkins and MIT and a member of the Board of Regents of the University System of Maryland. He has served on the Board of Directors of Lockheed Martin, Black and Decker, Procter and Gamble, and Conoco Phillips, and chaired the Gathering Storm study that recommended the creation of ARPA-E.

He was founding chair of In-Q-Tel, a member of the Board of Advisors to the Secretary of Energy, a founding member of the American Energy Innovation Council and a member of the MIT Energy Initiative External Advisory Board. He has been presented the Presidential Medal of Technology and received honorary degrees from 35 universities. He holds Bachelor's and Master's degrees in aeronautical engineering from Princeton University.

Esther S. Takeuchi is a SUNY Distinguished Professor and the William and Jane Knapp Chair in Energy and the Environment in the Departments of Materials Science and Chemical Engineering and Chemistry at Stony Brook University. She holds a joint appointment at Brookhaven National Laboratory as Chief Scientist in the Energy and Photon Sciences Directorate. Dr. Takeuchi is a member of National Academy of Engineering, was awarded the National Medal of Technology and Innovation, was inducted into the National Inventors Hall of Fame and is a Charter Member of the National Academy of Innovation. She received the E. V Murphree Award and Astellas Award from the American Chemical Society and the Electrochemical Society Battery Division Technology award. She is a Fellow of the Electrochemical Society (ECS) the American Institute of Medical and Biological Engineering (AIMBE) and American Association for the Advancement of Science (AAAS). Dr. Takeuchi is inventor > 150 patents and received the 2018 European Inventor Award in the category in the category of non-EPO countries.

Prior to her academic appointment, she was employed at Greatbatch, Inc., where her research focused on lithium battery research for implantable applications. Her work was instrumental in the success of the lithium/silver vanadium oxide (Li/SVO) battery the power source enabling the widespread adoption of life-saving implantable cardiac defibrillators (ICDs). She began her academic career at the University at

Buffalo in the Departments of Electrical Engineering and Chemical Engineering and relocated to Stony Brook University and Brookhaven National Laboratory in 2012. Dr. Takeuchi received a bachelor's degree from the University of Pennsylvania with a double major in chemistry and history and completed a Ph.D. in chemistry at the Ohio State University.

Kelvin Droegemeier is the Director of The White House Office of Science and Technology Policy (OSTP). Dr. Droegemeier serves as President Donald J. Trump's science advisor and leads OSTP in its coordination of science and technology initiatives across the Federal Government. Kelvin's background is in extreme weather, numerical weather prediction, and data assimilation.

Before joining The White House, Kelvin served as Vice President for Research and Regents' Professor of Meteorology at the University of Oklahoma, where he joined the faculty in 1985 as Assistant Professor of Meteorology. In his 33 years at the University of Oklahoma, Kelvin generated more than $40 million in research funding and authored or co-authored more than 80 refereed articles and 200 conference publications. He also co-founded, directed, and led the National Science Foundation (NSF) Science and Technology Center for Analysis and Prediction of Storms (CAPS) and served as co-founder and Deputy Director of the NSF Engineering Research Center for Collaborative Adaptive Sense of the Atmosphere (CASA).

Kelvin served two six-year terms on the National Science Board, the governing body of the NSF, including the last four years as Vice-Chairman, having been nominated by Presidents George W. Bush and Barack Obama and twice confirmed by the United States Senate. He has also served on and chaired numerous national boards and committees and is a Fellow of the American Meteorological Society and American Association for the Advancement of Science. He was appointed in 2017 as Oklahoma Cabinet Secretary of Science and Technology.

Born in Kansas, Kelvin earned a B.S. in meteorology from the University of Oklahoma and M.S. and Ph.D. degrees in atmospheric science from the University of Illinois at Urbana-Champaign.

SCIENCE TO TECHNOLOGY TRANSITION: PERSPECTIVES FROM DOE TECHNOLOGY OFFICES

- **Linda Horton** is the Director of the DOE Basic Energy Sciences (BES) Materials Sciences and Engineering Division. While at DOE, she also served as the team lead for the Energy Frontier Research Centers from 2011-2013 and has led the planning for several Basic Research Needs workshops and reports. Prior to joining DOE, she was at Oak Ridge National Laboratory for nearly 30 years, serving in a number of roles including Director for the Center for Nanophase Materials Sciences (CNMS).
- **Peter Faguy** manages the Applied Battery Research Program, a part of the Hybrid Electric Systems Group in the Vehicle Technologies Office in DOE Office of Energy Efficiency and Renewable Energy. He also serves as a technical expert in the areas of electrochemical energy storage and conversion (batteries, fuel cells, CO_2 conversion, and pollution remediation) and advanced materials manufacturing (nanomaterials, composites, reel-to-reel coatings, characterization, and nondestructive evaluation). Peter started his career as a professor at the University of Louisville, but left to help launch the stat-up company, MicroCoating Technology, before moving on to several energy related small businesses.
- **Eric Hsieh** is the Director of Grid Systems and Components for the DOE Office of Electricity. This group delivers grid modernization through technology innovation. The portfolio includes transformers, power electronics, robotics, and energy storage. Mr. Hsieh has over 15 years of experience in advancing energy delivery technology at several organizations, including A123 Systems and the Federal Energy Regulatory Commission. Mr. Hseih received his MPP in Public Policy from the University of California, Berkeley.
- **Mike McKittrick** is the Program Lead for R&D Consortia in the DOE Advanced Manufacturing Office. In this role, he is the DOE Lead for the Critical Materials Institute, a $120 million/5 year program to develop R&D solutions for challenges across the supply chain of critical materials for clean energy technologies, and the DOE Lead for the REMADE Manufacturing USA Institute, a $140 million/5 year program to develop technologies to reduce the cost and energy needed to recycle, reuse and remanufacturing key materials. Prior to his time at DOE, he worked as a chemical engineer at the US Environmental Protection Agency and a Professor at the University of Buffalo. Dr. McKittrick received his Ph.D. from Georgia Institute of Technology in Chemical Engineering.
- **Eric L. Miller** serves as a Program Manager for Hydrogen Production and Delivery in the DOE Fuel Cell Technologies Office. His professional career in alternative energy research has spanned more than 25 years, centering on solar energy conversion and on hydrogen and fuel cell technologies. He is widely recognized as a world leader in photoelectrochemical hydrogen production for his pioneering research in this field. Recently, Dr. Miller has played an instrumental role in the launch and management of DOE's Energy Materials Network, which aims to accelerate materials discovery and development critical to a broad spectrum of key clean energy technologies.
- **Avi Shultz** is the acting program manager for the Solar Energy Technologies Office (SETO) Concentrating Solar Power (CSP) team, which supports research, development, and demonstration of solar thermal components and systems that can enable wide-spread deployment of low-cost CSP with thermal energy storage. Dr. Shultz has been with SETO since 2013, where he started as a policy fellow and was hired as a federal technology manager, supporting the CSP subprogram on a wide variety of topics, including thermochemical energy storage, CSP systems and cost analysis, and non-electricity applications of solar thermal process heat. Prior to joining SETO, Dr. Shultz was a Rubicon Post-Doctoral Fellow at the University of

Amsterdam, where his research focused on developing supramolecular approaches to catalysts for artificial photosynthesis. Dr. Shultz holds a B.A. from Columbia University and a Ph.D. in chemistry from Northwestern University, performing his thesis research on the synthesis of catalytically active porous materials.

- **Sven Mumme** is a technology manager in the DOE Building Technologies Office (BTO). In this role he manages the Envelope subprogram within the Emerging Technologies program. He also leads BTO's Technology-to-Market Initiative, Small-Business Vouchers Program, and Small Business Innovation Research Program. Mumme originally joined the Department of Energy in 2012 as an ARPA-E Technology-to-Market Advisor, where he helped transition breakthrough energy technologies from lab to market. Prior to joining DOE, Mumme worked for W.R. Grace and Underwriters Laboratories (UL). Mumme earned a B.S. with honors in mechanical engineering from Queen's University in Kingston, Ontario, and an MBA from The Fuqua School of Business at Duke University.

PANEL: EFRC IMPACT ON SCIENCE AND TECHNOLOGY

- **Marc Kastner** is President of the Science Philanthropy Alliance, a coalition of leading nonprofit institutions and foundations dedicated to increasing financial support for basic science research by understanding the opportunities and complexities philanthropists face in funding basic science, and providing advice and learning opportunities for individual philanthropists and foundation staffs. Prior to leading the Alliance, he had a long career in a variety of senior positions at the Massachusetts Institute of Technology (MIT). Prof. Kastner joined MIT in 1973 and was named the Donner Professor of Physics in 1989. He became director of the Center for Materials Science and Engineering in 1993, head of the Department of Physics in 1998 and dean of the School of Science in 2007. Prof. Kastner's research has focused on the electronic structure of materials, including nanoscale semiconductor structures, in which the effects of electron correlations are crucial to understanding macroscopic properties.
- **Daniel Cosgrove** is Professor and Holder of the Eberly Family Chair in Biology at Pennsylvania State University and Director of the Center for Lignocellulose Structure and Formation (CLSF), an Energy Frontier Research Center funded by the US Department of Energy in 2009, a coordinate effort by 16 labs in five universities and Oak Ridge National Lab. His research group is focused on the structure of growing cell walls and the mechanisms of plant cell enlargement; they discovered expansins as the protein mediators of acid-induced wall loosening and have used biophysical, molecular biology and genomic approaches to understand the mechanisms of expansins, as well as their biological roles and evolution. After earning a B.A. in Botany at the University of Massachusetts and a PhD in Biological Sciences at Stanford, Cosgrove did postdoctoral stints at the University of Washington and the Nuclear Research Center in Julich, Germany, before starting as assistant professor at Penn State. He served as President of the American Society of Plant Biologists (ASPB 2001), Chairman of the ASPB Education Foundation (2002), member of the Science Advisory Board for the Danforth Plant Science Center (2009-2012), Director for the USDA Competitive Grants Panel on Plant Growth and Development, Director of ChloroFilms (2009-2012), an international contest for plant biology videos on YouTube, and member of the Science Advisory Board for the Australian Centre of Excellence for Plant Cell Walls (2009-2015).
- **Paul J. Dauenhauer** is currently the Lanny Schmidt Honorary Professor at the University of Minnesota in the Department of Chemical Engineering and Materials Science. He received a bachelor of science in chemical engineering and chemistry from the University of Wisconsin -

Madison in 2004, and a Ph.D. in chemical engineering from the University of Minnesota in 2008. Paul worked as a senior research engineer for the Dow Chemical Company within Core R&D Reaction Engineering in Midland, MI and the Hydrocarbons & Energy Department in Freeport, TX. In 2009, he joined the University of Massachusetts, Amherst, Department of Chemical Engineering as an assistant professor, before moving to Minnesota in 2014. His research has been highlighted by numerous awards including the NSF CAREER, the DOE Early Career, and the Camille-Dreyfus Teacher-Scholar award. He is the co-founder of Sironix Renewables and the inventor of the flagship technologies for Activated Research Company and enVerde, LLC. Website: http://dauenhauer.cems.umn.edu Twitter: @pauldauenhauer

- **Hunter McDaniel** founded UbiQD, Inc. in 2014, and serves as CEO. He previously worked at Los Alamos National Laboratory as a postdoc under Victor Klimov in the Center for Advanced Photophysics EFRC. Hunter has a PhD in Materials Science and Engineering from University of Illinois, and prior to that he studied Physics and Electrical Engineering at UC Santa Barbara. UbiQD produces copper indium sulfide and related quantum dots, and develops optical technologies such as luminescence concentrators. The company’s first commercial product is a greenhouse film that red-shifts the sun’s spectrum for improved crop outcomes, and sometimes electricity generation. UbiQD’s nanomaterials represent a platform technology with many applications beyond spectrum-optimized greenhouses, and their ambition is to become a leader in the growing multi-billion-dollar quantum dot industry.
- **Krista S. Walton** is Professor and Robert “Bud” Moeller Faculty Fellow in the School of Chemical and Biomolecular Engineering at Georgia Tech. She received her B.S.E. in chemical engineering from the University of Alabama-Huntsville in 2000 and obtained her Ph.D. in chemical engineering from Vanderbilt University in 2005, working with Prof. M. Douglas LeVan. Prof. Walton completed an ACS PRF Postdoctoral Fellowship at Northwestern University in 2006 under the direction of Prof. Randall Snurr. Her research program focuses on the design, synthesis, and characterization of functional porous materials for use in adsorption applications including CO2 capture and air purification. She has published close to 100 peer-reviewed articles and presented dozens of plenary lectures and invited seminars. Prof. Walton currently serves as an Associate Editor for the ACS Journal Industrial & Engineering Chemistry Research, and is the Director and Lead PI of Georgia Tech’s DOE Energy Frontier Research Center, UNCAGE-ME. Prof. Walton’s accomplishments have been recognized by many prestigious awards including the AIChE FRI/John G. Kunesh Award for Excellence in Separations Research (2016), the ACS Women Chemists Committee Rising Star Award (2015), the inaugural International Adsorption Society Award for Excellence in Publications by a Young Member of the Society (2013) and the Presidential Early Career Award for Scientists and Engineers (2008).

PANEL: EFRC IMPACT ON THE ENERGY WORKFORCE

- **Michelle Buchanan** is the Deputy for Science and Technology at Oak Ridge National Laboratory. Dr. Buchanan oversees one of the nation's most extensive portfolios of research and development, spanning physical and materials sciences, energy and engineering sciences, computing and computational sciences, biological and environmental sciences, neutron sciences, and global security, for the U.S. Department of Energy and other sponsors. Before assuming her current position in October 2017, Dr. Buchanan served in a series of senior leadership roles at Oak Ridge National Laboratory including Associate Laboratory Director for Physical Sciences and director of the ORNL Chemical Sciences Division. She joined ORNL in 1978 after earning a B.S. in chemistry from the University of Kansas in Lawrence, Kansas, and a Ph.D. in chemistry from the

University of Wisconsin in Madison, Wisconsin. Dr. Buchanan is the author or co-author of more than 150 scientific publications and reports, holds two patents, and was editor of a book on Fourier transform mass spectrometry. She received the 2019 Ellen Swallow Richards Diversity Award given by TMS, the Minerals, Metals & Materials Society. Dr. Buchanan is a Fellow of both the American Association for the Advancement of Science (AAAS) and a Fellow of the American Chemical Society (ACS).

- **Karena Chapman** is Joseph Lauher and Frank W. Fowler Endowed Chair in Materials Chemistry in the Department of Chemistry at Stony Brook University. Before moving the Stony Brook University, she was a chemist at Argonne National Laboratory, building the dedicated Pair Distribution Function instrument at the Advanced Photon Source. Her research focuses on understanding the coupling of structure and reactivity in energy-relevant materials using advanced synchrotron-based characterization tools. This work has been recognized as one of ACS' Talented 12 in 2016 and was awarded the 2015 MRS Outstanding Young Investigator Award. She is involved in 3 EFRCs: as a Thrust lead for the Northeast Center for Chemical Energy Storage (NECCES), as a PI for the Inorganometallic Catalyst Design Center (ICDC), and as Associate Director for the Next Generation Synthesis Center (GENESIS).
- **Brandi Cossairt** was born and raised in Miami, Florida. She is a first-generation college graduate, having obtained her B. S. in Chemistry from the California Institute of Technology in 2006. Brandi went on to pursue graduate studies at the Massachusetts Institute of Technology under the guidance of Professor Christopher C. Cummins and was awarded her Ph.D. in 2010. She then continued her academic career as an NIH NRSA Postdoctoral Fellow at Columbia University between 2010 and 2012 working with Professor Jonathan Owen. Brandi joined the Department of Chemistry at the University of Washington as an Assistant Professor in 2012 and was promoted to Associate Professor with Tenure in 2018. She has received a number of awards for her research including a Sloan Research Fellowship, a Packard Fellowship, an NSF CAREER Award, a Dreyfus Teacher-Scholar Award, and the National Fresenius Award from the American Chemical Society. Outside of the lab Brandi is an Associate Editor at the ACS journal Inorganic Chemistry and is the co-founder of the Chemistry Women Mentorship Network (ChemWMN).
- **Cary Hayner** is the co-founder and Chief Technology Officer of NanoGraf, Inc. Cary is a co-inventor of the core NanoGraf technology. He has expertise in research and development with graphene, silicon, and other materials. His work includes developing flexible, high-energy composite materials as anode and cathode technologies for Li-ion batteries. He is an author on ten publications and two patents. Cary holds a PhD in chemical engineering from Northwestern University and has dual bachelor's degrees in chemical engineering and chemistry from the University of Minnesota, as well as previous experience in computational chemistry, pharmaceuticals, and sustainability. He was a member of the Center for Electrochemical Energy Science (CEES) from 2009 – 2013.
- **Liam C. Palmer** received a B.S. in chemistry from the University of South Carolina in 1999. He completed his Ph.D. on molecular encapsulation under the supervision of Prof. Julius Rebek, Jr. at The Scripps Research Institute in 2005. He then started as a post-doc in the lab of Prof. Samuel Stupp at Northwestern University. Liam was promoted to a Research Assistant Professor in the Department of Chemistry in 2007 and again to a Research Associate Professor in 2015. He is also currently Director of Research for the Simpson Querrey Institute (SQI) and Executive Director of Research at the Center for Bio-Inspired Energy Science (CBES).

BES EARLY CAREER NETWORK ORGANIZED EVENTS

SOCIAL EXCURSIONS

SOCIAL EVENING AT DUKE'S COUNTER

When: Monday, July 29, 2019, 7:00 PM – Late
Who: Graduate students, postdocs, and early career scientists

Description: An evening socializing at Duke's Counter (3000 Connecticut Ave. NW, Suite J). The venue is about 0.5 miles from the hotel. A group will meet in the hotel lobby shortly after meeting activities end to walk over together. Others are free to join at any time. Participants are responsible for their own food and drinks.

BES Early Career Network Organizers:

- **Aaron Taggart (Chair)**, University of North Carolina at Chapel Hill, AMPED
- **Jefferson Dixon**, Stanford University, PTL
- **Robert Sacci**, Oak Ridge National Laboratory, FIRST
- **Janani Sampath**, University of Washington, CSSAS

Contact:

- Aaron Taggart (ataggart@live.unc.edu)

BASEBALL GAME AT NATIONALS PARK

When: Tuesday, July 30, 2019, 7:00 PM – Late
Who: All attendees and their friends and family

Description: Washington Nationals vs. Atlanta Braves at 7:05 pm. We will leave from the conference center and take the Metro (red line connected to green line ~31 minutes) to and from Nationals Stadium. Send $12 payment by June 19 through Google Wallet to Robert Sacci at imbellis@gmail.com to ensure a ticket at the discounted group rate.

BES Early Career Network Organizers:

- **Robert Sacci (Chair)**, Oak Ridge National Laboratory, FIRST
- **Aaron Taggart**, University of North Carolina at Chapel Hill, AMPED

Contacts:

- Robert Sacci (saccirl@ornl.gov)
- Aaron Taggart (ataggart@live.unc.edu)

LUNCH EVENTS

DIVERSITY IN ENERGY SCIENCE LUNCH

When: Monday, July 29, 2019, 12:30 – 1:30 PM
Where: Exhibition Hall C – Lincoln 2, 3, and 4
Who: All meeting attendees

Description: Ready to network, learn about diversity and have a great time at lunch? Join us at this year's Diversity in Energy Science Event. Through a dynamic networking-trivia game you will have the opportunity to talk to scientist from all around the world while exploring the relevance of diversity in the STEM fields. Compete with your collogues for the diversity-expert prize and get your next research idea as you interact one-on-one with PI's, graduate students and postdocs.

BES Early Career Network Organizers:

- **Natalia Rodriguez Quiroz (Chair)**, University of Delaware, CCEI
- **Liang Feng**, Texas A&M University, CGS
- **Lynnicia Massenburg**, Penn State University, CLSF
- **Santanu Roy**, Oak Ridge National Laboratory, MSEE

ELEVATOR PITCHES AND SCIENCE SPEED DATING LUNCH

When: Monday, July 29, 2019, 12:40 – 1:40 PM
Where: Lincoln 3&4
Who: All meeting attendees

Description: Elevator pitches can be the start of new projects, collaborations, and jobs and are essential for effective communication of scientific ideas between people of all levels of expertise. Come work on your pitch while networking with new people! We'll be hosting a short workshop on designing an elevator pitch, complete with a chance to create and hone your very own pitch. This will be followed by a round robin game where you'll have the chance to practice your pitch with a variety of people with different levels of expertise.

BES Early Career Network Organizers:

- **Samantha Johnson (Chair)**, Pacific Northwest National Laboratory, CME
- **Zhe Fan**, Oak Ridge National Laboratory, EDDE
- **Ryan Greer**, Florida State University, CAST
- **Annalise Maughan**, National Renewable Energy Laboratory, CHOISE
- **Ruocun (John) Wang**, North Carolina State University, FIRST

BES EARLY CAREER NETWORK (ECN) REPRESENTATIVES

The DOE Basic Energy Sciences - Early Career Network (BES ECN) is a group of graduate students, postdoctoral researchers, and early career scientists from current Energy Frontier Research Centers (EFRC), Energy Innovation Hubs, Computational Materials Sciences awards (CMS), and Computational Chemical Sciences awards (CCS). 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. The BES ECN plans webinars, hosts meet-ups at national meetings, and organizes early career events at biennial Principal Investigators Meetings. They also maintain a LinkedIn group, DOE BES - Early Career Network (ECN), for current members and alumni of the BES Early Career Network. Each active BES center is invited to have a representative on the BES ECN planning committee.

Name	Institution	Center
Farbod Alimohamadi	Temple University	Center for Complex Materials from First Principles (CCM)
Emma Anquillare	Boston University (current stationed at ALS/LBNL)	Joint Center for Energy Storage Research (JCESR)
Jacob Artz	National Renewal Energy Laboratory	Center for Biological Electron Transfer and Catalysis (BETCy)
Sage Bauers	National Renewal Energy Laboratory	Center for Next Generation of Materials by Design: Incorporating Metastability (CNGMD)
Marcos Calegari Andrade	Princeton University	Chemistry in Solution and at Interfaces (CSI)
Carmen Chen	Georgia Tech	Center for Understanding and Control of Acid Gas-induced Evolution of Materials for Energy (UNCAGE-ME)
Hyeyoung Cho	University of Utah	Multi-Scale Fluid-Solid Interactions in Architected and Natural Materials (MUSE)
Haelie Chung	University of California, San Diego	NorthEast Center for Chemical Energy Storage (NECCES)
Javier Del Valle	University of California, San Diego	Quantum Materials for Energy Efficient Neuromorphic Computing (Q-MEEN-C)
Carlos Diaz	University of Texas at El Paso	Fermi-Lowdin Oribtal Self-Interaction Correction Center (FLOSIC)
Jefferson Dixon	Stanford	Photonics at Thermodynamic Limits (PTL)
James Dombrowki	Northwestern University	Advanced Materials for Energy-Water Systems (AMEWS)
Joseph DuChene	Caltech	Joint Center for Artificial Photosynthesis (JCAP)
Zhe Fan	Oak Ridge National Laboratory	Energy Dissipation to Defect Evolution (EDDE)
Liang Feng	Texas A&M	Center for Gas Separations Relevant to Clean Energy Technologies (CGS)
George Giannakakis	Tufts University	Integrated Mesoscale Architectures for Sustainable Catalysis (IMASC)
Ryan Greer	Florida State University	Center for Actinide Science & Technology (CAST)
Nathan Harms	Northeastern University	Exascale Catalytic Chemistry Project (ECC)

Lingfeng He	Idaho National Laboratory	Center for Thermal Energy Transport under Irradiation (TETI)
Lisa Housel	Stony Brook University	Center for Mesoscale Transport Properties (m2mt)
Satcher Hsieh	Lawrence Berkeley National Laboratory/ University of California, Berkeley	Center for Novel Pathways to Quantum Coherence in Materials (NPQC)
Aysenur Iscen	Northwestern University	Center for Bio-Inspired Energy Science (CBES)
Na-Hyun Jo	Ames Laboratory/ Iowa State	Center for the Advancement of Topological Semimetals (CATS)
Samantha Johnson	Pacific Northwest National Laboratory	Center for Molecular Electrocatalysis (CME)
Tyler Josephson	University of Minnesota	Nanoporous Materials Genome Center (NMGC)
Jesse Ko	Stanford Synchrotron Radiation Lightsource/ SLAC National Accelerator Laboratory	Center for Synthetic Control Across Length-scales for Advancing Rechargeables (SCALAR)
Vancho Kocevski	University of South Carolina	Center for Hierarchical Waste Form Materials (CHWM)
Bryan Kudisch	Princeton University	Bioinspired Light-Escalated Chemistry (BioLEC)
Lynnicia Massenburg	Penn State University	Center for Lignocellulose Structure and Formation (CLSF)
Annalise Maughan	National Renewal Energy Laboratory	Center for Hybrid Organic Inorganic Semiconductors for Energy (CHOISE)
Saba Navabzadeh Esmaeely	Ohio State University	Center for Performance and Design of Nuclear Waste Forms and Containers (WastePD)
Hyunho Noh	Northwestern University	Center for Light Energy Activated Redox Processes (LEAP)
Bo Peng	Pacific Northwest National Laboratory	Center for Scalable Predictive methods for Excitations and Correlated Phenomena (SPEC)
Maria Philip	University of Illinois at Urbana-Champaign	Center for Electrochemical Energy Science (CEES)
Diana Qiu	Lawrence Berkeley National Laboratory	Center for Computational Study of Excited-State Phenomena in Energy Materials (C2SEPEM)
Rodolfo Rodriguez	University of California, Riverside	Spins and Heat in Nanoscale Electronic Systems (SHINES)
Natalia Rodriguez Quiroz	University of Delaware	Catalysis Center for Energy Innovation (CCEI)
Santanu Roy	Oak Ridge National Laboratory	Molten Salts in Extreme Environments (MSEE)
Janani Sampath	University of Washington	The Center for the Science of Synthesis Across Scales (CSSAS)
William (Will) Smith	Washington State University	Interfacial Dynamics in Radioactive Environments and Materials (IDREAM)
Aaron Sternbach	Columbia University	Programmable Quantum Materials (Pro-QM)

David Stewart	University of Maryland	Nanostructures for Electrical Energy Storage (NEES)
Rahul Sujanani	University of Texas at Austin	Center for Materials for Water and Energy Systems (M-WET)
Jindi Sun	University of Wyoming	Center for Mechanistic Control of Water-Hydrocarbon-Rock Interactions in Unconventional and Tight Oil Formations (CMC-UF)
Aaron Taggart	UNC Chapel Hill	Alliance for Molecular PhotoElectrode Design for Solar Fuels (AMPED)
Paul Todd	Colorado State University	A Next Generation Synthesis Center (GENESIS)
Ruocun (John) Wang	North Carolina State University	Fluid Interface Reactions, Structures and Transport Center (FIRST)
Yishu Wang	Johns Hopkins University	Institute for Quantum Matter (IQM)
Nicholas Winner	University of California, Berkeley	Fundamental Understanding of Transport Under Reactor Extremes (FUTURE)
Peng Xu	Iowa State University	Exascale Software for Heterogeneous and Interfacial Catalysis (ESHIC)
Yao Yang	Cornell University	Center for Alkaline-Based Energy Solutions (CABES)
Maher Yazback	University of Florida	Center for Molecular Magnetic Quantum Materials (M2QM)

2019 EFRC PI MEETING – GRAPHIC AGENDA FOR TUESDAY, JULY 30, 2019

	Time	Lincoln 2	Lincoln 3&4	Lincoln 5	Lincoln 6	Thurgood Marshall East	Thurgood Marshall North	Thurgood Marshall West	Thurgood Marshall South
I	8:00 - 9:40 AM	K. Solar Energy	H. Quantum Materials I	B. Catalysis I	A. Bio-inspired Science	D. Energy Storage	J. Separation Science	F. Materials and Chemistry by Design	G. Nuclear Energy
II	11:00 – 12:20 PM	L. Subsurface Science			M. Synthesis Science		E. Energy - Water		
III	1:45 – 3:45 PM	I. Quantum Materials II			C. Catalysis II				

		A. Bio-inspired Science	B. Catalysis I	D. Energy Storage	F. Materials and Chemistry by Design	G. Nuclear Energy	H. Quantum Materials I	J. Separation Science	K. Solar Energy
Room		***Lincoln 6***	***Lincoln 5***	***Thurgood Marshall East***	***Thurgood Marshall West***	***Thurgood Marshall South***	***Lincoln 3&4***	***Thurgood Marshall North***	***Lincoln 2***
Chair		*Robert Stack*	*Chris Bradley*	*Refik Kortan*	*Mike Markowitz*	*Philip Wilk*	*P. Thiyagarajan*	*Daniel Matuszak*	*Christopher Fecko*
I-1	**8:00 AM**	[**CLSF**] Charles T. Anderson *Penn State* Life in The Construction Zone: Dynamic Assembly of Plant Cell Walls	[**CME**] James M. Mayer *Yale* Developing and Using Scaling Relationships for Molecular Electrocatalysis of the Oxygen Reduction Reaction	[**NECCES**] Shirley Meng *UC San Diego* Pushing the Limit of Intercalation - Combining Theory, Computation and Experiments to Control Cation and Anion Redox	[**FIRST**] Yury Gogotsi *Drexel* MXene Pseudocapacitive Energy Storage Systems with High Energy Density	[**CAST**] Christopher Dares *Florida International U* Simple Methods to Quantitatively Generate Hexavalent Americium	[**SHINES**] Víctor H. Ortiz, Qiming Shao* *UC Riverside, UC Los Angeles* Ferrimagnetic Insulator for Ultrafast and Ultralow-power Spintronic Devices	[**CGS**] Jeffrey R. Long *UC Berkeley* Cooperative Adsorption and Gas Separations in Metal–Organic Frameworks	[**AMPED**] Rachel E. Bangle, Jenny Schneider* *UNC Chapel Hill* Transparent Conducting Oxides As Highly Versatile Dye-Sensitized Photoelectrodes
I-2	**8:20 AM**	[**CSSAS**] F. Akif Tezcan *UC San Diego* Multiscale control of the self-assembly pathways and morphologies of 2D protein assemblies	[**CCM**] Jianwei Sun *Tulane* Tuning the Catalytic Activity of Metal-Intercalated Layered Materials	[**FIRST**] Veronica Augustyn *NC State* Importance of Structural Stability for Fast, Pseudo-capacitive Energy Storage in Oxides Revealed by Operando AFM	[**ICDC**] Rachel Getman, Heather Kulik *Clemson, MIT* Inorganometallic Catalyst Design Center: Theory Driving Next-Generation Catalyst Design	[**CHWM**] Hans-Conrad zur Loye *U South Carolina* Synthesis, Structure and Ion Exchange Potential of New Uranyl Salt Inclusion Phases	[**M^{2}QM**] Jie-Xiang Yu, Ashlyn Hale* *U Florida* Synthesis, Characterization and Predictive First-Principles Calculations	[**UNCAGE-ME**] J. R. Schmidt *U Wisconsin - Madison* Acid-Gas Induced Defects in Zeolitic Imidazolate Frameworks	[**LEAP**] Tobin J. Marks *Northwestern* Soft Matter and Hybrid Solar Cell Interface Science and Engineering

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2019 EFRC PI MEETING – GRAPHIC AGENDA FOR TUESDAY, JULY 30, 2019

		A. Bio-inspired Science	**B. Catalysis I**	**D. Energy Storage**	**F. Materials and Chemistry by Design**	**G. Nuclear Energy**	**H. Quantum Materials I**	**J. Separation Science**	**K. Solar Energy**
Room		***Lincoln 6***	***Lincoln 5***	***Thurgood Marshall East***	***Thurgood Marshall West***	***Thurgood Marshall South***	***Lincoln 3&4***	***Thurgood Marshall North***	***Lincoln 2***
I-3	**8:40 AM**	[**CBES**] Kyle J. M. Bishop *Columbia* Autonomous Navigation of Synthetic Microrobots	[**CABES**] Héctor Abruña *Cornell* Electrocatalysis in Alkaline Media: Novel Materials and Architectures and Operando Methods	[**m2M/t**] Kenneth Takeuchi, Yimei Zhu *Stony Brook, BNL* 1D materials: Improved structural resiliency via atomic level design	[**CNGMD**] Sage Bauers, Chris Bartel* *NREL, U Colorado* Designing New Nitride Semiconductors: From Computational Discovery to Experimental Realization	[**CAST**] Ryan Baumbach *National High Magnetic Field Lab, Florida State* Environments for Actinides: Synthesis, Structure and Electronic State	[**Q-MEEN-C**] Eric Fullerton *UC San Diego* Spin Hall Effects in Novel Materials	[**CHWM**] Natalia Shustova *U South Carolina* Thermodynamics and Electronic Properties of Heterometallic Multinuclear Actinide-MOFs	[**AMPED**] Gerald J. Meyer *UNC Chapel Hill* Conductive Oxides as Photoelectrodes that Support Long-Lived Charge-Separation and Water Oxidation Catalysis
I-4	**9:00 AM**	[**BioLEC**] Kyle F. Biegasiewicz, Bryan Kudisch* *Princeton* Discovery of a new photobiocatalyst platform: Non-natural radical photochemistry enabled by flavoproteins	[**AMPED**] Alexander J. M. Miller *UNC Chapel Hill* Controlling Orbitals in Molecular Electrocatalysts to Unlock New Pathways Towards Solar Fuels	[**NECCES**] Zachary Lebens-Higgins, Antonin Grenier, Julija Vinckeviciute* *Binghamton, Stony Brook, UC Santa Barbara* From Cation to Anion Redox: Pushing the ultimate limit of layered oxides	[**GENESIS**] John B. Parise *Stony Brook* GENESIS: A Next Generation Synthesis Center	[**IDREAM**] Thomas M. Orlando *Georgia Tech* Radiation effects at complex interfaces: Energy exchange and reactions during radiolysis of Boehmite (γ-AlOOH) nanoplates	[**SHINES**] Igor Barsukov *UC Riverside* Thermally driven magnon condensation in YIG/Py nanowires	[**CGS**] Michael Tsapatsis *U Minnesota* High Performance Membranes Made by Ligand-Induced PermSelectivation (LIPS)	[**CME**] Thatcher Root *U Wisconsin–Madison* Mediated Electrolysis Approaches to Energy Conversion
I-5	**9:20 AM**	[**CLSF**] James D. Kubicki *UT El Paso* Density Functional Theory Modeling of Elementary Cellulose Microfibrils	[**CME**] Daniel J. Martin, Samantha I. Johnson* *Yale, PNNL* The Effect of Electrostatics on Small Molecule Binding and Catalysis Using a Polycationic Iron Porphyrin	[**SCALAR**] Rebecca Kubena, Josh Zak* *UCLA, U Southern California, Caltech* Investigating the Redox Activity & Lithiation of Icosahedral Boron Clusters in the Solid State	[**WastePD**] Jianwei Wang *Louisiana State* Ceramic Waste Form Design and Performance Prediction – A SEDMAT Approach	[**CAST**] Eric Schelter *Penn State* Towards New Methods for Separating Actinide sand Relevant Anions from Waste Through Redox Processes and Supramolecular Anion Recognition	[**IQM**] David Vanderbilt *Rutgers* Recent Progress on 3D Axion Insulators		[**LEAP**] Alex B.F. Martinson *ANL* Acid Compatible Halide Perovskite Photocathodes: Solar-Assisted Hydrogen Production Enabled By Atomic Layer Deposition

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2019 EFRC PI MEETING – GRAPHIC AGENDA FOR TUESDAY, JULY 30, 2019

9:40 – 11:00 AM **Poster Session I (refreshments provided)**

		B. Catalysis I	**D. Energy Storage**	**E. Energy - Water**	**F. Materials and Chemistry by Design**	**G. Nuclear Energy**	**H. Quantum Materials I**	**L. Subsurface Science**	**M. Synthesis Science**
Room		***Lincoln 5***	***Thurgood Marshall East***	***Thurgood Marshall North***	***Thurgood Marshall West***	***Thurgood Marshall South***	***Lincoln 3&4***	***Lincoln 2***	***Lincoln 6***
Chair		*Wade Sisk*	*Tom Russell*	*Eliane Lessner*	*George Maracas*	*Tim Fitzsimmons*	*Michael Pechan*	*James Rustad*	*Bonnie Gersten*
II-1	**11:00 AM**	[**ICDC**] Bruce Gates *UC Davis* Inorganometallic Catalyst Design Center: Metal Organic Framework Catalysts Assessed at the Scale of Catalytic Sites	[**NEES**] A. Alec Talin *SNL* Determining Potentials across Solid State Battery Systems	[**M-WET**] Ségolène Antoine, Rahul Sujanani, Sally Jiao, Malgorzata Chwatko* *UC Santa Barbara, UT Austin* Understanding the Impact of Mesoscale Membrane Architecture on Water Transport	[**CLSF**] Jochen Zimmer *U Virginia* Molecular Basis for Cellulose Microfibril Formation	[**EDDE**] Yanwen Zhang *ORNL* Nanostructured High-entropy Alloys under Extreme Environments	[**Q-MEEN-C**] Ivan Schuller, Javier del Valle *UC San Diego* Quantum Materials for Energy Efficient Neuromorphic Computing and First Implementation of Neuristors and Synaptors Based on Charge	[**MUSE**] Viktoriya Semeykina *U Utah* Geo-Architectured Material Synthesis, Characterization and Modeling	[**CSSAS**] Chun-Long Chen *PNNL* Peptoid-controlled synthesis of hierarchical materials
II-2	**11:20 AM**	[**IMASC**] Georgios Giannakakis, Kaining Duanmu, Paul Kress, Zhen Qi* *Tufts, UC Los Angeles, LLNL* Mechanistic Studies Of Non-Oxidative Ethanol Dehydrogenation On NiAu Single Atom Alloys	[**CEES**] Jeffrey Greeley *Purdue* Molecular structure of solid state electrode/ electrolyte interfaces: thermodynamic properties and automated algorithms for structure determination	[**AMEWS**] Giulia Galli *U Chicago/ANL* First Principles and Multi-Scale Simulations of Materials for Energy-Water Systems	[**CBES**] Samuel I. Stupp *Northwestern* Supramolecular Polymer-Covalent Network Hybrid Materials for Light-Activated Robotic Functions	[**FUTURE**] Farida Selim *Bowling Green State University* Understanding the Defect Structure in Irradiated Materials	[**Pro-QM**] Dmitri N.Basov *Columbia* Programmable Quantum Materials	[**CMC-UF**] Bowen Ling *Stanford* Microfluidics for probing reactive transport in fractured media	[**CNGMD**] Wenhao Sun, Feng Wang *LBNL, BNL* Complex Metal Oxides: Moving from Materials by Design to Synthesis by Design

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2019 EFRC PI MEETING – GRAPHIC AGENDA FOR TUESDAY, JULY 30, 2019

		B. Catalysis I	D. Energy Storage	E. Energy - Water	F. Materials and Chemistry by Design	G. Nuclear Energy	H. Quantum Materials I	L. Subsurface Science	M. Synthesis Science
Room		*Lincoln 5*	*Thurgood Marshall East*	*Thurgood Marshall North*	*Thurgood Marshall West*	*Thurgood Marshall South*	*Lincoln 3&4*	*Lincoln 2*	*Lincoln 6*
II-3	**11:40 AM**	[**CCEI**] Dongxia Liu *U Maryland* Synthesis of Ultra-Low Loadings of Catalysts for Hydrodeoxygenation (HDO) of Biomass	[**m2M/t**] Esther Takeuchi, Lynden Archer *Stony Brook, Cornell* Productive and parasitic reactions: The role of interfacial chemistry and structure	[**CABES**] T.A. Arias *Cornell University* Ab initio theory of fundamental processes underlying fuel cell performance of alkaline membranes	[**UNCAGE-ME**] Tina M. Nenoff *SNL* Acid Gas Stability and Selectivity of Rare Earth MOFs	[**TETI**] Maniesha Singh *Purdue* Equilibrium and non-equilibrium defect disorder in U-doped ThO2 and implications for lattice thermal conductivity	[**NPQC**] Joel Moore *LBNL* Introduction, with Selected Highlights, to the Center for Novel Pathways to Quantum Coherence in Materials	[**MUSE**] Hyeyoung Cho, Jiaoyan Li, Hassnain Asgar* *U Utah, INL, U Wisconsin* Property changes under confinement in architected materials	[**GENESIS**] James R. Neilson *Colorado State* Enabling Prescriptive Synthesis of Metastable and Ternary Oxides
II-4	**12:00 PM**	[**IMASC**] Philippe Sautet *UC Los Angeles* Stability, dynamics and catalytic reactivity of surface sites at bimetallic catalysts from first principles	[**FIRST**] Tyler Mathis , Xuehang Wang, Matthew W. Thompson* *Drexel, Vanderbilt* Dynamics of Electrolytes Under Confinement in Next Generation (Pseudo)Capacitive Materials	[**M-WET**] Scott Shell *UC Santa Barbara* Surface Programming of Hydration Water Structure, Dynamics, and Thermodynamics	[**BEES**] Thomas A. Zawodzinski *U Tennessee* The Interplay Between Structure, Dynamics and Electrochemistry in Microemulsions	[**FUTURE**] Peter Hosemann *UC Berkeley* Quantification of Pressure in Helium Bubbles via 4DSTEM and Computer Simulations	[**M^{2}QM**] Steven Hill *Florida State* Spectroscopic Studies of Molecular Magnetic Quantum Materials	[**CMC-UF**] A. R. Kovscek *Stanford* A Multiscale, Multiphysics, and Multidiscipinary EFRC to Achieve Control of Water-Hydrocarbon-Rock Interactions in Unconventional and Tight-Oil Formations	[**CNGMD**] David Ginley, Shyam Dwaraknath *NREL, LBNL* Identification and Functionality of New Polar Materials and Interfaces

12:20 – 1:45 PM **Lunch (buffet lunch provided)**
12:40 – 1:40 PM **ECN Event: Elevator Pitches and Science Speed Dating (all welcome)**

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2019 EFRC PI MEETING – GRAPHIC AGENDA FOR TUESDAY, JULY 30, 2019

		B. Catalysis I	**C. Catalysis II**	**D. Energy Storage**	**E. Energy - Water**	**F. Materials and Chemistry by Design**	**G. Nuclear Energy**	**H. Quantum Materials I**	**I. Quantum Materials II**
Room		***Lincoln 5***	***Lincoln 6***	***Thurgood Marshall East***	***Thurgood Marshall North***	***Thurgood Marshall West***	***Thurgood Marshall South***	***Lincoln 3&4***	***Lincoln 2***
Chair		*Chris Bradley*	*Viviane Schwartz*	*Craig Henderson*	*Peter Lee*	*James Davenport*	*John Vetrano*	*Matthias Graf*	*Thomas Settersten*
III-1	**1:45 PM**	[**IMASC**] Robert J. Madix *Harvard* Predicting reactor performance of npAu catalysts from studies on single crystals in ultrahigh vacuum	[**BETCy**] Jacob H. Artz *Washington State* Tuning catalytic bias of hydrogen gas producing hydrogenases	[**SCALAR**] Sarah Tolbert *UC Los Angeles* Overview of battery research from the center for synthetic control across length-scales for advancing rechargeables	[**AMEWS**] Seth Darling *ANL* Overview of the AMEWS EFRC	[**MSEE**] Santanu Roy, Fei Wu, Haimeng Wang* *ORNL, U Iowa, Notre Dame* Bridging the gap between theory & experiments on the structure, dynamics, & thermodynamics of molten salts	[**TETI**] Michael Manley *ORNL* Phonon transport in $Th_{1-x}U_xO_2$ from Ueutron Scattering and First-Principles Computation	[**PTL**] Prineha Narang *Harvard* Predicting Optically Excited Phenomena in Quantum Materials	[**CHOISE**] Matthew C. Beard *NREL* Controlling Optical, Electrical, and Spin Properties within Lead-Halide Inspired Hybrid Semiconductors
III-2	**2:05 PM**	[**CCEI**] Paul Dauenhauer *U Minnesota* Dynamic Catalysis Resonance for Chemical Conversion Acceleration	[**CBES**] Emil A. Weiss *Northwestern* Hierarchical Photocatalysis and Strategies to Control It	[**NECCES**] Karena Chapman *Stony Brook* Operando X-ray Characterization of Multi-Scale Kinetic Limitations in Battery Electrodes	[**M-WET**] Benny Freeman *UT Austin* Overview of Center for Materials for Water and Energy Systems (M-WET)	[**WastePD**] Joseph V. Ryan *PNNL* The Science of Environmental Degradation of Glass Materials	[**EDDE**] Takeshi Egami *U Tennessee; ORNL* Local Lattice Distortions in High-entropy Alloys	[**CCM**] Arun Bansil *Northeastern* SCAN and the Challenge of Cuprates and Other Complex Materials	[**PTL**] Jennifer Dionne *Stanford* The Light Years: Combined optical and environmental electron microscopy to visualize plasmonic processes w/ atomic-scale resolution
III-3	**2:25 PM**	[**UNCAGE-ME**] Zili Wu *ORNL* Role of Surface Structure and Dopants on the Interaction And Conversion of Acid Gases over Metal Oxide and Sulfide Catalysts	[**CME**] Brandi M. Cossairt *U Washington* Understanding and Controlling Electrocatalytic Transformations at Transition Metal Phosphide Interfaces	[**m2M/t**] Amy Marschilok, Alan West *Stony Brook, Columbia* Progress towards scalable electrodes: Experimental results & continuum simulation	[**CENT**] Narayana Aluru *University of Illinois* Multiscale modeling of fluids in single digit nanopores	[**BEES**] Edward Maginn *Notre Dame* Liquid Structure, Orientation Dynamics, & Charge Transport of Deep Eutectic Solvents: An Experimental and Molecular Simulation Study	[**WastePD**] Gerald S. Frankel *Ohio State* Science of Environmental Degradation of Materials for Corrosion Resistant Alloys	[**CATS**] Linlin Wang *Ames* Computational search for magnetic Weyl semimetals in Eu compounds	[**CHOISE**] Adrienne Stiff-Roberts *Duke* Tunable internal quantum well alignment in rationally designed oligomer-based perovskites

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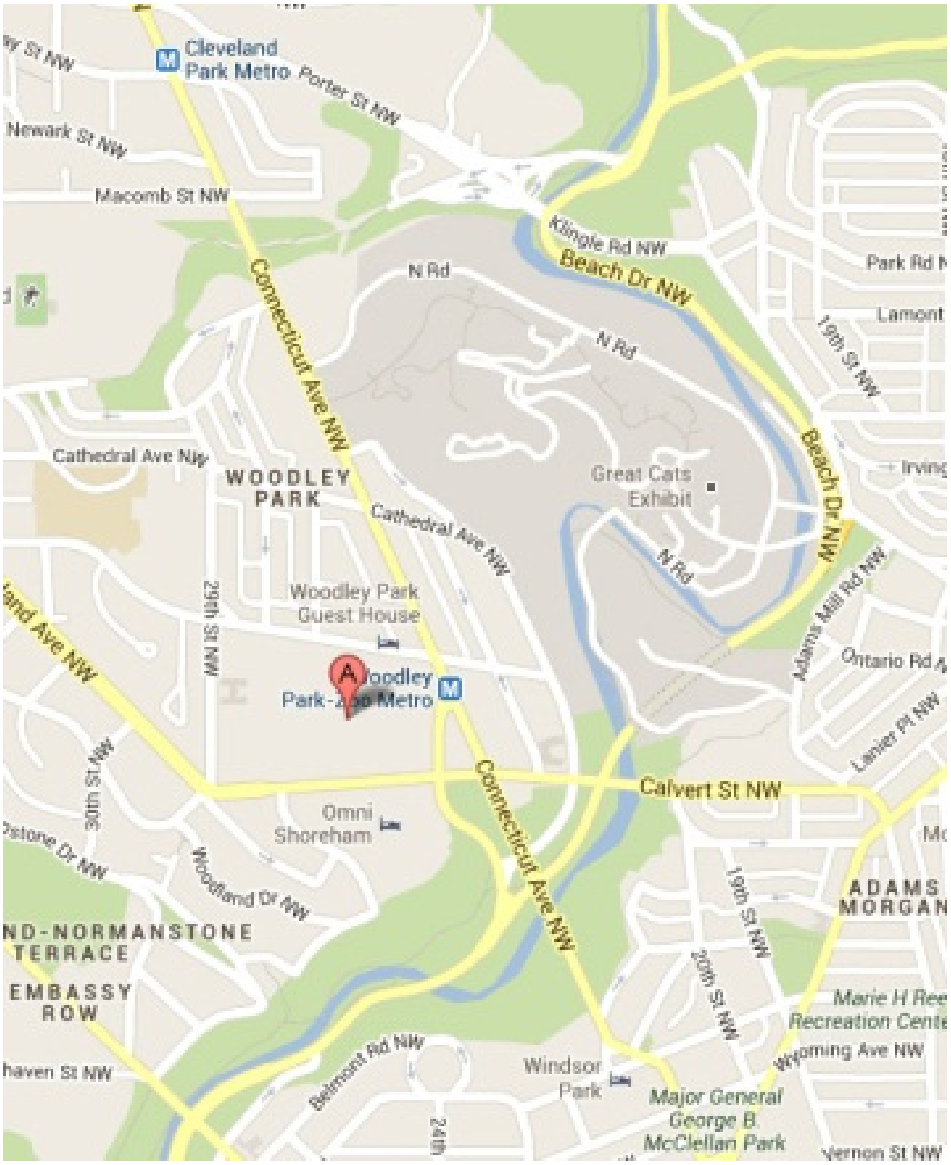
2019 EFRC PI Meeting – Graphic Agenda for Tuesday, July 30, 2019

		B. Catalysis I	C. Catalysis II	D. Energy Storage	E. Energy - Water	F. Materials and Chemistry by Design	G. Nuclear Energy	H. Quantum Materials I	I. Quantum Materials II
Room		***Lincoln 5***	***Lincoln 6***	***Thurgood Marshall East***	***Thurgood Marshall North***	***Thurgood Marshall West***	***Thurgood Marshall South***	***Lincoln 3&4***	***Lincoln 2***
III-4	**2:45 PM**	[**BioLEC**] Todd Hyster *Princeton* Radical Biocatalysis - Using Light to Reveal New Enzyme Functions	[**CCEI**] Dionisios G. Vlachos *U Delaware* An Overview of Focus and Accomplishments of the Catalysis Center for Energy Innovation	[**NEES**] Gary Rubloff *U Maryland* Mesoscale Architectures for Solid State Energy Storage	[**FIRST**] T Egami *ORNL/U Tennessee* Local Ionic Dynamics of Electrolytes in Real Space And Time	[**MSEE**] S. Gill *BNL* Investigating Chemical Speciation & Thermodynamics of Metals in Molten Salts Using in situ X-ray Absorption Spectroscopy	[**EDDE**] Yang Tong, Xing Wang* *ORNL* Tuning Local Atomic Environments to Control Radiation Damage	[**SHINES**] Chia-Ling Chien *Johns Hopkins* Half quantum flux in unconventional superconductor b-Bi_2Pd	[**Pro-QM**] Xiaodong Xu *U Washington* Switching 2D Magnetic States via Pressure Tuning of Layer Stacking
III-5	**3:05 PM**	[**BETCy**] Shelley C. Minteer *U Utah* Developing electroanalytical techniques for evaluating nitrogenase thermodynamics and mechanisms	[**ICDC**] J. Hupp *Northwestern* Inorganometallic Catalyst Design Center: Chemical Transformations of Small Hydrocarbons Using Atomically Precise Heterogeneous Catalysts	[**CEES**] Tim T. Fister *ANL* Overcoming Interfacial Reaction Barriers in Conversion Reactions	[**MUSE**] Greeshma Gadikota, Michael Hoepfner *U Wisconsin,* *U Utah* Dynamic Characterization of Fluids in Confined Space	[**IDREAM**] Hsiu-Wen Wang *ORNL* Advances in understanding concentrated water-in-salt solution: Structure, dynamics and nucleation mechanisms	[**MSEE**] Lingfeng He *INL* Multi-Scale Characterization of Interfacial and Corrosion Processes in Molten Salt Environments	[**IQM**] Yi Li *Johns Hopkins* Towards Monopole Superconductivity	[**NPQC**] James Analytis *LBNL* Frustration, Disorder and Coherence in a New Class of Antiferromagnetic Spintronics
III-6	**3:25 PM**	[**BioLEC**] Abigail Doyle *Princeton* Photocatalysis with Nickel	[**IMASC**] Eric A. Stach *U Pennsylvania* Characterizing the structure of dilute alloy catalysts in reaction conditions	[**SCALAR**] Xiangfeng Duan, Philippe Sautet *UC Los Angeles* Electrocatalyst design for sulfur reduction reaction	[**IDREAM**] Elias Nakouzi *PNNL* From nanoparticle forces, interfacial structure, & aggregation to macroscopic response dynamics and rheological properties: A complementary & cross-correlated study across scales	[**CENT**] Aleksandr Noy *LLNL* High electro-osmotic coupling in ion conductance of 1.5 nm diameter carbon nanotube porins	[**CHWM**] Scott Misture *Alfred U* New Methods For Characterizing Nanoscale Structural Features: Clear Links To Properties	[**CATS**] Dmitry Yarotski *LANL* Probing Ultrafast Photocurrents in the Weyl Semimetal TaAs using THz Emission Spectroscopy	[**M^2QM**] Vivien Zapf *LANL* Magnetoelectric coupling in molecular materials

3:45 – 5:15 PM	**Poster Session II (refreshments provided)**
4:30 PM	**Announce winners of the *Graduate Student and Postdoc Team Science Competition***
7:00 PM – late	**ECN Event: Baseball Game at Nationals Park (all welcome)**

* Team Science Finalist

HOTEL MAPS

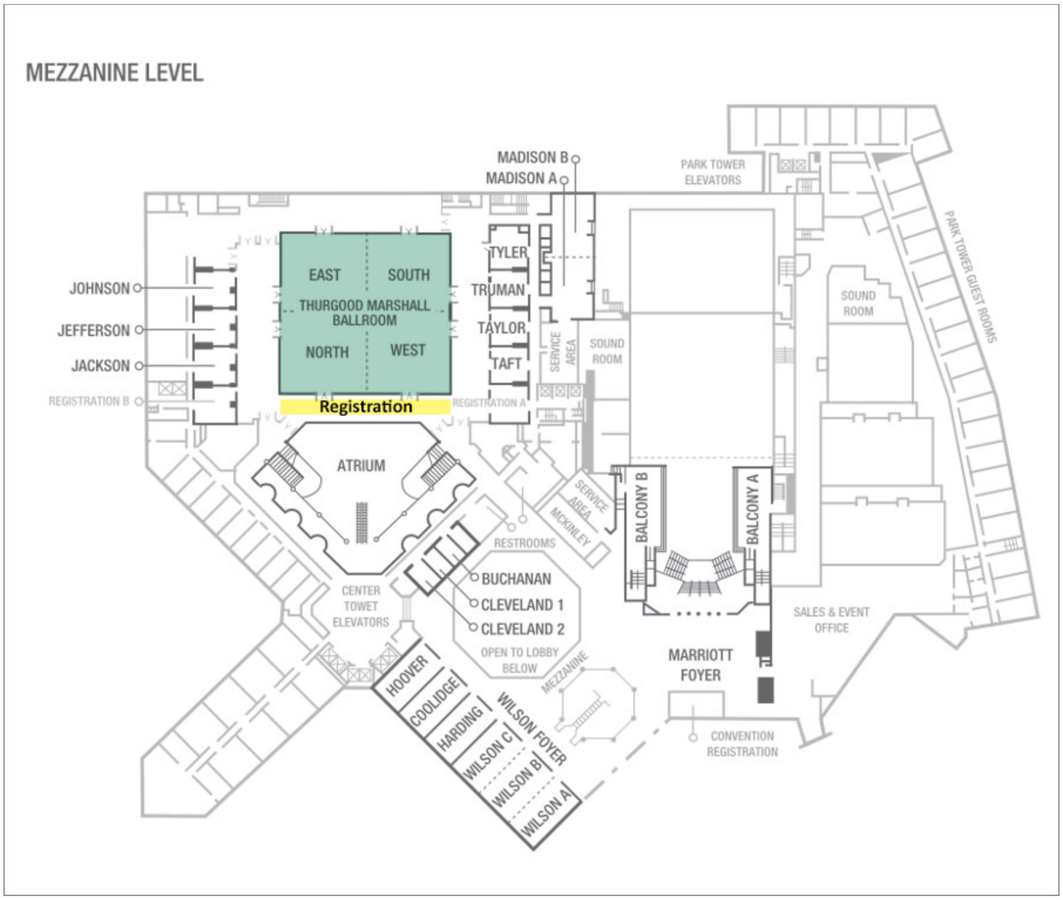


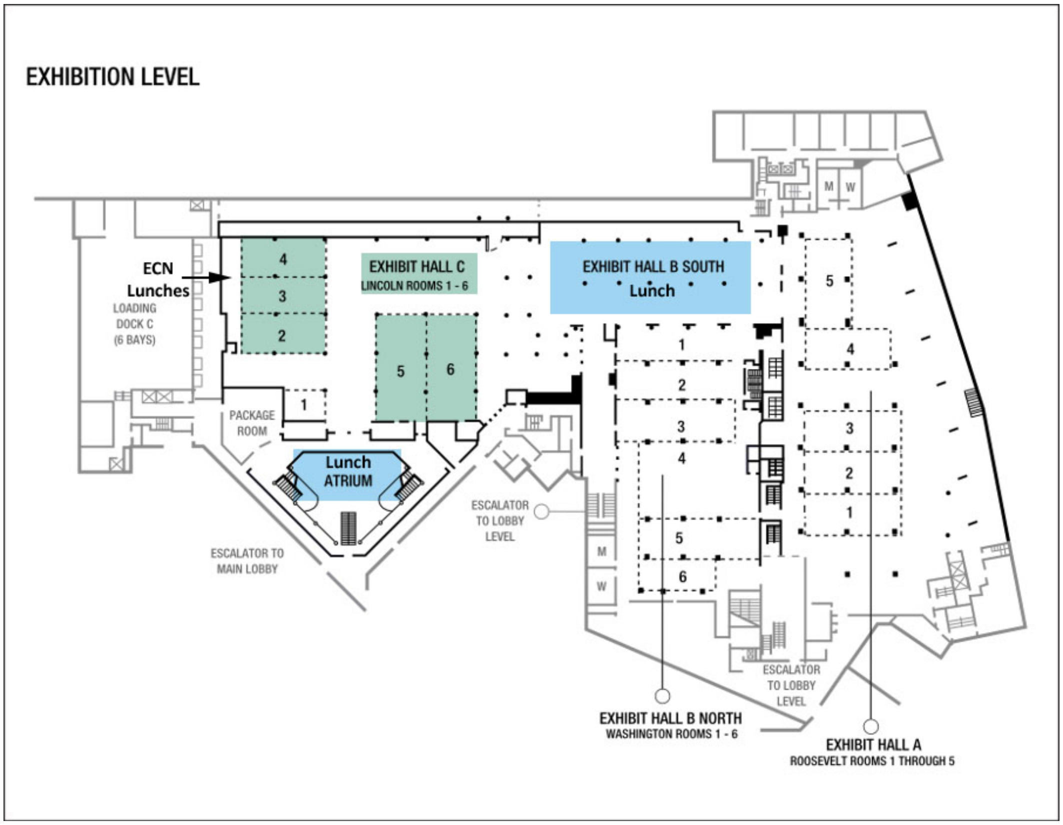
Washington Marriott Wardman Park
2660 Woodley Road NW
Washington, DC 20008

Subway Station: Woodley Park-Zoo/Adams Morgan Metro Red line

Meeting Rooms:
Thurgood Marshall: E, N, S, W
Lincoln: 2, 3 & 4, 5, 6

2019 EFRC PI MEETING – HOTEL MAPS





TECHNICAL TALK ABSTRACTS

A. BIO-INSPIRED SCIENCE

SESSION I: TUESDAY, JULY 30, 2019; 8:00 – 9:40 AM; LINCOLN 6

8:00 AM

A-I-1: LIFE IN THE CONSTRUCTION ZONE: DYNAMIC ASSEMBLY OF PLANT CELL WALLS

[CLSF] William J. Barnes, Xiaoyu Zhu, Daniel D. McClosky, Yunzhen Zheng, Xiaoran Xin, Joseph L. Hill, Chaowen Xiao, Shundai Li, Ming Tien, Ying Gu, Daniel J. Cosgrove, Charles T. Anderson
The Pennsylvania State University

Plant cell walls are dynamic structures that are built in layers by plant cells, and different wall components are brought together for wall assembly by distinct mechanisms. For example, cellulose is polymerized at the cell surface, matrix polysaccharides are polymerized in the cell and trafficked to the wall via exocytosis, and lignin is polymerized in the wall itself. CLSF has revealed new elements of the wall assembly machinery, including proteins that control cellulose synthase delivery, guidance, and removal from the cell surface, those that provide the raw materials for the synthesis of wall polysaccharides, and those that help deliver wall polysaccharides to the correct location after their polymerization. CLSF has also shown that deficiencies in one wall component lead to wholesale remodeling of the wall assembly machinery, resulting in abnormal wall structures that can nonetheless enable some plant growth. We are gaining the capability to detect and manipulate wall components before and immediately after their delivery to the cell surface, allowing for the possibility of controlling wall assembly to modulate the physical properties of the plant cell wall.

8:20 AM

A-I-2: MULTISCALE CONTROL OF THE SELF-ASSEMBLY PATHWAYS AND MORPHOLOGIES OF 2D PROTEIN ASSEMBLIES

[CSSAS] Shuai Zhang[1], Robert G. Alberstein[2], Harley Pyles[3], Brittney Hellner[3], François Baneyx[3], James J. De Yoreo[1], David Baker[3], F. Akif Tezcan[2]
[1]Pacific Northwest National Laboratory; [2]University of California San Diego; [3]University of Washington

A primary goal of CSSAS is to control the spatiotemporal organization of matter through bottom-up design of molecular building blocks. As nanoscale building blocks that are chiefly responsible for generating cellular complexity, proteins offer unique advantages, including absolute structural monodispersity and precise genetic and chemical tunability. To fully harness these advantages, CSSAS is taking a multi-pronged approach.

In the ***first approach***, the Baker Lab at the University of Washington (UW) is using the Rosetta software suite to computationally design protein-mineral interfaces as well as multiple modes of protein-protein interactions to control protein self-assembly on inorganic crystals.

In the ***second approach***, the Baneyx Lab (UW) focuses on solid-binding proteins that incorporate amino acid sequences selected for their ability to bind to inorganic materials. Through a detailed understanding of how these proteins bind to interfaces, they construct dynamic protein-nanoparticle systems that alter the solid-state structure of titania synthesized from soluble precursors at ambient conditions.

Lastly, highlighted in this talk, the Tezcan Lab (UCSD), uses a chemical-bond-centered approach, which enables the self-assembly of an engineered protein with simultaneous control from four different sources of interactions (covalent bonding, electrostatic surface templating, dipole-dipole interactions and salting out) to yield four distinct, precisely patterned 2D crystals. These assemblies were characterized through *in situ* atomic force microscopy and semi-quantitative thermodynamic analysis, which delineated the contribution of protein-protein and -surface interactions to the underlying free-energy landscape, demonstrating the rich phase behavior obtainable from a single, patchy protein building block when interactions acting over multiple length scales are exploited.

8:40 AM

A-I-3: AUTONOMOUS NAVIGATION OF SYNTHETIC MICROROBOTS

[CBES] Yong Dou[1], Zhengyan Zhang[1], Zhiqiang Pei[2], Paul M. Chaikin[3], Samuel I. Stupp[2], Kyle J. M. Bishop[1]
[1]Columbia University; [2]Northwestern University; [3]New York University

Living cells navigate complex environments to perform diverse functions by integrating the capabilities of sensing, computation, and actuation. The pursuit of similar capabilities in synthetic "microrobots" requires strategies for directing self-propulsion in response to environmental cues such as chemical gradients. We show that the 3D shape of a colloidal particle can be used to direct its motion along complex trajectories powered by different energy inputs (electric, acoustic, chemical). We describe how shape-based programming can enable autonomous navigation by coupling particle motions to external stimuli using responsive shape-changing materials. Different material programs can encode a variety of functional behaviors such as stimulus seeking, avoidance, and regulation. These design concepts are demonstrated in silico using physical models of self-phoretic colloids connected by with stimuli-responsive linkers. We discuss recent progress and outstanding challenges in the experimental realization of synthetic microrobots capable of autonomous navigation.

9:00 AM – Team Science Finalist

A-I-4: DISCOVERY OF A NEW PHOTOBIOCATALYST PLATFORM: NON-NATURAL RADICAL PHOTOCHEMISTRY ENABLED BY FLAVOPROTEINS

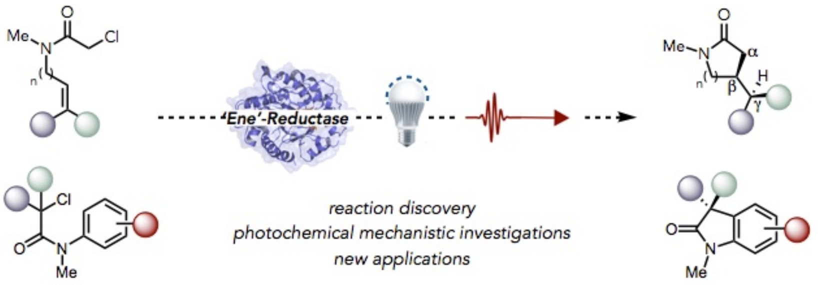
[BioLEC] Kyle F. Biegasiewicz[1], Bryan Kudisch[1], Simon J. Cooper`, Xin Gao[1], Michael Black[1], JiHye Kim[1], Daniel Oblinsky[1], Braddock A. Sandoval[1], Andrew Meichan[1], Samuel E. Garfinkle[1], Gregory D. Scholes[1], and Todd K. Hyster[1]

[1]*Princeton University*

Photobiocatalysis is a field that attempts to mimic the utility and efficiency of natural photosynthesis but with the goal of driving non-natural chemical reactions. The grand challenge associated with this task is that enzymes have naturally evolved to catalyze their own specific set of natural reactions, and as a result, the versatility of their inherent mechanistic machinery has largely been underexplored. Further, biological photochemistry is already a rare occurrence, oftentimes requiring whole "photosystems" worth of unique proteins (ie photosynthesis), such that the use of existing photochemical architectures in biology for new catalysis is a Herculean effort.

Surmounting these challenges, we discovered a new class of radical-mediated photobiochemical transformations using visible light, where our key shift in thinking was in the use of flavin-dependent 'ene'-reductases, which are enzymes without any natural photochemical activity. By surveying of a library of structurally homologous flavoproteins and their respective mutants, we have demonstrated a plethora of novel enantioselective transformations on a wide-variety of non-natural substrates. Critical to the success of these studies was the identification of the photochemical mechanisms of the various oxidation states of flavin using ultrafast spectroscopy, taking optical snapshots of various chemical intermediate species in the catalytic cycle and uncovering the disparate photophysics present in these 'ene'-reducatases as compared to all previously studied flavoproteins.

With the knowledge that we've gained regarding the synthetic utility and photochemical workings of these systems, we are poised to move forward towards traditionally difficult bond activations for diverse applications.



Contributions: T.K.H., K.F.B., S.J.C., X.G., J.-H.K. designed the experiments. K.F.B., S.J.C., X.G., J.-H.K. performed and analyzed results. B.A.S. cloned the improved variant used in the study, S.E.G. obtained x-ray quality crystals and solved the crystal structures. L.A.J. determined the absolute configuration. B.K. and D.G.O. conducted the photophysical and photochemical mechanistic investigation, which B.K., D.G.O., and G.D.S. analyzed and interpreted. T.K.H. and G.D.S. supervised the project.

9:20 AM

A-I-5: DENSITY FUNCTIONAL THEORY MODELING OF ELEMENTARY CELLULOSE MICROFIBRILS

[CLSF] Hui Yang[1], Mei Hong[2], Seong H. Kim[1], James D. Kubicki[3]
[1]The Pennsylvania State University; [2]Massachusetts Institute of Technology; [3]The University of Texas at El Paso

This presentation focuses on the complementary nature of density functional theory (DFT) calculations and spectroscopic studies related to cellulose and its interactions within plant cell walls (PCWs). The complexity, structural disorder and nanoscale nature of PCWs make them difficult to analyze and understand, but advances in sum-frequency generation (SFG) and nuclear magnetic resonance (NMR) spectroscopies as well as DFT have made it possible to elucidate structure not observable previously. Combined with other techniques such as wide-angle X-ray scattering (WAXS) and neutron diffraction, details of PCW components (e.g., cellulose, lignin, pectin, etc.) and their interactions with one another can be modeled. These techniques provide new insight into biological and biochemical studies and provide a basis for creating improved models of the PCW. Topics covered include the habit of the cellulose microfibril as originally generated in PCWs, the surface structure of cellulose microfibrils, and interactions with water and xylan.

B. CATALYSIS I

SESSION I: TUESDAY, JULY 30, 2019; 8:00 – 9:40 AM; LINCOLN 5

8:00 AM

B-I-1: DEVELOPING AND USING SCALING RELATIONSHIPS FOR MOLECULAR ELECTROCATALYSIS OF THE OXYGEN REDUCTION REACTION

[CME] Daniel Martin[1], Michael Pegis[1], Catherine Wise[1], Anna Brezny[1], Yu-Heng Wang[2], Colin W. Anson[2], James B. Gerken[2], Zachary K. Goldsmith[1], Patrick E. Schneider[1], Soumya Ghosh[1], Sharon Hammes-Schiffer[1], and Shannon S. Stahl[2], Samantha I. Johnson[3], Simone Raugei[3], James M. Mayer[1]
[1]Yale University; [2]University of Wisconsin–Madison; [3]Pacific Northwest National Laboratory

The rapid and efficient reduction of dioxygen to water is a critical challenge in the development of many new chemical energy technologies. The use of well-characterized molecular electrocatalysts provides new insights into the factors that control both the rates (turnover frequencies, TOF) and energy efficiencies (overpotential, η), and how to use earth abundant metals. Our studies of iron porphyrin complexes initially showed a single scaling relationship between TOF and η as the catalyst $E_{1/2}$ was varied. However, broader studies at Yale, Wisconsin and throughout the CME have revealed a variety of scaling relations that depend on the reaction mechanism and the specific catalyst system component that was varied. We have found that these scaling relationships can be *derived* from first principles, from the rate law and the Nernst equation for the particular system. They are explanatory and can be predictive. Since developing them for iron-porphyrins, these relationships have been applied to cobalt complexes, including examples that form H_2O_2 at remarkably low overpotentials. An iron electrocatalyst with a polycationic porphyrin ligand shows a dramatic improvement in the catalytic efficiency – high TOF at low η – in a way that can be predicted from a combination of *two* scaling relationships. Applications to other proton-coupled electron transfer catalytic energy challenges are in progress.

8:20 AM

B-I-2: TUNING THE CATALYTIC ACTIVITY OF METAL-INTERCALATED LAYERED MATERIALS

[CCM] Jianwei Sun[1], Michel L. Klein[2], Daniel R. Strongin[2], Jinliang Ning[1], James W. Furness[1],
Yubo Zhang[1], Akila C. Thenuwara[2], Richard C. Remsing[2]
[1]Tulane University, [2]Temple University

The lowering of reaction overpotentials is a persistent and universal goal in the development of catalysts for (photo)electrochemistry, which can usually be facilitated by selectively stabilizing one reaction intermediate over another. In this mechanistic study of the oxygen evolution reaction (OER) catalyzed by cobalt-intercalated layered MnO_2, we show that confinement effects and local cobalt atomic ordering in the interlayer space can be synergistically used to tune the adsorption energies of O, OH, and OOH reaction intermediates and the scaling relationship between them. In general, the interlayer confinement destabilizes the adsorption of intermediates for the OER, but clustering Co atoms can selectively stabilize the adsorption of OOH in particular. After considering both effects, our model predicts an overpotential of 0.30 V for the Co-intercalated MnO_2 catalyzed OER, in excellent agreement with the experimental result of 0.36 V. These new insights explain the enhanced catalytic performance of MnO_2 by intercalating atoms and illuminate a route for engineering non-toxic precious-metal-free catalysts through designed layered materials.

8:40 AM

B-I-3: ELECTROCATALYSIS IN ALKALINE MEDIA: NOVEL MATERIALS AND ARCHITECTURES AND OPERANDO METHODS

[CABES] *Yao Yang[1], Yin Xiong[1], Hongsen Wang[1], Elliot Padgett[1], Can Li[2], Pengtao Xu[1], Xi Yin[3], Francis DiSalvo[1], Jiye Fang[2], Jin Suntivich[1], Piotr Zelenay[3], David Muller[1], Héctor Abruña[1]*
[1]Cornell University, [2]Binghamton University, [3]Los Alamos National Lab

The use of alkaline media has opened new opportunities for the ORR (oxygen reduction reaction) and HOR (hydrogen oxidation reaction) and enabled the use of non-precious-metal-based electrocatalysts. This presentation will deal with the design, synthesis and characterization of high performance electrocatalysts for both ORR and HOR. The use of multimetallic oxides for the ORR and novel alloys for the HOR will be emphasized. For the ORR we have developed multimetallic (Mn, Co, Fe) oxide architectures with high activity and stability. The use of operando X-ray absorption spectroscopy and diffraction along with high resolution TEM (including EELS elemental mapping) have provided unprecedented insights into the complex interplay of composition and structure on activity and lifetime. For the HOR, we have developed new families of metal alloys, such as $Ir_aPd_bRu_c$ nanoparticles, that have dramatically lowered the overpotential for the HOR in base. More recently we have developed a family of Rh-based alloys (with Pt, Ir, Cu, Pd) that exhibit very high activity and lifetime. A size effect was observed for the HOR on Rh/C, where small Rh nanoparticle catalysts exhibited a much higher HOR activity than bulk Rh. A synergistic effect was noted for the HOR on PtRh and IrRh alloy catalysts.

We will also discuss ongoing efforts employing Fe and Co-containing nitrogen doped carbons, single crystal single facet of perovskite films and shape selected electrocatalysts for the ORR.
The presentation will conclude with an assessment of future work and potential new opportunities.

9:00 AM

B-I-4: CONTROLLING ORBITALS IN MOLECULAR ELECTROCATALYSTS TO UNLOCK NEW PATHWAYS TOWARDS SOLAR FUELS

[AMPED] Alexander J. M. Miller
University of North Carolina at Chapel Hill

Catalyst development represents an important thrust in the Alliance for Molecular PhotoElectrode Design (AMPED), with an emphasis on establishing design principles in the electrochemical reduction of CO_2 to fuel candidates. This presentation introduces a new strategy in molecular electrocatalysis in which supporting ligands enforce the spatial positioning and energies of frontier orbital to achieve high activity at low overpotential. A redox-active ligand has unoccupied orbitals that dictate the onset potential of electrocatalysis, while a redox-inactive supporting ligand independently adjusts the nucleophilicity of catalytic intermediates. Mechanistic studies have elucidated the role of the trans effect in accelerating catalysis and have explored structure-function relationships on the chelate. Forays into new reaction chemistry and new catalyst structures will be presented and considered in the context of light-driven catalysis.

9:20 AM – Team Science Finalist

B-I-5: THE EFFECT OF ELECTROSTATICS ON SMALL MOLECULE BINDING AND CATALYSIS USING A POLYCATIONIC IRON PORPHYRIN

[CME] Daniel J. Martin[1], Samantha I. Johnson[2], James M. Mayer[1], Simone Raugei[2]
[1]Yale University, [2]Pacific Northwest National Laboratory (PNNL)

The Center for Molecular Electrocatalysis (CME) aims to store and harvest chemical energy using small, abundant molecules (e.g. O_2, NH_3 and N_2). However, these small molecules are often quite stable and difficult to activate. The oxygen reduction reaction (ORR) is one such quintessential chemical-to-electrical energy conversion reaction and is common to most fuel cells. The reaction is kinetically challenging and typically requires expensive metals (e.g. high-surface area platinum) or high overpotentials. Iron porphyrins are well-established molecular analogues for studying the ORR, as they are easily functionalized, use an earth-abundant metal, and are known for their ability to bind and activate O_2.[1]

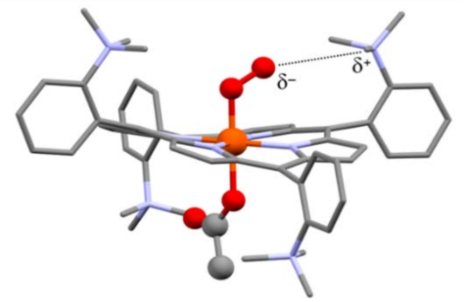


Fig 1. A computed model of $Fe^{III}(O_2^{\bullet-})(OAc)$, a probable intermediate during catalytic turnover, highlighting the subtle electrostatic interactions between the substrate and the charged ligand.

Iron αβαβ-*tetra*(*o-N*,*N'*,*N''*-trimethylanilinium)porphyrin (Fe-*o*-TMA), which features cationic trimethylaminium groups, has been reported as an exceptional catalyst for electrochemical CO_2 reduction. The cationic groups in the ligand were proposed to electrostatically stabilize a high-energy CO_2 adduct, $Fe^{I}(CO_2^{\bullet-})$.[2] Current CME studies have shown that Fe-o-TMA with buffered acetic acid is an ORR catalyst. However, in this case, O_2 binding is not significantly enhanced via through-space coulombic interactions. Rather, the interactions between Fe-*o*-TMA and carboxylate axial ligands are more important.

This work seeks to understand the molecular nature of small molecule binding and activation to Fe-*o*-TMA. Both experimental studies and density functional theory calculations were used cooperatively to understand the electrostatic interactions between the positively charged trimethyaminium groups and bound O_2, CO_2, and carboxylate adducts. With a focus on Fe-*o*-TMA catalyzed ORR, we show that the $Fe^{III/II}$ reduction potential is sensitive to coordinating anions in solution and that the O_2 binding energies for this catalyst are similar to those for porphyrin systems lacking the cationic moieties. This counterintuitive result sheds light on the difference between electrostatic effects on O_2 vs. CO_2 binding and highlights how secondary sphere interactions and metal-center electronics affect small molecule binding and activation. These results have broad applications, from energy storage in small molecules to understanding how biological structures use their environments to control reactivity.

Contributions: As a continuation of ongoing collaborations between the authors, DJM initiated this new direction and executed the experimental work, with advice from JMM. SIJ and SR designed the computational research, and SIJ executed and interpreted the calculations.

[1] a) B. D. Matson, et al., *Chem. Commun.* **2012**, *48*, 11100-11102; b) M. L. Pegis, et al., *ACS Cent. Sci.* **2016**, *2*, 850-856; c) M. L. Pegis, et al., *Chem. Rev.* **2018**, *118*, 2340-2391.
[2] I. Azcarate, et al., *J. Am. Chem. Soc.* **2016**, *138*, 16639-16644.

SESSION II: TUESDAY, JULY 30, 2019; 11:00 – 12:20 PM; LINCOLN 5

11:00 AM

B-II-1: INORGANOMETALLIC CATALYST DESIGN CENTER: METAL ORGANIC FRAMEWORK CATALYSTS ASSESSED AT THE SCALE OF CATALYTIC SITES

[ICDC] Bruce C. Gates[1]
[1]University of California, Davis

Metal organic frameworks (MOFs) have drawn wide attention as potential catalysts, offering high densities of catalytic sites in high-area porous solids, some with stabilities at high temperatures. We summarize opportunities for application of MOFs as catalysts and fundamental issues affecting their applications. MOF framework compositions and pore structures can strongly influence catalytic performance, allowing, for example, shape-selective and bifunctional catalysis. Identification and manipulation of the catalytic sites in MOFs are helping to advance guidelines for synthesizing optimum catalysts. For example, MOF catalytic sites can be tuned by incorporating groups such as formate, acetate, benzoate, and trifluoroacetate on Zr_6O_8 MOF nodes and $-NH_2$, -OH, $-NO_2$, and phenyl substituents on the benzene rings of MOF linkers. The effects of these groups on the electronic properties of the nodes that can serve as catalytic sites have been quantified with IR spectra of the node μ_3-OH groups and by DFT calculations, which are in good agreement with each other.

We present data illustrating the ability of mononuclear, high spin, Fe(II) sites in the nodes of the MOF MIL-100(Fe) to convert propane via dehydrogenation, hydroxylation, and over-oxidation with an atomic oxidant. Some examples of MOF catalysis provide insight into subtle issues of the heterogeneity of catalytic sites associated with the presence of defects in the MOFs. An example involves MOFs that incorporate Zr_6O_8 nodes that may be hydroxylated and provide catalytic sites for acid-base-catalyzed reactions. We report elucidation of the chemistry of these nodes UiO-66 and UiO-67, having used IR and NMR spectroscopies to determine the ligands on the node surfaces originating from the solvents and modifiers used in the syntheses.

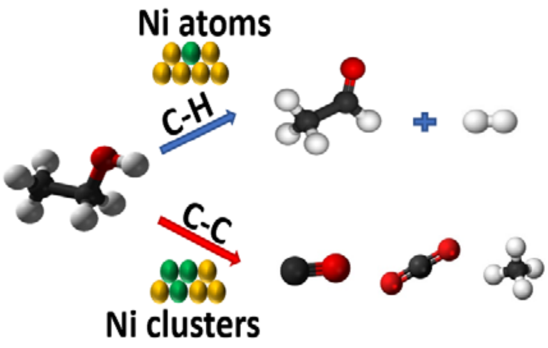
11:20 AM – Team Science Finalist

B-II-2: MECHANISTIC STUDIES OF NON-OXIDATIVE ETHANOL DEHYDROGENATION ON NIAU SINGLE ATOM ALLOYS

[IMASC] Georgios Giannakakis[1]; Kaining Duanmu[2]; Paul Kress[1]; Zhen Qi[4]; Jurgen Biener[3]; Simon R. Bare[4]; Charles Sykes[1]; Philippe Sautet[2]; Maria Flytzani-Stephanopoulos[1]
[1]Tufts University, [2]University of California, Los Angeles, [3]LLNL, [4]SLAC

Non-oxidative dehydrogenation of ethanol to acetaldehyde is of much practical interest since the main byproduct is hydrogen, which does not require additional separation steps unlike water, the byproduct under oxidative conditions. Mechanistically, ethanol dehydrogenation is also of interest as the first step in both ethanol steam reforming and ethanol oxidation. The commercial copper-based catalysts suffer from sintering, leading to deactivation. Gold (Au) catalysts are an alternative, as Au provides enhanced stability and exhibits 100% selectivity, albeit at the cost of low conversion. Here, we report the beneficial effect of alloying the Au surface with nickel (Ni) atoms, and the catalytic behavior of the resulting single atom alloy (SAA).

We have successfully deposited single atoms of Ni in Au surfaces[1], forming NiAu SAAs either supported on silica or in unsupported nanoporous form. The alloying of isolated Ni atoms with Au effectively suppressed the sintering of Au in both cases, based on SEM and TEM. It also lowered the activation energy of the ethanol dehydrogenation reaction significantly (from 96±3 to 59±5 kJ/mol), while the high selectivity of Au was maintained even at high temperatures (280 °C), at which point Ni forms clusters that catalyze the ethanol decomposition reaction (see scheme). The evolution of the catalytic structure was followed by CO-DRIFTS, allowing for structure-activity correlations. The Ni structure before reaction, after reduction, and during reaction was determined in-situ by EXAFS. The formation of Ni ensembles affected selectivity, as confirmed by TPD experiments performed under UHV conditions on single Au crystals doped with Ni. Ethanol drives Ni to the Au surface from the sub-surface where it exists after reduction, thereby activating the catalyst, as shown by XPS and confirmed by DFT calculations. *In-operando* mechanistic studies were performed on the NiAu SAAs via ethanol DRIFTS, high energy resolution fluorescence detection (HERFD) XAS, and Kinetic isotope effects (KIE) studies, which showed that both O-H and C-H bond activation are kinetically relevant steps. This was corroborated by density functional theory (DFT) calculations of the reaction mechanisms on NiAu SAA and Au surfaces, which also showed that the overall barrier on NiAu SAA is much lower than on Au surfaces, in agreement with experiments. Last, PdAu SAAs, which have been reported as promising selective hydrogenation catalysts[2], were also tested under similar reaction conditions but did not improve the catalytic activity to the same extent as Ni, as shown by kinetic measurements, ethanol DRIFTS, and verified by DFT. This difference, identified first in our EFRC work, will be further probed in other reaction systems of interest to the EFRC.



References:

[1]Giannakakis, G. *et al.* ,*Top. Catal.* **2018,** 61, 475
[2]Liu, J. *et al.* , *Catal. Sci. Technol.* **2017,** 7, 4276

Contributions:

G.G. performed kinetic, isotopic and spectroscopic studies, conducted XAS, TEM and XPS measurements. K.D. performed DFT calculations. P.K. conducted surface science studies. Z.Q. synthesized nanoporous materials and took SEM images.

11:40 AM

B-II-3: SYNTHESIS OF ULTRA-LOW LOADINGS OF CATALYSTS FOR HYDRODEOXYGENATION (HDO) OF BIOMASS

[CCEI] Dongxia Liu[1], Yuan Zhang [1], Emily Shulman[1], Jiayi Fu[2], Weiqing Zheng[2], Dionisios G. Vlachos[2]
[1]University of Maryland; [2]University of Delaware

Ultra-low loadings (ULLs) of metal catalysts, including single-atom catalysts or metal cluster catalysts, are being studied for catalytic reactions. These ULL catalysts show unexpectedly high specific activity, selectivity and maximized metal utilization but are challenged by stability and long-term durability in catalytic reactions. The single atoms or small metal clusters on catalyst supports can be mobile and aggregate into nanoparticles when exposed to elevated temperatures or liquid solvents. This causes detrimental consequences for catalytic performance. Therefore, our research is focused around the development of robust and stable ULL catalysts to advance their practical applications, especially for HDO reactions in biomass processing under hydrothermal conditions. In this presentation, we highlight the progress we have made on the synthesis of ULL catalysts by employing three strategies. The first strategy is to increase the surface area of the support materials. For this purpose, we synthesized low-dimensional (e.g., nanosheet and nanotube) metal oxide materials. Laser induced thermal shock technique (LTS) has primarily been used to increase fatigue resistance in metal alloys and modify surface structure and chemistry of metallic materials. In the second strategy, we employed LTS technique to treat the ULL catalysts to manipulate the microenvironment for metal residence. The support and/or metal-support interactions could change the electronic structures of ULL metals. In the third strategy, we employed metal oxide supports with different reducibility to examine its influence on the ULL stability. All these syntheses contribute to creation of ULLs with fine-tuned structural and compositional specifications for HDO application.

12:00 PM

B-II-4: STABILITY, DYNAMICS AND CATALYTIC REACTIVITY OF SURFACE SITES AT BIMETALLIC CATALYSTS FROM FIRST PRINCIPLES

[IMASC] Kaining Duanmu[1], Wei Chen[2], Jin Soo Lim[2], Nicola Molinari[2], Lixin Sun[2], Romain Réocreux[3], Michail Stamatakis[3], Boris Kozinsky[2], Philippe Sautet[1]
[1]University of California, Los Angeles, [2]Harvard University, [3]University College London

As shown by experiments, notably from the IMASC EFRC, catalysts formed by the combination of two transition metals show unique catalytic properties. In these catalysts, important structural reconstructions are linked with thermodynamic stability and dynamics of the surface site under reaction conditions for dilute alloys of group 10 metals (Pd or Ni) in group 11 ones (Ag or Au). In this presentation, I will survey recent results from the team of computational chemists of the IMASC EFRC on this topic, in interaction with surface science or catalysis experiments. For the catalytic property, it is of utmost importance to understand which metal is on the surface, and the structure of the surface site. Thermodynamic calculations can first be involved to understand how various conditions—vacuum, oxidative (O_2) or reductive (H_2) environments—affect the stability and the presence of the active group 10 metal at the surface. The formation of metastable surface structures is here key for the activity. However, this thermodynamic approach needs to be completed with a dynamic and kinetic understanding of the surface restructuring. In IMASC we combine two approaches. One approach links semi-empirical molecular dynamics calculations with DFT, to unravel the family of elementary steps responsible for the restructuring of the surface. The other approach combines these elementary steps in a Kinetic Monte-Carlo simulation. Finally, the unique catalytic activity of metastable bimetallic sites can be explored from reaction pathway calculations.

SESSION III: TUESDAY, JULY 30, 2019; 1:45 – 3:45 PM; LINCOLN 5

1:45 PM

B-III-1: PREDICTING REACTOR PERFORMANCE OF NPAU CATALYSTS FROM STUDIES ON SINGLE CRYSTALS IN ULTRAHIGH VACUUM

[IMASC] Robert J. Madix[1]
[1]Harvard University

The utility of the surface reactivity observed for model systems under ultra-high vacuum for predicting the performance of catalytic materials under ambient flow conditions is a highly debated topic in heterogeneous catalysis. We have shown that vast differences in selectivity observed for methanol self-coupling across wide ranges of temperature and reactant pressure can be accurately predicted utilizing the kinetics and mechanism obtained from model studies on gold single crystals in ultrahigh vacuum regressed to fit transient pulse responses over nanoporous gold ($Ag_{0.03}Au_{0.97}$) at low pressures (TAP). Specifically, microkinetic modelling of the complex sequence of elementary steps governing this reaction predicts the dramatic effect of reactant partial pressure on the product distribution and leads to conclusion that the gas phase partial pressures of both reactants and the reaction temperature determine the changes in selectivity to methyl formate formation. Moreover, thorough analysis of the reaction network indicates that the product distribution becomes increasingly insensitive to kinetic effects at pressures approaching 1 bar, leading toward 100% selectivity methyl formate. A rigorous kinetic sensitivity analysis also demonstrates the complex interplay of the kinetics of the elementary steps and the overall catalytic behavior.

2:05 PM

B-III-2: DYNAMIC CATALYSIS RESONANCE FOR CHEMICAL CONVERSION ACCELERATION

[CCEI] Paul Dauenhauer[1]
[1]University of Minnesota

The emergence of competitive renewable energy from solar and wind heightens the importance of moving energy from the place of origin to the places where people live and work. Chemically capturing energy as compressed hydrogen or energy liquids including hydrocarbons and ammonia remains the leading method of energy storage based on density and fungibility, but the catalytic technology necessary for transformation of electricity into chemicals in small, distributed energy systems is the key challenge for implementation. In this work, the general approach of dynamic catalyst operation is described as oscillatory binding energy of sorbates on active sites as a method to dramatically accelerate the rate of catalytic reaction. Surface oscillations in sinusoidal and square waveforms of transient binding energy are imposed on catalyst surfaces with varying amplitude and frequency to identify the resonance conditions leading to 10,000x enhancement in overall reaction rate. The results are presented in the context of catalyst-reaction behavior and with regard to implementation in industrial reactor technologies necessary for moving and storing renewable energy.

2:25 PM

B-III-3: ROLE OF SURFACE STRUCTURE AND DOPANTS ON THE INTERACTION AND CONVERSION OF ACID GASES OVER METAL OXIDE AND SULFIDE CATALYSTS

[UNCAGE-ME] Si Luo[1], Uma Tumuluri[1], Jun-Kun Lai[2], Lohit Sharma[2], Monica Vasiliu[3], Joshua Howe[4], David Sholl[4], Katherine Page[5], Meijun Li[1], David A. Dixon[3], Jonas Baltrisaitis[2], Israel E. Wachs[2], Zili Wu[1]
[1]Chemical Science Division, Oak Ridge National Laboratory; [2]Lehigh University; [3]University of Alabama; [4]Georgia Institute of Technology; [5]Neutron Scattering Division, Oak Ridge National Laboratory

The nature of the interaction of acid gases including SO_2, CO_2 and NO_x with metal oxides was investigated and found to be sensitive to both the surface structure of the oxides as well as the type of dopants. We utilized single component oxides such as CeO_2, TiO_2, and ZnO with different morphologies to understand the effect of surface crystallographic termination on the interaction with the acid gases, supported mixed oxides including WO_x-doped Vox and K_2O-doped WO_x to understand the dopant promotion effect. In addition to the critical role of surface structure, the oxygen vacancies in the metal oxides were also found to play an important role in the interaction with the acid gases. The conversion of acid gases was also found impacted by the dopants as wells as defects, as illustrated in the selective catalytic reduction (SCR) NO_x with NH_3 over supported VO_x/TiO_2 catalysts and CO_2 hydrogenation (reverse water gas shift - rWGS) over MoS_2. The cooperativity between the redox sites of VO_x and the acid sites associated with WO_x was responsible for the increase of the total activity of the SCR reaction. The impact of H_2S on the rWGS reaction was carefully studied and found to be bifunctional as either an inhibitor or a co-reactant over MoS_2. The detailed investigations on the structure of the active sites and the reaction mechanism of the acid gas conversion will also be discussed.

2:45 PM

B-III-4: RADICAL BIOCATALYSIS – USING LIGHT TO REVEAL NEW ENZYME FUNCTIONS

[BioLEC] Todd K. Hyster[1]
[1]Princeton University

Enzymes are exquisite catalysts for chemical synthesis, capable of providing unparalleled levels selectivity. Unfortunately, biocatalysts are often limited to the reactivity patterns found in nature. In this talk, I will share my groups efforts to use light to expand the reactivity profile of enzymes. In our studies, we have exploited the photoexcited state of common biological cofactors, such as NADH and FMN to facilitate electron transfer to substrates bound within enzyme active sites. In other studies, we found that enzymes will electronically activate bound substrates for electron transfer. In the presence of common photoredox catalysts, this activation can be used to direct radical formation to enzyme active sites. Using these approaches, we are able to develop biocatalysts to solve long-standing selectivity challenges in chemical synthesis.

3:05 PM

B-III-5: DEVELOPING ELECTROANALYTICAL TECHNIQUES FOR EVALUATING NITROGENASE THERMODYNAMICS AND MECHANISMS

[BETCy] David P. Hickey[1], Rong Cai[1], Zhi-Yong Yang[2], Lance Seefeldt[2], and Shelley D. Minteer[1]
[1]University of Utah, [2]Utah State University

In the last 5 years, there have been extensive studies and new materials designed for catalytic reduction of nitrogen to ammonia. This is a very difficult reductive transformation for traditional electrocatalysts and photocatalysts, but nature can provide an inspiration. Nitrogenase is the only enzyme known to reduce nitrogen to ammonia. This intriguing enzyme is typically studied by a range of spectroscopies and due to the complexity of the nitrogenase system (including the dynamics of both a catalytic protein containing a FeMo-cofactor and an Fe protein), it is hard to directly study enzyme mechanism with standard spectroscopic techniques and assays. This talk will discuss electroanalytical techniques for studying the enzyme mechanism of nitrogenase, including both mediated bioelectrocatalysis and direct bioelectrocatalysis. The talk will discuss electrode materials innovation for interfacing these complex proteins with electrode surfaces as well as the use of square wave voltammetry and amperometric titrations to evaluate thermodynamics and mechanism, including inhibition studies, mutant enzyme studies, and kinetic isotope effect studies.

3:25 PM

B-III-6: PHOTOCATALYSIS WITH NICKEL

[BioLEC] Stephen Ting[1], Sofia Garakyaraghi[1], Chelsea M. Taliaffero[2], Gregory D. Scholes[1], Felix N. Castellano[2], Abigail Doyle[1].
[1]Princeton University; [2]North Carolina State University

Ni-photoredox catalysis has recently emerged as an enabling strategy to promote previously challenging or impossible cross-coupling reactions. Although these reactions involve the irradiation of Ni complexes and an increasing number of these reactions are proposed to involve excited Ni complexes, little is known about the excited states of Ni complexes and their relevance to catalytic cross coupling. In this seminar, I will describe our collaborative efforts to characterize the photophysics of Ni complexes relevant to Ni-photoredox. These studies could lead to the development of improved catalyst systems and the discovery of novel reactions

C. CATALYSIS II

SESSION III: TUESDAY, JULY 30, 2019; 1:45 – 3:45 PM; LINCOLN 5

1:45 PM

C-III-1: TUNING CATALYTIC BIAS OF HYDROGEN GAS PRODUCING HYDROGENASES

[BETCy] Jacob H. Artz[1,2], Oleg A. Zadvornyy[1], David W. Mulder[2], Stephen M. Keable[3], Aina E. Cohen[4], Michael W. Ratzloff[2], S. Garrett Williams[5], Bojana Ginovska[6], Neeraj Kumar[6], Jinhu Song[4], Scott E. McPhillips[4], Catherine M. Davidson[4], Artem Y. Lyubimov[4], Natasha Pence[1], Gerrit J. Schut[7], Anne K. Jones[5], S. Michael Soltis[4], Michael W. W. Adams[7], Simone Raugei[1,6], Paul W. King[2], and John W. Peters[1,3,6]
[1]Washington State University, [2]National Renewable Energy Laboratory, [3]Montana State University, [4]SLAC National Accelerator Laboratory, [5]Arizona State University, [6]Pacific Northwest National Laboratory, [7]University of Georgia.

Hydrogenases catalyze the seemingly simple interconversion of protons and electrons with hydrogen gas, and are significant in hydrogen gas cycling and interspecies hydrogen gas transfer as well as in the energetics of many microbial systems. Hydrogenases display a wide range of catalytic rates and biases in reversible hydrogen gas oxidation catalysis. The interactions of the iron-sulfur containing catalytic site with the local protein environment are thought to contribute to differences in reactivity, but this has not been demonstrated. The microbe *Clostridium pasteurianum* produces three [FeFe]-hydrogenases that differ in their "catalytic bias" exerting a disproportionate rate acceleration in one direction or the other spanning a remarkable seven orders of magnitude. The combination of high-resolution structural work, biochemical and biophysical analyses, and computational modeling demonstrate the catalytic bias can be explained through a simple yet elegant model involving the relative stabilization and destabilization of different states of the catalytic active site metal cluster through protein secondary interactions which allow it to operate under different reduction-oxidation regimes. The design features used by the [FeFe]-hydrogenases to tune and control reactivity will serve as a platform by which to develop novel biased catalysts.

2:05 PM

C-III-2: HIERARCHICAL PHOTOCATALYSIS AND STRATEGIES TO CONTROL IT

[CBES] Mohamad Kodaimati[1], James Schwabacher[1], Ofer Kedem[1], Jinghan Zhu[1], Namrata Ramani[1], Chad A. Mirkin[1], George C. Schatz[1], Emily A. Weiss[1]

A feature of natural photosynthetic systems is their ability to operate with the low photon flux of sunlight, where the absorption of light and transport of photochemical potential to the catalytic centers is efficiency-limiting. Natural systems overcome this limitation through a process called energy transfer, where quanta of energy are gathered by many weakly coupled light absorbing centers that pass the energy among themselves to funnel it to a single catalytic reaction center. This talk describes the use of quantum dot (QD) assemblies as artificial light harvesting-reaction center units for the photocatalytic reduction of H^+ to H_2, where excitons are funneled through EnT from sensitizer QDs (sQDs) to catalyst QDs (cQDs). At the optimized sensitizer-to-catalyst ratio of 4:1, the internal quantum efficiency (*IQE*) of the reaction system is 4.0±0.3%, a factor of 13 greater than the *IQE* of a sample that is identical except that EnT is suppressed due to the relative core sizes of the sQDs and cQDs. A kinetic model supports the proposed exciton funneling mechanism for enhancement of the catalytic activity. Prior to this work this type of energy migration-based approach to light-powered chemistry has not been employed in artificial photocatalytic systems. This talk also describes ongoing work to modulate the catalytic efficiencies of such systems by controlling interparticle distances through pH-dependent DNA linkers and hydrogel matrices.

2:25 PM

C-III-3: UNDERSTANDING AND CONTROLLING ELECTROCATALYTIC TRANSFORMATIONS AT TRANSITION METAL PHOSPHIDE INTERFACES

[CME] Ian Murphy[1], David Ung[1], Murielle Delley[2], Jeffrey T. Miller[3], James M. Mayer[2], Brandi M. Cossairt[1]
[1]University of Washington; [2]Yale University; [3]Purdue University

Electrocatalysis is inherently interfacial, and almost always involves the motion of electrons and protons in energy-related transformations. The Heterogeneous Interfaces thrust in CME seeks to achieve molecular-level control of e^- and H^+ motion and to understand and develop inner-sphere reactivity at heterogeneous interfaces. This talk will highlight our new efforts for one class of heterogeneous materials – transition metal phosphides. TMPs have gained increasing interest as earth-abundant electrocatalytic materials from their origins as industrially-applied hydroprocessing catalysts. We have developed a series of TMP model compounds in nanocrystal form with diameters ranging from 5 to 500 nm. These compounds are being used to explore how surface-dependent reactivity can be quantified, characterized, and tuned. Through a combination of physical, spectroscopic, and structural characterization, stoichiometric reactivity studies, and electrocatalytic benchmarking in both aqueous and organic media, we seek to understand and exploit tunable interfaces for a variety of multi-proton, multi-electron small-molecule transformations. Specific highlights of the work will include: (1) direct experimental quantification of reactive H_2-derived TMP-H moieties, (2) demonstration of covalent modification of TMP surfaces resulting in altered electrocatalytic performance, and (3) modeling the physical and electronic structure evolution under ambient and catalytic conditions using synchrotron X-ray spectroscopies.

2:45 PM

C-III-4: AN OVERVIEW OF FOCUS AND ACCOMPLISHMENTS OF THE CATALYSIS CENTER FOR ENERGY INNOVATION

[CCEI] Dionisios G. Vlachos[1]
[1]University of Delaware

In this talk, an overview of the research thrusts and accomplishments of the Catalysis Center for Energy Innovation will be presented. This will cover the development of new, renewable, performance-advantaged materials as well as direct replacement molecules, new catalysts and functionalities, novel reaction mechanisms, and new analytical and computational tools. Examples of renewable molecules include high performance lubricants, surfactants, dienes, and high-pressure sensitive adhesives. Examples of new catalysts include the family of P-zeosils, P-containing acid catalysts on pure siliceous supports, which are very selective for dehydration without catalyzing oligomerization and other side reactions.

3:05 PM

C-III-5: INORGANOMETALLIC CATALYST DESIGN CENTER: CHEMICAL TRANSFORMATIONS OF SMALL HYDROCARBONS USING ATOMICALLY PRECISE HETEROGENEOUS CATALYSTS

[ICDC] Joseph T. Hupp[1]
[1]*Northwestern University*

The discovery of enormous amounts of fracking-accessible shale gas within the United States has changed the national and global energy landscape, most obviously in the realm of fuel. Less obvious is the transformative effect of the discovery upon large-scale chemical manufacturing. Replacing crude oil with wet shale gas (*i.e.*, C_1, C_2, C_3, and C_4) has tremendous implications for catalytic chemistry. The initial tasks for heterogeneous catalysts with shale gas are to chemically activate and then combine C_1, C_2, C_3, and/or C_4 species. For C_1-C_4 and related intermediate compounds, the tasks include controlled carbon-carbon bond formation, selective oxygenation, dehydrogenation, and selective hydrogenation. Thus, the structures of well-defined model catalysts, before, during, and after catalysis, can, in principle, be assessed, and the information can be used to motivate hypothesis-driven investigations of mechanisms, structure/activity relationships, and composition/activity relationships.

As supports for assembly and evaluation of atomically precise metal-oxide, metal-sulfur, and metal(0) clusters, the ICDC exploits chemically and thermally robust MOFs – with assembly of the catalysts themselves being accomplished via self-limiting grafting chemistry. The MOFs of interest present hexa-metal(IV)-oxo, hydroxo, aqua nodes that can be viewed as uniform arrays of spatially isolated pieces of zirconia, hafnium, or ceria.

Via an iterative loop, computational and experimental structural and reactivity studies serve to advance catalyst design, elucidate design rules, and potentially reveal new mechanisms. Finally, understanding the extent to which theory, computations, and machine learning can describe, predict, and reveal catalyst behavior, and developing theory methods that can advance this understanding, are central to ICDC's mission.

3:25 PM

C-III-6: CHARACTERIZING THE STRUCTURE OF DILUTE ALLOY CATALYSTS IN REACTION CONDITIONS

[IMASC] Alexandre Foucher[1], Erjia Guan[2], Nicholas Marcella[2], Mathilde Luneau[3], J. Anilbal Boscoboinik[4], Dario J. Stacchiola[4], Anatoli I. Frenkel[2], Cynthia M. Friend[3], Eric A. Stach[1]
[1]*University of Pennsylvania,* [2]*Stony Brook University,*[3]*Harvard University,*[4]*Brookhaven National Laboratory*

The IMASC EFRC is investigating how dilute alloy catalysts can be used to tune selectivity and reactivity of selective oxidation and hydrogenation reactions. In these materials the active element is the minor component of a bimetallic system. This leads to significant complications in determining local structure, morphology and composition, complications that are further exacerbated by the fact that reaction conditions lead to dynamic restructuring of the catalysts and in some cases their support. The characterization cross-cut within IMASC is developing a suite of techniques to track these dynamic changes as they occur (both in-situ and using operando methods), and to systematically correlate the data across different analytical techniques. This presentation will highlight the ways that synchrotron probes such as x-ray absorption and x-ray photoelectron spectroscopy can be used to track features such as oxidation state, chemical restructuring and local morphology on the global scale, as well as how the use of local probes such as electron microscopy and scanned probes can provide nanometer and atomic scale information, all in reactive conditions.

D. ENERGY STORAGE

SESSION I: TUESDAY, JULY 30, 2019; 8:00 – 9:40 AM; THURGOOD MARSHALL EAST

8:00 AM

D-I-1: Pushing the Limit of Intercalation - Combining Theory, Computation and Experiments to Control Cation and Anion Redox

[NECCES] Y. Shirley Meng[1], Hyeseung Haelie Chung[1], Minghao Zhang[1], Oleg Shpyrko[1], Maxwell D. Radin[2], Anton Van der Ven[2], Antonin Grenier,[3,4] Karena W. Chapman,[3,4] Zachary Lebens-Higgins,[5] Louis F. J. Piper[5], M. Stanley Whittingham[5], Clare P. Grey[6]
[1]UC San Diego, [2]UC Santa Barbara, [3.]Stony Brook University, [3]Argonne National Laboratory, [5]Binghamton University, [6]University of Cambridge

Oxygen-redox reactions are believed to be responsible for the excess energy available in lithium rich layered oxides, this leads to a new class of cathode materials called anion redox materials for energy storage. Nevertheless, the major issue of anionic redox is the irreversibility correlated with defects generation, which results in serious structure degradation and the voltage decay during extended cycles. In comparison to the classical layered oxides, deep understanding of the defects formation and its effect on anion redox materials has not been explored yet. NECCES team combine theory and first principles calculations with advanced experiments to demonstrate the unique metastable structure of the cycled anion redox materials. Using operando Bragg coherent diffractive imaging, our team directly confirm dislocations and strain form more readily in the anion redox materials as compared with classical layered oxides. The distinct behaviors can be attributed to the different defect formation mechanisms, which leads to the different anion redox properties in these intercalation materials. Understanding and controlling the anion redox behavior will enable us to further push the limit of intercalation chemistry.

8:20 AM

D-I-2: IMPORTANCE OF STRUCTURAL STABILITY FOR FAST, PSEUDOCAPACITIVE ENERGY STORAGE IN OXIDES REVEALED BY OPERANDO AFM

[FIRST] Veronica Augustyn,[1] Ruocun Wang,[1] Wan-Yu Tsai,[2] Qiang Gao,[2] Simon Fleischmann,[1] Naresh Osti,[2] Eugene Mamontov,[2] Alexander Koleshnikov,[2] Yangyunli Sung,[3] De-en Jiang,[3] Nina Balke[2]
[1]North Carolina State University, [2]Oak Ridge National Laboratory, [3]University of California, Riverside

The intercalation of cations into the vacant sites of materials represents one of the most important electrochemical energy storage mechanisms and is widely used in commercialized rechargeable batteries. Achieving high power capability while maintaining high energy density is desirable for numerous energy storage applications. Redox-based pseudocapacitance is an energy storage mechanism whereby transport processes in the solid state, such as diffusion, do not limit the faradaic reactions rendering it achieving both high energy and power densities. In the specific case of tungsten oxide, the presence of structural water leads to a transition in the energy storage mechanism from battery-type intercalation to pseudocapacitance. We will demonstrate that these electrochemical mechanisms are linked to the mechanical response of the materials during insertion of protons. For the first time, *operando* electrochemical strain microscopy (ESM) is used to measure the deformation of redox-active energy storage materials, and to link the local nanoscale deformation to the global current response. This technique reveals that the local mechanical deformation of the hydrated tungsten oxide is smaller and more gradual than the anhydrous oxide, and occurs without hysteresis during the intercalation and de-intercalation processes. The ability of layered materials with confined structural water to minimize mechanical deformation likely contributes to their fast energy storage kinetics. This is a very important finding which connects, for the first time, the mechanical signature of electrochemical redox-processes. This opens up a unique opportunity to study local electrochemical redox-processes which are not attainable with current-based techniques.

8:40 AM

D-I-3: 1D MATERIALS: IMPROVED STRUCTURAL RESILIENCY VIA ATOMIC LEVEL DESIGN

[m2M/t] Kenneth J. Takeuchi[1], Yimei Zhu[2], Ping Liu[2], Lijun Wu[2], Bingjie Zhang[1], Xiaobing Hu[2], Lisa M. Housel[1], Jianping Huang[1], Seung-Yong Lee[2], Alexander B. Brady[1], Altug S. Poyraz[2], Killian R. Tallman[1], Paul F. Smith[1], Shaobo Cheng[2], Diana M. Lutz[1], Mikaela R. Dunkin[1], Qingping Meng[2], Shize Yang[2], Mark S. Hybertsen[2], Amy C. Marschilok[1], Esther S. Takeuchi[1]
[1]Stony Brook University; [2]Brookhaven National Laboratory

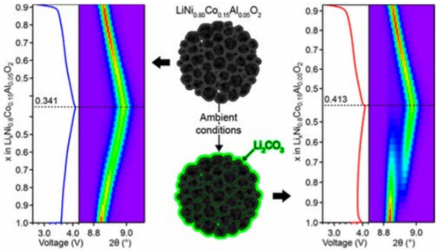
When considering ion insertion materials, a common structural form is the layered motif providing ion diffusion in two dimensions. However, lattice expansion and contraction associated with ion movement and electron transfer can also be accompanied by structural degradation and amorphization with loss of functional capacity. In contrast, tunnel type structures with a more rigid framework can accommodate the presence of multiple cations and provide opportunities for detailed design of structurally robust systems. The tunnel size of the host structure can be matched to the size of the mobile ion, including consideration of the guest cation solvation effects. Structural defects such as oxygen vacancies can be manipulated to play a beneficial role in facilitating the desired ion transport. Targeted synthesis provided meaningful insight into design for structurally robust materials through statistical atomic level analysis of the materials by local probes, coupled with theory, bulk characterization and electrochemistry.

9:00 AM – Team Science Finalist

D-I-4: FROM CATION TO ANION REDOX: PUSHING THE ULTIMATE LIMIT OF LAYERED OXIDES

[NECCES] Zachary W. Lebens-Higgins[1], Antonin Grenier[2], Julija Vinckeviciute[3], Anton Van der Ven[3], Karena Chapman[2], Louis F. J. Piper[1]
[1]Binghamton University; [2]Stony Brook University; [3]University of California, Santa Barbara

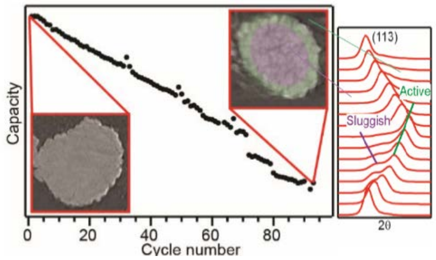
Narrowing the gap between theoretical and practical reversible capacities of layered oxide cathodes remains a critical challenge for next generation Li-ion batteries.[1] NECCES identified $LiNi_{0.8}Co_{0.15}Al_{0.05}O_2$ (NCA) as a model system for understanding the chemical reactions at various length scales that govern cycling performance of layered oxides. The solid solution behavior of the NCA ternary system is effectively modeled by an O3 phase ($R\bar{3}m$) up to 90 % Li-extraction with aluminum inhibiting phase transitions from O3 to O1.[2]



Li_2CO_3 overlayer [3]

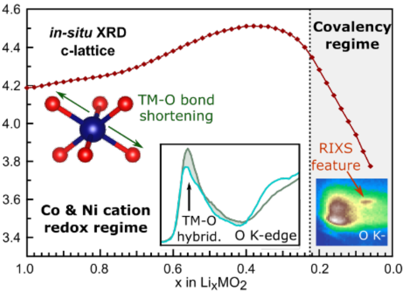
The electrochemistry of Ni-rich cathodes is strongly influenced by their sensitivity to air-exposure. In the first charge of NCA, high impedance from surface Li_2CO_3 gives rise to reaction heterogeneity during delithiation.[3] Without this overlayer the heterogeneity is eliminated resulting in the intrinsic solid-solution behavior.

Suppressing Li_2CO_3 and related overlayer species is key for long-term cycling performance,[4] yet challenges remain in retaining high capacities when operating above 4.3 V vs. Li+/Li0. Among the high voltage operating challenges, operando x-ray diffraction revealed intergranular fracturing to be a dominant capacity fading mechanism between 2.7-4.5V, accounting for up to 20% capacity loss [5]. Primary particles lose electrical contact and become "sluggish" because of fracturing due to large mechanical stress associated with lattice breathing.



Intergranular fracturing fade mechanism [5]

The c-lattice collapse at high voltages above 4.3 V vs. Li+/Li0 is considered to arise from covalency-driven oxygen redox and plays a key role in the mechanical induced fracturing. A combination of resonant inelastic x-ray scattering (RIXS) with an array of structural and electronic probes were used to provide direct insight into the charge compensation process. Nickel and cobalt redox were found to occur in tandem below 4.25 V resolving a long-standing issue. Oxidized oxygen signatures in O K-edge RIXS maps were observed to emerge concurrently with the c-lattice collapse. The RIXS feature's evolution with delithiation presents evidence of depopulating O 2p states,[6] and suggests that covalency may be utilized elsewhere for rational design of anionic redox.



Cation and anion charge compensation considered in delithiation of NCA

NECCES references: [1.] Adv. Energy Mater. (2017) 160288; [2] *J. Mater. Chem. A* (2018) **6**, 4189-4198; [3] *Chem. Mater.* (2017) **29**, 7345-7352; [4] J. Electrochem. Soc. (2017) A3727-A3741; [5] *Nano Lett.* (2017) **17**, 3452−3457;

Contributions: Z. W. L.-H. & L. F. J. Piper conducted x-ray spectroscopy experiments regarding charge compensation. A. G. & K. C. conducted operando synchrotron x-ray diffraction and structural analysis. J. V & A. V. V. performed supporting density functional theory calculations.

9:20 AM – Team Science Finalist

D-I-5: Investigating the Redox Activity and Lithiation of Icosahedral Boron Clusters in the Solid State

[SCALAR] Rebecca M. Kubena[1], Dahee Jung[1], Zeeshan Parvez[1], Jonathan C. Axtell[1], Nicholas H. Bashian[2], Andrew Dawson[1], Josh Zak[3], Anton Van der Ven[4]*, Brent C. Melot[2]*, Kimberly A. See[3]*, Sarah H. Tolbert[1]* & Alexander M. Spokoyny[1]*
[1]UC Los Angeles; [2]University of Southern California; [3]Caltech; [4]UC Santa Barbara

Molecular borane clusters are well-known to exhibit reversible redox activity in solution. Specifically, icosahedral dodecaborate (B_{12}) clusters exhibit two sequential one-electron redox processes that can occur at different potentials depending on the nature of the organic substituents decorating the boron. This tunability, along with multiple accessible redox states, make these clusters appealing targets for developing new materials for rechargeable batteries. Within SCALAR, the Spokoyny group has been preparing several new insoluble redox-active B_{12} derivatives for use as novel cathode materials. They work closely with the Tolbert and Melot groups to study the fundamental electrochemical performance of these materials using potentio- and galvanostatic techniques. Cyclic voltammetry indicates a single distinct reversible Faradaic feature in several forms of the cluster that have been precipitated by derivatizing with Zn(II) ions, styrene, and carboxylic acid (Fig. 1a), which supports the idea that Li-ions can be inserted into the network of clusters. Further galvanostatic studies for the styrene cluster have showed promising reversibility on extended cycling (Fig. 1b). The Raman expertise of the See group is being leveraged to understand the stability of the organic functional groups decorating the surface of the clusters (Fig. 1c). The ability directly to monitor the vibrational mode during *operando* cycling experiments allows us to directly understand the impact of redox processes on the local structure of the clusters and quickly identify parasitic attacks on the organic groups. In parallel, the Melot group is performing *operando* X-ray diffraction measurements to monitor global changes in the bulk crystal structure. This complementary approach using extremely sensitive techniques leads to a more holistic understanding of the entire material system and provides deeper mechanistic insight. Supporting these efforts, the Van der Ven group is using computational modelling to determine stabile phases and stability limits. The complex and multi-faceted nature of these unique boron based materials necessitates the range of methods made available through multiple research groups. Utilizing the combined expertise of this multi-university effort allows for a fully comprehensive study of the synthetic, structural, and electrochemical dynamics of this new class of boron clusters based electrodes.

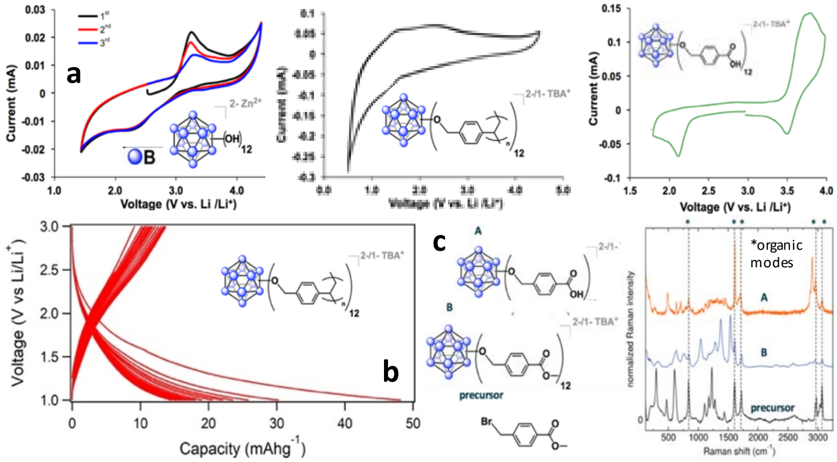


Figure 1. Preliminary data consisting of **(a)** cyclic voltammetry, **(b)** galvanostatic voltammetry, and **(c)** Raman spectroscopy of several B_{12}

Contributions: R.M.K, D.J, Z.P, and J.C.A synthesized and characterized the boron cluster based materials. N.H.B and A.D performed electrochemical experiments, N.H.B. conducted operando XRD measurements. J.K performed Raman measurements. A.V. and colleagues did all theoretical modeling.

SESSION II: TUESDAY, JULY 30, 2019; 11:00 – 12:20 PM; THURGOOD MARSHALL EAST

11:00 AM

D-II-1: DETERMINING POTENTIALS ACROSS SOLID STATE BATTERY SYSTEMS

[NEES] Elliot J. Fuller[1], Evgheni Strelcov[2,3], Michael W. Swift[4], Joshua D. Sugar[1], Yue Qi[4], Nikolai Zhitenev[2], Jabez J. McClelland[2] and A. Alec Talin[1]
[1]Sandia National Lab Livermore, [2]National Institute for Standards and Technology, [3]Maryland NanoCenter, [4]Michigan State University

A primary scientific challenge in solid state energy storage is to understand, in a coordinated fashion, how the roles of electrons and ions play out and interact across electrode/electrolyte interfaces. The interaction is bidirectional and profound: electronic structure of the materials defines band structure, space charge, and electric fields in the material which influence ion as well as electron transport. In turn, ion transport from charge/discharge cycles can significantly alter the electrode materials, changing their electronic structure and the very fields which that alter transport. Electrostatic potential distributions across solid state batteries (SSBs), and particularly at interfaces, reflect these critical interactions and are the target of NEES experimental and computational research. We have developed Kelvin probe force microscopy (KPFM) to reveal voltage and mechanical gradients in cross-sectional SSBs as a function of state-of-charge, mapping these for a Si/LiPON/Li_xCO_2 SSB. We have also established a theoretical first-principles-informed framework to predict these gradients for a Li/LiPON/Li_xCO_2 cell, predicting that transport and the sign of the field at the LiPON/Li_xCO_2 will depend on the state-of-charge in the Li_xCO_2 cathode. This collaboration of experiment and theory are promising for shining light on these central questions of solid state energy storage.

11:20 AM

D-II-2: MOLECULAR STRUCTURE OF SOLID STATE ELECTRODE/ELECTROLYTE INTERFACES: THERMODYNAMIC PROPERTIES AND AUTOMATED ALGORITHMS FOR STRUCTURE DETERMINATION

[CEES] Robert Warburton[1], Siddharth Deshpande[1], Liang Li[2], Shane Patel[3], Jason Howard[2], Christopher Wolverton[3], Maria Chan[2], Tim Fister[2], Paul Fenter[2], Larry Curtiss[2], Jeffrey Greeley[1]
[1]Purdue University, [2]Argonne National Laboratory, [3]Northwestern University

Widespread interest in the use of solid state electrolytes for applications in lithium ion batteries has recently led to the development of a broad spectrum of experimental and computational techniques to characterize the structure of such materials. Although remarkable progress has been made in the determination of bulk properties, less information is available for corresponding interfacial features of the solid/solid electrode/electrolyte interfaces. In this presentation, we describe work within CEES that has led to the development of computational algorithms for prediction of molecular-level details of such properties, including atomic structure, electronic, and transport effects. We employ these techniques to interpret detailed X-ray scattering results for the interface between lithium-manganese-oxide cathodes and lithium-lanthanum-titanium-oxide electrolytes, and we suggest future avenues for generalizing the results to larger classes of solid/solid interfaces.

11:40 AM

D-II-3: PRODUCTIVE AND PARASITIC REACTIONS: THE ROLE OF INTERFACIAL CHEMISTRY AND STRUCTURE

[m2M/t] Esther S. Takeuchi[1], Lynden A. Archer[2], David C. Bock[3], Kent Jingxu Zheng[2], Prayag Biswal[2], Matthew M. Huie[1], Qing Zhao[2], Andrea M. Bruck[1], Xiaotun Liu[2], Tian Tang[2], Jiefu Yin[2], Killian R. Tallman[1], Lisa M. Housel[1], Wenzao Li[1], Lei Wang[3], Juergen Thieme[3], Amy C. Marschilok[1], Kenneth J. Takeuchi[1]
[1]Stony Brook University; [2]Cornell University; [3]Brookhaven National Laboratory

Despite their importance, interfaces are rarely formed by design. The spontaneous formation of uncontrolled interfaces determined by the thermodynamic stability of the electrolyte at the potential of the requisite surface is typical. Modification of the electrolyte through inclusion of electrolyte additives can change the onset potential of electrolyte decomposition as well as the overpotential for metal deposition where the effect of the electrolyte additive on electrochemistry can be profound extending the cycle stability or modifying the morphology of deposits at the negative electrode surface. Notably, we demonstrate the impact of electrolyte additives. Further, we show that it is possible to effectively probe the reaction of the electrolyte with the active electrode surface using operando methods in conjunction with electrochemistry. For example, the onset of the surface electrolyte interphase formation can be determined at a systems level using x-ray absorption spectroscopy of the active material coupled with detailed analysis of the thermal profile of an electrochemical cell using isothermal microcalorimetry.

12:00 PM – Team Science Finalist

D-II-4: Dynamics of Electrolytes under Confinement in Next Generation (Pseudo)capacitive Materials

[FIRST] X. Wang[1], L. Vlcek[2], M.W. Thompson[3], T.S. Mathis[1], R. Matsumoto[3], N.C. Sanders[4]
[1]Drexel University, [2]ORNL/UTK, [3]Vanderbilt University, [4]Oak Ridge National Laboratory

The key challenges impeding the predictive design of novel electrode materials and electrolytes for faster, lighter, thinner electrochemical energy storage devices include 1.) lack of understanding of the electrochemical processes occurring at electrode-electrolyte interfaces, and 2.) lack of knowledge about the transport of charge-storing ions and solvents in electrolyte systems, both in the bulk and under confinement. The FIRST Center has brought together a team of researchers from various institutions with expertise in advanced characterization techniques, materials synthesis, and computational modeling for probing in-depth the fundamental science of electrochemical fluid-solid interfaces and transport in electrolyte systems. Of particular interest are two-dimensional (2D) electrode materials with nano-confined fluids, which show rapid ion transport and surface-redox reaction rates. One such group of materials are 2D transition metal carbides and nitrides referred to as MXenes, which are metallically conductive, ionophilic materials with highly reactive surfaces capable of high-rate, pseudocapacitive charge storage. Recently we demonstrated how changing the organic solvent of lithium-ion-containing electrolytes can double the charge stored by the Ti_3C_2 MXene.[1] The fundamental science behind this unconventional finding was investigated by a combination of *in situ* electrochemical characterization, molecular dynamics (MD) simulations, and quasi-elastic neutron scattering (QENS) to reveal that when a carbonate-based solvent is used, the lithium ions will intercalate into the Ti_3C_2 layers in a de-solvated state. The opposite is true when a nitrile- or sulfoxide-based solvent is used, where solvent molecules will co-intercalate with the lithium ions, lowering the overall charge storage capability of Ti_3C_2, as shown by the MD simulation in **Figure 1** of a charged Ti_3C_2 electrode with the different electrolytes used in this study. To better understand and make use of this observation, we have conducted computational and experimental studies to screen optimal combinations of electrolyte ions and solvents for maximizing ion transport in room-temperature ionic liquids (RTILs), which are notorious for their slow transport properties. By surveying a diverse set of organic solvents using a Molecular Simulation Design Framework (MoSDeF) suite of software tools and MD simulations, we found that pure solvent diffusivity dominates the conductivity of RTIL-solvent mixtures.[2] This builds on our previous studies showing how solvent polarity impacts the transport properties in these types of electrolyte mixtures.[3] Altogether, our work shows how rigorous study of the interplay between charge-storing ions, organic solvents, and novel electrode materials can be used in the design of high-power and high-energy (pseudo)capacitive systems.

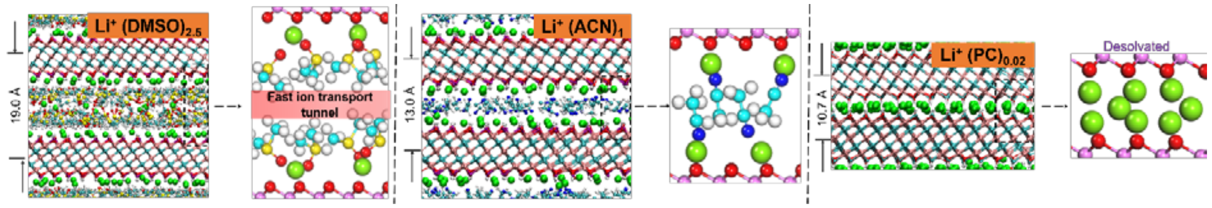


Figure 1. Molecular dynamics simulations showing the differing degrees of Li^+ ion confinement for charged Ti_3C_2 electrodes for $[Li^+][TFSI^-]$ dissolved in different electrolyte solvents[1].

References: [1]X. Wang et al., *Nature Energy* **2019,** *4* (3), 241-248; [2]M.W. Thompson et al., *J. Phys. Chem. B* **2019,** *123* (6), 1340-1347; [3]N.C. Osti et al., *J. Phys. Chem. Lett.* **2017,** *8* (1), 167-171.

Contributions: X.W. and T.M. conducted electrochemical experiments; N.C.S. made electrolyte conductivity measurements; M.W.T. and R.M. conducted computational screening within the MoSDeF framework; L.V. conducted MD simulations integrated with quasielastic neutron scattering results.

SESSION III: TUESDAY, JULY 30, 2019; 1:45 – 3:45 PM; THURGOOD MARSHALL EAST

1:45 PM

D-III-1: OVERVIEW OF BATTERY RESEARCH FROM THE CENTER FOR SYNTHETIC CONTROL ACROSS LENGTH-SCALES FOR ADVANCING RECHARGEABLES (SCALAR)

[SCALAR] Bradley Chmelka[1], Xiangfeng Duan[2], Bruce S. Dunn[2], Jian Luo[3], Brent C. Melot[4], Thomas F. Miller III[5], Sri R. Narayan[4], Laurent Pilon[2], Philippe Sautet[2], Kimberly A. See[5], Rachel Segalman[1], Ram Seshadri[1], Alex Spokoyny[2], Barry C. Thompson[4], Sarah H. Tolbert[2], Anton Van der Ven[1], and Johanna Nelson Weker[6]
[1]University of California (UC) Santa Barbara; [2]UC Los Angeles; [3]UC San Diego; [4]University of Southern California; [5]California Institute of Technology; [6]SLAC National Accelerator Laboratory

In this talk, we overview the new SCALAR EFRC, which aims to expand the range of materials that can be used for electrochemical energy storage beyond traditional metal-ion redox, while simultaneously bridging atomistic and nanometer length-scales to improve cycling stability and transport. The center is composed of three thrusts. Thrust I focuses on the atomic scale, with an emphasis on anion redox reactions in an effort to combine anion and cation redox for increased capacity. Projects within this thrust include pure anionic systems such as redox-stable boron clusters, mixed anion/cation redox systems based on metal chalcogenides, and fluoride ion intercalation hosts. Thrust III complements Thrust I using a multi-length scale approach to rethink battery materials at the nanometer level. Here, the goal is to develop synthetic methods to create architectures and interfaces that achieve enhanced electrochemical reversibility and cycling stability. Projects include the development of flexible, conductive scaffolds, both for integration with materials in thrust I, and to stabilize volume changes upon cycling in more established electrode materials. This thrust also aims to stabilize interfaces, using both new methods to create artificial SEI layers, and through integration of redox catalysts into surfaces. Finally, thrust II bridges the atomic and nanometer scales by developing approaches to enhance ion and electron transport. In two parallel approaches, we focus on conductive polymer binders to enhance electrical conductivity in slurry networks, and on synthesizing new intercalation hosts with highly connected metal-oxygen polyhedra to provide intrinsic electrical conductivity. Electrochemical calorimetry complements both efforts.

2:05 PM

D-III-2: OPERANDO X-RAY CHARACTERIZATION OF MULTI-SCALE KINETIC LIMITATIONS IN BATTERY ELECTRODES

[NECCES] Karena W. Chapman,[1,2] Antonin Grenier,[1,2] Hao Liu,[2,3] Kamila M. Wiaderek,[2] Saeed Kazemiabnavi,[4] Katsuyo Thornton,[4] Philip J. Reeves,[5] Ieuan D. Seymour,[5] Clare P. Grey,[5] Peter J. Chupas,[1,2]
[1]Stony Brook University, [2]Argonne National Laboratory, [3]Binghamton University, [4]University of Michigan, [5]University of Cambridge

NECCES has developed high fidelity operando tools, including the AMPIX and RATIX electrochemical cells, that allow us to probe energy storage reactions in battery electrodes on multiple length and time scales. For the NCA ($LiNi_{0.8}Co_{0.15}Al_{0.05}O_2$) and LFP ($LiFePO_4$) model systems that are a focus of the NECCES EFRC, we have identified limitations in reaction kinetics on the atomic, particle and electrode scale that underlie limitations in effective energy storage capacity, efficiency and lifetime. Using spatially resolved operando high energy X-ray diffraction computed tomography, we have identified accelerated reactions at the faces of a composite battery electrode that is linked to local limitations in ionic and electronic transport. Non-uniformity of the electrode reaction leads to variability in the charge/discharge rate, both as a function of time and position within the electrode: this local variability means that the maximum rate experienced by individual cathode particles is 2-5 times faster than the average, controlled cycling rate. This rate heterogeneity may accelerate rate-dependent degradation pathways in regions of the composite

electrode experiencing faster-than-average reaction and has important implications for optimizing rate-dependent battery performance. In high fidelity operando diffraction studies of NCA, we have resolved the apparent first cycle capacity loss evident in NCA and other Ni-containing Li layered transition metal oxide cathodes. Limitations in Li transport kinetics within the electrode at Li concentrations approaching unity retard the reaction and give rise to reaction heterogeneity and a low first cycle Coulombic efficiency under Galvanostatic cycling conditions.

2:25 PM

D-III-3: PROGRESS TOWARDS SCALABLE ELECTRODES: EXPERIMENTAL RESULTS AND CONTINUUM SIMULATION

[m2M/t] Amy C. Marschilok[1], Alan C. West[2], Lei Wang[3], Alison H. McCarthy[1], Nicholas W. Brady[2], Christianna Lininger[2], Andrea M. Bruck[1], David C. Bock[3], Alexander B. Brady[1], Karthik Mayilvahanan[2], Killian R. Tallman[1], Calvin D. Quilty[1], Lisa M. Housel[1], Kenneth J. Takeuchi[1], Esther S. Takeuchi[1]
[1]Stony Brook University; [2]Columbia University; [3]Brookhaven National Laboratory

Fundamental understanding of transport properties across multiple size regimes is critical for the rational design of electrodes based on insertion and conversion materials. Charge transport through the bulk material is governed by the various phase transformations occurring at the atomic level. However, minimizing diffusion length at both the crystallite level and the particle level is also critical to achieve high capacity utilization at a given rate. Porous-electrode theory allows for the simulation of ion and electron transport over multiple length scales (allowing the analysis of tailored architectures), the kinetics of electrochemical and chemical reactions, and phase change kinetics (and how new phases impact transport processes). Synchrotron based operando experiments can enable time and spatially resolved visualization of phase (re)distribution under kinetically limited use conditions. Thus, through an iterative, interactive process, experiment and theory can provide complementary information to inform the rational design of scalable electrode systems.

2:45 PM

D-III-4: MESOSCALE ARCHITECTURES FOR SOLID STATE ENERGY STORAGE

[NEES] Gary Rubloff [1], Sang Bok Lee [1], Keith Gregorczyk [1], A. Alec Talin [2]
[1]University of Maryland, [2]Sandia National Lab Livermore

NEES research has realized a sequence of mesoscale energy storage architectures that achieve simultaneous high energy and high power by synthesis of 3D nanostructure arrays. Several of these rely upon a 3D scaffold of high aspect ratio (depth/width) pores in self-assembled anodic aluminum oxide or trenches formed by anisotropic dry etching of Si substrates. For solid state batteries (SSBs) this is followed by conformal deposition of active battery layers over the 3D topography, using either atomic layer or electrochemical deposition to achieve a “vertical SSB array”. These thin film synthesis approaches offer a high degree of control over shapes and composition of nano- and micro- structures. They also enable functional solid electrolyte layers which are much thinner (~40nm) than normally employed in solid state batteries (~1μm). Furthermore, lateral patternability of the battery structures provides for versatile placement of battery elements and wiring at the mesoscale. A different embodiment of the same design principles employs planar batteries stacked one on top of the other as a “lateral SSB array”, avoiding need for a 3D scaffold but requiring a more complex wiring scheme. The vertical and lateral configurations require very different fabrication strategies and present different scientific challenges at both the nano and meso scale, underscoring the diversity presented by mesoscale design and synthesis.

3:05 PM

D-III-5: OVERCOMING INTERFACIAL REACTION BARRIERS IN CONVERSION REACTIONS

[CEES] Tim T. Fister[1], Robert Warburton[2], Guena Evmenenko[3], Jae Jin Kim[1], Fernando Castro[3], Jeffrey Greeley[2], Chris Wolverton[3], Maria Chan[1], Vinayak Dravid[3], Michael Bedzyk[3], Paul Fenter[1]
[1]Argonne National Laboratory, [2]Purdue University, [3]Northwestern University

The reaction of a metal oxide with lithium to form metal nanoclusters and lithium oxide is a classic example of a conversion reaction. This broad class of reactions, where lithium reacts directly with the anion species, often has many times the specific capacity of intercalation materials, but is usually limited in reversibility. Problems with Coulombic inefficiency, voltage hysteresis, and poor transport properties originate with the formation of interfaces between lithium-rich and reduced metal species during the first discharge. In the Center for Electrochemical Energy Science (CEES), we have studied the formation of these interfaces in spinel and rock salt metal oxides using *in situ* transmission electron microscopy and x-ray scattering methods. Pairing these operando methods with first principles calculations, we have discovered the existence of local metastable crystal structures during this initial lithiation. We also find lithium accumulation in charged grain boundaries that leads to barrier-free lithiation at these solid/solid interfaces. Using these design principles and novel synthesis methods developed in CEES, we have used the features to design nanostructure battery electrodes with improved reversibility and energy density. These studies could be useful not only for enabling oxide conversion reactions, but could also be important for understanding interfacial reactivity and transport in solid state batteries.

3:25 PM

D-III-6: ELECTROCATALYST DESIGN FOR SULFUR REDUCTION REACTION

Lele Peng[1], Ziyang Wei[2], Phillippe Sautet[1], Xiangfeng Duan[1]
[1]University of California, Los Angeles

Lithium-sulfur (Li-S) chemistry exhibits considerable potential for ultrahigh density energy storage. However, polysulfide shuttling remains a persistent challenge that limits long-term stability and practical applications of Li-S batteries. Here we aim to develop electrocatalysts for sulfur reduction reaction (SRR) to enable rapid and complete sulfur reduction and minimize polysulfide formation. During past period, we primarily focused on developing a robust protocol to rapidly prepare, evaluate and understand a series catalytic systems. Heteroatom doped holey graphene frameworks (HGF) was explored as a model initial system. In this presentation, we discuss the research progress on SRR electrocatalyst design and investigation. By using the heteroatom doped holey graphene frameworks as model system, we start with experimental investigation of electrocatalytic SRR activity, focusing on probing reduction kinetics and determining reduction activation energy. We will then discuss some theoretical simulations to explore the nature of the active site and possible SRR pathways and understand the origin of the catalytic activity and by analyzing the Gibbs free energy of lithium polysulfide evolution. We will further explore the optimized SRR catalyst materials in the practical device, probing their impact to some critical device parameters, including, energy density, rate capability and cycling endurance. Together, by closely integrating the experimental and theoretical efforts, we hope to formulate a set of material design principles that can help guide the fabrication of advanced Li-S battery cathodes for the next generation energy storage devices.

E. ENERGY - WATER

SESSION II: TUESDAY, JULY 30, 2019; 11:00 – 12:20 PM; THURGOOD MARSHALL NORTH

11:00 AM – Team Science Finalist

E-II-1: Understanding the Impact of Mesoscale Membrane Architecture on Water Transport

[M-WET] Segolene Antoine[1], Malgorzata Chwatko[2], Dipak Aryal[2], Rahul Sujanani[2], Sally Jiao[1], Venkat Ganesan[2], Nathaniel Lynd[2], Rachel Segalman[1], Lynn Katz[2], Benny Freeman[2]

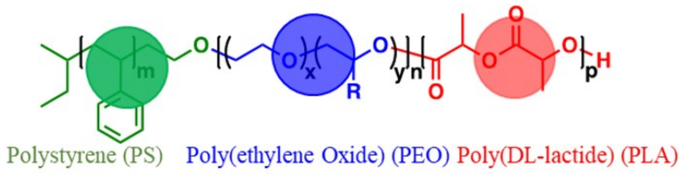
[1]University of California, Santa Barbara; [2]The University of Texas at Austin

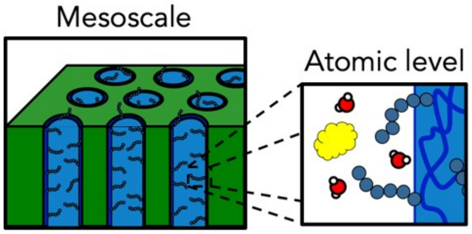
Water and energy are crucial resources for humanity but are interconnected as it takes copious amounts of energy to produce clean water. Synthetic membranes are widely used for purifying relatively clean water (e.g., seawater and brackish water desalination etc.) due to low energy requirements of membranes relative to alternatives (e.g., thermally-based separations).

However, current membranes were not designed to treat highly impaired water, such as produced water, due to extensive fouling and poor separation properties. Furthermore, there is a lack of fundamental and systematic studies probing the impact of polymer structure and membrane morphology on transport properties. Block copolymers (BCPs) self-assembly offers a highly tunable platform to achieve novel water filtration membranes with uniform pore sizes, well-defined pore size distributions (PSDs) and varied morphologies.

To study the impact of pore size on the water diffusion, both experimental and simulation approaches were utilized. The BCPs were synthesized *via* anionic polymerization and controlled ring-opening polymerization. BCPs were composed of polystyrene (PS), poly(ethylene oxide) (PEO) and polylactide (PLA) (PS-*b*-PEO-*b*-PLA). Membrane morphology was controlled via polymer composition such that the hydrophilic PEO block coats the pores. We propose that tuning the length of the hydrophilic block (PEO) will change both the size and hydrophilicity of the pores and consequently water diffusion through them. To achieve this, we varied the PEO block volume fraction from 0 to 20% while adjusting the PLA block volume fraction. Simulation results show that with increasing PEO block length the diffusion of water seems to decrease. Macroscopic water permeation measurements, which are used to characterize commercial materials, are being performed.

These results validated the simulation models that will be used in an inverse design strategy to determine the best morphologies exhibiting high water flux and subsequently target them experimentally. A key goal of this study is to understand how mesoscale architecture (i.e., pore geometry and chemistry) affects transport. This supports the broad goals of M-WET by providing optimized geometrical parameters used in future M-WET studies to design new membranes that can provide fit for purpose water and recover valuable solutes with less energy. This effort will bridge the polymer chemistry, membrane science, modelling, and water chemistry communities together.





Contributions: SA, MC synthesized the polymers used in this work. SA, RS tested macroscopic membrane performance. DA and SJ performed the simulations. VG, NL, RS, LK, BF helped to design the experiments and analyze data, supervised the work.

11:20 AM

E-II-2: FIRST PRINCIPLES AND MULTI-SCALE SIMULATIONS OF MATERIALS FOR ENERGY-WATER SYSTEMS

[AMEWS] Juan de Pablo[1,2], Giulia Galli[1,2], George Schatz[3], Gregory Voth[2]
[1]Argonne National Laboratory; [2]University of Chicago; [3]Northwestern University

We present an overview of multi-scale and first principles simulations of materials for energy-water systems, with a focus on aqueous spectra and the characterization of aqueous interfaces.

11:40 AM

E-II-3: AB INITIO THEORY OF FUNDAMENTAL PROCESSES UNDERLYING FUEL CELL PERFORMANCE OF ALKALINE MEMBRANES

[CABES] J.F. Mendez-Valderrama, Mariel Tader, Brian Ernst, Robert A. Distasio, T.A. Arias
Cornell University

With the recent advent of stable alkaline membranes and the opportunities they present to upend current acid-based fuel cell technologies, understanding the fundamental atomic-scale processes underlying the stability of, and OH^- transport through, such membranes has become of prime importance. Whereas much is understood regarding such processes in acid-stable membranes such as Nafion, relatively little is known regarding the performance and stability of alkaline membranes. In this talk, we will present a number of recent *ab initio* results of direct relevance to further improving the stability and transport properties of alkaline membranes as garnered through cutting edge techniques optimized for the particular challenges presented by these new systems.

12:00 PM

E-II-4: SURFACE PROGRAMMING OF HYDRATION WATER STRUCTURE, DYNAMICS, AND THERMODYNAMICS

[M-WET] Scott Shell[1], Songi Han[1], Nathaniel Lynd[2], Gosia Chwatko[2], Ben Pedretti[2], Rachel Segalman[1], Mikayla Barry[1], Audra DeStefano[1], Thomas Webber[1], Dennis Robinson-Brown[1], Nicholas Sherck[1], Timothy Keller[1], Sally Jiao[2], Jacob Monroe[2], Pinar Gokturk[3], and Ethan Crumlin[3]
University of California at Santa Barbara[1], University of Texas at Austin[2], Lawrence Berkeley National Labs[3]

Controlling the interaction of water with polymer surfaces is crucial for the success of membrane-based separations and for the design of efficient membrane technologies. The primary knowledge gap that this project seeks to address is the nature of the hydration layer as influenced by the polymer surface chemistry and topology, which in turn play a key role in determining solute and ion surface affinity, foulant propensity, and interfacial transport. Restructuring of polymeric surfaces in response to hydration is also of interest. The studies rely on parallel polymer platforms with polymer surface chemistry controlled via sequence-defined peptoids and the surface hydrophobicity of crosslinked polyethers. Multiple, state-of-the-art, experimental and computational tools are employed to generate an integrated and mechanistic understanding of surface water structure, dynamics, and thermodynamics on polymer surfaces.

SESSION III: TUESDAY, JULY 30, 2019; 1:45 – 3:45 PM; THURGOOD MARSHALL NORTH

1:45 PM

E-III-1: OVERVIEW OF THE ADVANCED MATERIALS FOR ENERGY-WATER SYSTEMS EFRC

[AMEWS] Wei Chen[1], Seth Darling[1], Juan de Pablo[1,2], Jeffrey Elam[1], Giulia Galli[1,2], Harold Kung[3], Alex Martinson[1], Karen Mulfort[1], Paul Nealey[1,2], George Schatz[3], Steven Sibener[2], Dmitri Talapin[1,2], David Tiede[1], Matthew Tirrell[1,2], Andrei Tokmakoff[2], Gregory Voth[2], Nestor Zaluzec[1]
[1]Argonne National Laboratory (lead institution); [2]University of Chicago; [3]Northwestern University

The AMEWS center targets the three legs of water/solid interfaces: adsorption, reactivity, and transport. Our program aims to: (1) Design and synthesize responsive interfaces to selectively and reversibly adsorb specific components from a complex aqueous fluid; (2) Decipher and harness the interplay between confinement and charge on catalytic reactivity at water/solid interfaces; and (3) Predictively describe the transport of water, aqueous solutions, and charged species across multiple time and length scales, especially under extreme confinement and in the presence of charged interfaces.

2:05 PM

E-III-2: OVERVIEW OF CENTER FOR MATERIALS FOR WATER AND ENERGY SYSTEMS (M-WET)

[M-WET] Benny Freeman[1], Lynn Katz[1], Rachel Segalman[2], Venkat Ganesan[1], Desmond Lawler[1], Nathaniel Lynd[1], Thomas Truskett[1], Mukul Sharma[1], Michael Webber[1], Mahdi Abu-Omar[2], Christopher Bates[2], Songi Han[2], Craig Hawker[2], Scott Shell[2], Todd Squires[2], Michael Doherty[2], Glenn Fredrickson[2], Ethan Crumlin[3], and Alex Hexemer[3]
University of Texas at Austin[1], University of California at Santa Barbara[2], Lawrence Berkeley National Labs[3]

This presentation will provide a general introduction to M-WET, highlighting our approach to addressing water/energy nexus basic science challenges important for design, synthesis, and characterization of new polymer-based membranes for water purification. Novel synthetic approaches, fundamental theory and simulation spanning many length/time scales, and advanced characterization methods are being applied to discover basic understanding to underpin progress in membranes to treat water sources important in energy applications, such as produced water purification.

2:25 PM

E-III-3: MULTISCALE MODELING OF FLUIDS IN SINGLE DIGIT NANOPORES

[CENT] Narayana R Aluru[1], Mohammad Heiranian[1], Archith Rayabharam[1], Samuel Faucher[2], Michael Strano[2], Alex Noy[3], John Fourkas[4], Zuzanna Siwy[5], Haoran Qu[4], YuHuang Wang[4], Tuan Anh Pham[3]
[1]University of Illinois at Urbana-Champaign; [2]Massachusetts Institute of Technology; [3]Lawrence Livermore National Laboratory; [4]University of Maryland; [5]University of California, Irvine

Structure, dynamics and transport of fluids in single digit nanopores (SDNs) can be vastly different from their macroscopic counterparts. For example, water transport through carbon nanotubes has been shown to exhibit flow rates which are many orders of magnitude larger compared to those obtained from classical theories. While classical theories are fast, they do not account for the microscopic mechanisms that are important in single digit nanopores. Quantum and atomistic simulations can provide good accuracy, but they are limited in the length and time scales that can be dealt with. In this talk, we will present multiscale theories to describe fluidic behavior in SDNs. First, we will discuss multiscale approaches to calculate fluidic properties such as structure, interfacial friction, viscosity, permittivity, slip,

etc. in SDNs. We will show that these properties can be vastly different when compared to their bulk counterparts. Second, we will discuss the development of nanofluidic theories incorporating microscopic physics and show that these theories can predict water flow rates which are consistent with experimental measurements. Third, we will discuss the physics of electrical double layers (EDLs) and show that the structure and dynamical properties of ions and water in EDLs of SDNs can be different from those in larger pores/channels. Finally, we will present evidence of molecular sieving of simple organic molecules using SDNs.

2:45 PM

E-III-4: LOCAL IONIC DYNAMICS OF ELECTROLYTES IN REAL SPACE AND TIME

[FIRST] T. Egami[1,2], P.T. Cummings[3], Y. Shinohara[1], W. Dmowski[2], C.W. Ryu[2], M.W. Thompson[3], R. Matsumoto[3], R. Sacci[1], R.L. Sanders[1], S. Dai[1]
[1]Oak Ridge National Laboratory, [2]University of Tennessee, [3]Vanderbilt University

In solids atomic dynamics is described in terms of phonons and diffusion. In liquids, however, the time-scales of the two are similar, of the order of ps, and consequently phonons are strongly damped and diffusive steps are dynamically correlated. To describe such dynamics the conventional approach in the momentum (Q) and energy (E) space in terms of the dynamic structure factor, S(Q, E), is grossly inadequate. Instead we propose to describe the local dynamics in real space and time, using the Van Hove function (VHF), G(r, t). We demonstrated recently that the VHF can be determined by inelastic x-ray or neutron scattering (IXS or INS) experiments as the double-Fourier-transform of S(Q, E). The VHF of water determined by IXS is reproduced by simulation, to visualize correlated local dynamics of water molecules. The lifetime of the local environment determined by the VHF explains quantitatively the origin of viscosity. We are currently studying how the water dynamics is modified by addition of ionic salts. Most of salts, such as NaCl, increase viscosity of aqueous solution, but some, such as NaI, decrease it. However, the microscopic mechanism is controversial. We plan to apply this approach to the study of local dynamics in liquid electrolytes to understand the effect of mixing, dimensionality, confinement, interface, applied field, and other factors. The knowledge garnered shall contribute to the bottom-up design of better electrolytes.

3:05 PM

E-III-5: DYNAMIC CHARACTERIZATION OF FLUIDS IN CONFINED SPACE

[MUSE] Hassnain Asgar[1], Siddarth Agrawal[2], Greeshma Gadikota[1], and Michael Hoepfner[2]
[1]University of Wisconsin, [2]University of Utah

The MUSE Energy Frontier Research Center's (EFRC) objectives range from fabrication and characterization of geomaterials with repeatable hierarchal heterogeneity, to understanding the fundamental thermodynamics and transport properties of confined fluids. In this talk, we will discuss the thermophysical properties of confined fluids and *in situ* multi-scale characterization of *geo-architected* porous media. Steric and surface effects cause significant deviations between fluid properties (e.g., bubble points) from the bulk to confined state. To assess the physical and chemical origins of these properties on the molecular scale, we employ static and dynamic characterization tools. Specifically, we will discuss total neutron scattering to assess the fluid structure and thermodynamics, and nuclear magnetic resonance (NMR) to understand confined kinetic transport properties. To advance the common scientific theme of connecting fluid properties in confined and unconfined environments to the chemo-morphological characteristics of the materials, custom microreactors compatible with synchrotron characterization

techniques were developed. This approach has facilitated cross-scale *in-operando* characterization of fluid-solid interactions using cross-scale X-ray and neutron scattering and tomography techniques. Our future experimental investigations are supported by predictions of wettability alterations at solid interfaces, and organization and transport of light and heavy hydrocarbon molecules and CH_4 confined in the nanopores of silica using molecular-scale models. These predictions suggest that the chemistry of the solid interfaces, the fluids of interest, and the resulting interactions yield competing adsorption selectivity for solid interfaces.

3:25 PM

E-III-6: FROM NANOPARTICLE FORCES, INTERFACIAL STRUCTURE, AND AGGREGATION TO MACROSCOPIC RESPONSE DYNAMICS AND RHEOLOGICAL PROPERTIES: A COMPLEMENTARY AND CROSS-CORRELATED STUDY ACROSS SCALES

[IDREAM] Elias Nakouzi[1], Anthony J. Krzysko[2], Jaewon Lee[1], Lance E. Edens[2], Sidhant Pednekar[1], Patricia L. Huestis[6], Jennifer A. Soltis[1], Enrique Alvarado[2], Xin Zhang[1], Trent R. Graham[1], Dongsheng Li[1], , Cornelius F. Ivory[2], Kevin M. Rosso[1], Andrew G. Stack[4], Lawrence A. Anovitz[4], Aurora E. Clark [2,1], Greg K. Schenter[1,2], James J. De Yoreo[1,3], Jaehun Chun[1]
[1]Pacific Northwest National Laboratory, [2]Washington State University, [4]Oak Ridge National Laboratory, [6]University of Notre Dame

Nanoparticle interactions, surface chemistry, and aggregation, coupled with radiation, are linked to the response dynamics and rheological properties of complex solutions, a challenging problem exemplified by radioactive waste. Understanding this problem requires coupling phenomena across scales, from the molecular details at the particle-solution interface through the macroscopic complexities of aggregation. Using boehmite as a case study, we developed a 3D atomic force microscopy (AFM) capability and observed hydration layers within one nanometer of the surface templated by the boehmite crystal lattice. Moreover, measurements using customized AFM probes showed stronger adhesive forces between boehmite crystals over a range of increasing salt concentrations. These results were further validated by light and small angle neutron scattering (SANS) measurements combined with scaling theory that showed significantly faster boehmite aggregation rates at high pH and ionic strength. Importantly, we found that the irregular particle shape affects the rotational/translational diffusivity, the hydrodynamic forces between particles, and ultimately the aggregate structures, which are surprisingly dense as determined by SANS measurements and Monte Carlo simulations. We also found that aggregation is influenced by radiation using SANS measurements with irradiated boehmite. Furthermore, rheometric scattering techniques probed the connection between particle forces under flow and macroscopic response dynamics. These were complemented by simulations and network analysis, which demonstrate unexpected, non-monotonic viscosities as a function of flow rate. Our results provide a foundation for building a predictive understanding that bridges the gap between physicochemical behavior of individual nanoparticles and emergent properties of complex mixtures.

F. MATERIALS AND CHEMISTRY BY DESIGN

SESSION I: TUESDAY, JULY 30, 2019; 8:00 – 9:40 AM; THURGOOD MARSHALL WEST

8:00 AM

F-I-1: MXENE PSEUDOCAPACITIVE ENERGY STORAGE SYSTEMS WITH HIGH ENERGY DENSITY

[FIRST] Yury Gogotsi,[1] Xuehang Wang,[1] Tyler S. Mathis,[1] Cheng Zhan,[2] De-en Jiang,[2] Naresh C. Osti,[3] Eugene Mamontov,[3] Lukas Vlcek[3] and Matthew W. Thompson[4]
[1]Drexel University; [2]University of California, Riverside; [3]Oak Ridge National Laboratory; [4]Vanderbilt University

Pseudocapacitive charge storage is defined by fast, surface-confined redox reactions, making pseudocapacitive materials promising candidates for electrochemical energy storage systems with both, high energy and high power. 2D transition metal carbides and nitrides (MXenes) have shown great potential for pseudocapacitor applications due to their metallic conductivity and redox active surfaces. Ti3C2Tx, a prototypical MXene, is capable of delivering a remarkable capacitance of 1500 F/cm3 in acidic aqueous electrolyte, when well-designed electrode architectures are used. Considering the diversity of the large MXene family, we have conducted a computational screening of energy storage properties among twenty-four MXenes with different electronic structure, magnetism, and hydrogen adsorption energy. The simulation results suggest that most nitrides tend to have better capacitive performance than carbides. More positive hydrogen adsorption free energy (weak binding to H) and smaller change of the potential at the point of zero charge after H binding lead to higher capacitance. Besides further enhancing the capacitance of MXenes, improving the voltage window of a MXene pseudocapacitors is another key to enhancing the energy density. High-performance pseudocapacitive positive electrode materials, such as conductive polymers and ruthenium oxide, have been combined with MXenes to make all-pseudocapacitive asymmetric devices with expanded voltage window and increased energy density in aqueous electrolyte. Using ionic liquids can further enhance the energy density by expanding the applicable voltage window, provided the efficient intercalation of large organic ions in MXene is achieved. Observed directly by ex-situ neutron scattering, the diffusion of ionic liquid in the MXene can be accelerated by optimizing the concentration of the ionic liquid in the bulk electrolyte.

8:20 AM

F-I-2: INORGANOMETALLIC CATALYST DESIGN CENTER: THEORY DRIVING NEXT-GENERATION CATALYST DESIGN

[ICDC] Rachel B. Getman[1] and Heather J. Kulik[2]
[1]Clemson University; [2]Massachusetts Institute of Technology

An overview of the latest achievements in catalyst design as part of the activities of ICDC will be presented. This will include both the development and application of new methods. Two examples in catalyst design will be highlighted, one involving elucidating the catalytic mechanism of ethylene hydrogenation on single metal cation catalysts and one involving high-valent metal-oxo energetics relevant to selective partial oxidation. To provide insight into the catalytic mechanism, we performed a combined experimental and computational analysis using microkinetic modeling with a dual site mechanism and high throughput flow reactor experiments. We determined the reaction mechanism as a function of catalyst composition and reaction conditions and are presently working to link catalytic function to material properties of the catalyst, such as the electron configuration of the metal cation active site. As a complementary approach, we have developed machine learning models trained on electronic structure (here, density functional theory, or DFT) energetics for metal-oxo formation and hydrogen atom abstraction as representative catalytic steps. These artificial neural network models trained on compositional, inorganic chemistry-tailored representations enable near-DFT accuracy property prediction after modest training (100s of compounds). Using these trained models with awareness of their domain of applicability, we explore large compound spaces (10k-30k) in seconds instead of the days or weeks conventional theoretical chemistry calculations would require. We pair this approach with evolutionary algorithm optimization to both confirm expected design rules (e.g., scaling relations) but also identify opportunity for overcoming known trade-offs in catalysis.

8:40 AM – Team Science Finalist

F-I-3: DESIGNING NEW NITRIDE SEMICONDUCTORS: FROM COMPUTATIONAL DISCOVERY TO EXPERIMENTAL REALIZATION

[CNGMD] S.R. Bauers[1], C.J. Bartel[2], R. Woods-Robinson[3], J.S. Mangum[4], B.R. Chen[5], K. Heinselman[1], E. Arca[1], W. Sun[6], A.M. Holder[2], A. Zakutayev[1], S. Lany[1], G. Ceder[3, 6], L. Schelhas[5], M. Toney[5]
[1]National Renewable Energy Laboratory, [2]University of Colorado Boulder, [3]University of California, Berkeley, [4]Colorado School of Mines, [5]SLAC National Laboratory, [6]Lawrence Berkeley National Laboratory

To accelerate materials discovery, the Center for Next Generation of Materials Design (CNGMD) couples first-principles theory with high-throughput and directed synthesis as well as advanced characterization to understand and predict structure, properties, and phenomena. This approach is exemplified by our successful and on-going quest to discover new metal nitride semiconductors.

Despite nitrogen being approximately four times more prevalent than oxygen in Earth's atmosphere, there are ten times fewer known nitrides than oxides, a consequence of the stability of molecular nitrogen.[1] However, the same chemistry in nitrogen that leads to its highly stable diatomic form imparts unique chemical and physical traits when successfully incorporated in the solid state. In this work, we rationally targeted new spaces for nitride discovery, realized these materials in the lab, and identified new chemical mechanisms that determine the stability and optical properties of solid-state nitrides.

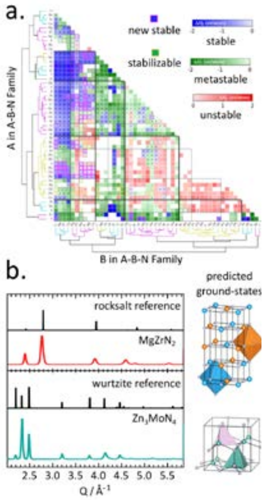


Fig 1: (a) Stability map of the ternary metal nitrides led to (b) experimental discovery of several new ternary nitrides.

As a core component of this work, we created a stability map of inorganic ternary nitrides using an ionic substitution algorithm and high-throughput density functional theory calculations (Fig 1a).[2] From this map, we 1) revealed the space of stable ternary nitrides to be twice as large as was previously known, with 203 new predicted stable compounds, and 2) extracted insights into the chemical origin of these new materials. Leveraging these predictions, we synthesized several compelling materials as thin-films using elevated nitrogen chemical potentials and confirmed their structures through a combination of synchrotron X-ray diffraction (Fig 1b) and high-resolution transmission electron microscopy. These discoveries—$ZnMoN_2$, Zn_3MoN_4, Zn_3WN_4, Zn_2SbN_3, $MgTiN_2$, $MgZrN_2$, $MgHfN_2$, Mg_2NbN_3, and Mg_2SbN_3—span a wide range of structures and chemistries and exhibit a diverse set of useful properties including tunable band gaps, redox-mediated stabilization, large dielectric constants, defect tolerance, small effective masses, and structural compatibility with known nitrides.[3,4,5] The full map of materials (Fig. 1a) was also assessed with a novel set of chemical bonding descriptors parsed from the computed electronic structure. In doing so, we partitioned the nitrides into those stabilized by the classical inductive effect and those stabilized by a newly proposed chemical mechanism, where nitrogen *donates* electron density, reducing the metals, which we term the *reductive* effect.

This work directly demonstrates and expands the materials development pipeline, integrating theory, computation, synthesis, and characterization to not only predict and realize new functional materials, but also to probe and understand the chemical mechanisms underlying their stability and properties. Looking beyond nitrides, this integrative materials-design approach will enable future efforts to explore under-developed chemical spaces for discovery of new functional materials for a range of applications.

References: [1]Sun et al. *Chem. Mater.* 29, 6936 (2017); [2]Sun et al. *Nat. Mater.* in press; [3]Arca et al. *J. Am. Chem. Soc.* 140, 4293 (2018); [4]Bauers et al. *arXiv*: 1810.05668; [5]Bauers et al. *Jpn. J. Appl. Phys.* in press.

Contributions: SB, KH and EA synthesized and characterized new nitrides; CB performed the chemical bonding analysis; RWR contributed experimentally and computationally; JM performed TEM characterization; BRC performed synchrotron characterization.

9:00 AM

F-I-4: GENESIS: A NEXT GENERATION SYNTHESIS CENTER

[GENESIS] John B. Parise,[1] Karena W. Chapman,[1] Peter G. Khalifah,[1] Simon J.L. Billinge,[2] Peter J. Chupas,[1] Kristin A. Persson,[3] Gabriel M. Veith,[4] Brian L. Phillips,[1] James R. Neilson,[5] Katsuyo S. Thornton,[6] Line Pouchard,[7] Eric Dooryhee,[7] Ping Liu,[8] Jack W. Simonson[9]
[1]Stony Brook University; [2]Columbia University; [3]Lawrence Berkeley National Laboratory; [4]Oak Ridge National Laboratory; [5]Colorado State University; [6]University of Michigan; [7]Brookhaven National Laboratory; [8]University of California San Diego; [9]Farmingdale State University

GENESIS develops a new paradigm for synthesis that accelerates the discovery of materials, by understanding how key structural and chemical transformations during synthesis are governed by the synthesis variables. Combinations of in-situ experimental protocols and real-time data analytics allow adaptive control over reaction pathways. Deep understanding of the role of precursors, additives, intermediates and their effects on redirecting the pathway toward desired products, will enable purposefully navigation of reaction pathways leading to new functional materials. While intuition-guided synthesis remains a mainstay, this iterative process is slow, and often poorly achieved. The physical realization of novel predicted materials through rational and efficient synthesis by exploiting advanced operando diagnostics coupled with data science tools will accelerate the synthesis of new materials by steering along those pathways most likely to lead to desired outcomes. The tightly integrated computational and experimental effort in GENESIS addresses the role of chemical and energy transport, across multiple length scales and how it limits reaction progress; identifying the incipient stages of reactant/product differentiation; and controlling reactions through adaptive feedback.

9:20 AM

F-I-5: CERAMIC WASTE FORM DESIGN AND PERFORMANCE PREDICTION – A SEDMAT APPROACH

[WastePD] Zelong Zhang,[1] Tiankai Yao,[2] Jie Lian,[2] Jianwei Wang[1]
[1]Louisianan State University; [2]Rensselaer Polytechnic Institute

Science of Environmental Degradation of Materials (SEDMat) is a science-based framework being developed by WastePD for nuclear waste form design and performance prediction. Fundamental understanding in the dissolution mechanisms/kinetics has been deepened for ceramic degradation, and some key materials parameters governing the chemical durability of ceramics were identified, representing a significant advancement for a science-based prediction of dissolution rates. Machine-learning accelerated materials discovery and experimental validation of ceramic materials dissolution testing are being combined in this effort. Specifically, artificial neural networks were used to predict a collection of new Ti-based and non-Ti-based hollandite compositions with well-defined crystallographic channel sizes and structural tolerance factors suitable to incorporate Cs. A methodology for evaluating chemical durability of nuclear waste forms was demonstrated for single phase ceramic iodoapatite based on the mechanisms of critical dissolution processes. Such a mechanistic approach, which is generally applicable to other nuclear waste forms and minerals, can be used to predict the dissolution rate in various environmental conditions and to evaluate the long-term durability. A correlation between the dissolution rate and reacting fluid flux has been derived and successfully applied for the modeling of experimental observations of dissolution kinetics of a number of oxides under various conditions. By introducing the reacting fluid flux as a thermodynamic rate controlling variable, the rate equation was modified to include environmental variables of temperature, pH, and fluid flux and parameters intrinsic to the material to describe responses of dissolution kinetics of the materials to these environmental variables.

SESSION II: TUESDAY, JULY 30, 2019; 11:00 – 12:20 PM; THURGOOD MARSHALL WEST

11:00 AM

F-I-1: MOLECULAR BASIS FOR CELLULOSE MICROFIBRIL FORMATION

[CLSF] Purushotham Pallinti[1], Sung Hyun Cho[2], Manish Kumar[2], Tracy Nixon[2], Jochen Zimmer[1]
[1]*University of Virginia;* [2]*The Pennsylvania State University*

A fundamental difference between animal and plant cells is the presence of a cell wall, which performs numerous essential functions in plant physiology. It determines cell shape by forming a strong outer structure that is selectively loosened to enable cell enlargement. Plant cell walls are supramolecular assemblies of diverse polymers hierarchically ordered at the nanoscale. Cellulose microfibrils (CMFs) are stiff load-bearing elements of the wall. On a molecular level, CMFs consist of multiple, precisely aligned cellulose chains, which in turn are linear polymers of glucose molecules. Cellulose is formed by cellulose synthase (CesA), a membrane-embedded enzyme that synthesizes cellulose from UDP-activated glucose molecules and secretes the polymer to the cell surface in a coupled reaction.

While the biosynthesis of individual cellulose polymers is well understood, how plants produce CMFs and how they are integrated into the cell wall remains unknown. Most likely, CMF formation is due to the organization of multiple CesA enzymes into supramolecular complexes in the plasma membrane, leading to coordinated secretion of multiple cellulose chains in close proximity, facilitating precise chain alignment. CLSF is testing this hypothesis by establishing the structural and functional basis for CMF biosynthesis in plants. We use a multi-pronged approach including functional reconstitution of CMF formation in vitro, structural analyses of CesAs and complexes thereof, as well as in vivo imaging of CesA clusters to delineate the mechanism of CMF biosynthesis in plants, thereby providing the molecular basis for cell wall engineering.

11:20 AM

F-I-2: SUPRAMOLECULAR POLYMER-COVALENT NETWORK HYBRID MATERIALS FOR LIGHT-ACTIVATED ROBOTIC FUNCTIONS

[CBES] Chuang Li[1], Aysenur Iscen[1], Hiroaki Sai[1], Kohei Sato[1], Nicholas A. Sather[1], Stacey Chin[1], Zaida Álvarez[1], Liam C. Palmer[1], George C. Schatz[1], Samuel I. Stupp[1]
[1]*Northwestern University*

The development of soft matter that mimics living organisms in its capacity to autonomously translate or morph reversibly is a grand challenge for science. Such materials could be transformative in emerging areas such as soft robotics, interactive actuators, and sensor-effector devices. We report here on experiments and computer simulations of a hybrid material in which supramolecular polymers are chemically bonded to a crosslinked network that reversibly expels and absorbs water in response to visible light. The supramolecular polymer reinforces the network at very low levels of covalent crosslinking, potentially acts as a conduit for water molecules, and facilitates faster photo-driven contraction. These effects enable a greater bending actuation and also lead to longer steps during the light-driven crawling motion of macroscopic films. Our work suggests that integrated systems of covalent networks and supramolecular assemblies could be highly tailorable to design autonomous robotic soft matter.

11:40 AM

F-I-3: ACID GAS STABILITY AND SELECTIVITY OF RARE EARTH MOFS

[UNCAGE-ME] Tina M. Nenoff[1], Dorina Sava Gallis[1], Grace Vincent[1], D. Jon Vogel[1], Jessica Rimsza[1], Katharine Page[2], Ryan P. Lively[3]
[1]Sandia National Laboratories; [2]Oak Ridge National Laboratory, [3]Georgia Institute of Technology

Herein, we report on the novel application and study of isostructural metal organic framework (MOF) materials platform based on RE-DOBDC (RE= Y, Yb, Tb, Eu; DOBDC= 2,5-dihydroxyterephthalic acid) containing coordinatively unsaturated open metal sites. In particular, we are interested in understanding the structural and thermal stability of these analogs to caustic gases (NO_x, SO_x). To do this, we investigated the preferential adsorption of these gases as function of metal identity; examined performance in complex gas environments and/or over long exposure; and used synergistic predictive molecular modeling to inform the experiment.

Materials characterization included neutron and X-ray diffraction, BET adsorption, FTIR, and photoluminescence. Acid gas adsorption studies were undertaken both in bulk adsorption and in ppm concentrations. DFT modeling of the structure-property relationship of the acid gas stability, and of the electronic and optical structures of the RE-DOBDC MOFs is concurrent to the experimentation. A combination of modeling packages including VASP, PBEsol functionals, projector augmented wave (PAW) psuedopotentials and van der waals interactions are being used.

Pure phases of the MOF were successfully synthesized and characterized. RE-DOBDC MOFs retain crystallinity under NO_x exposure. Uniquely, emission is quenched upon NO_x adsorption, indicative of stimuli responsive nature in this multifunctional material system. Modeling indicates the DOBDC ligand reorganizes in the MOF to accommodate gas molecules into the most favorable coordination with the unsaturated RE site. On-going work is expanding into adsorption selectivity and materials durability in mixed acid gas streams and developing an understanding of the structural robustness over extended exposure times.

12:00 PM

F-I-4: THE INTERPLAY BETWEEN STRUCTURE, DYNAMICS AND ELECTROCHEMISTRY IN MICROEMULSIONS

[BEES] Thomas A. Zawodzinski[1], Tessa Calhoun[1], Joshua Sangoro[1], Mark D. Dadmun[1], Alan Bard[2], Douglas G. Hayes[1]
[1]University of Tennessee, Knoxville and [2]University of Texas, Austin

The BEES EFRC is exploring various structured liquids as possible electrolytes for energy storage and other electrochemical applications. Here we describe our first studies of the electrochemical behavior of oil-in-water microemulsions. Stable microemulsion systems were prepared with water (plus salt), toluene (oil phase) and a Tween/butanol surfactant system. Ferrocene was loaded into the toluene phase and its electrochemical behavior observed. Results indicate remarkably reversible (fast) electrochemical kinetics in the region in which oil-in-water droplets or bicontinuous phases are present. Fast voltammetry and single droplet detection were used to probe the limits of rapid kinetics and to estimate typical droplet size. To understand this process further and understand the properties of each component, we have used a series of characterization methods. We have explored the structure of the droplets using X-Ray scattering and Second Harmonic Generation methods. We probed the interaction of the droplet with the interface with Neutron Reflectivity. We have used broadband dielectric and NMR spectroscopy to probe mobility of components in the microemulsion. In addition, the effects of various chemical variants (redox molecules, supporting electrolyte composition) we determined. Based on this, we will present our working picture of the droplet behavior and the electrochemical process with unprecedented detail.

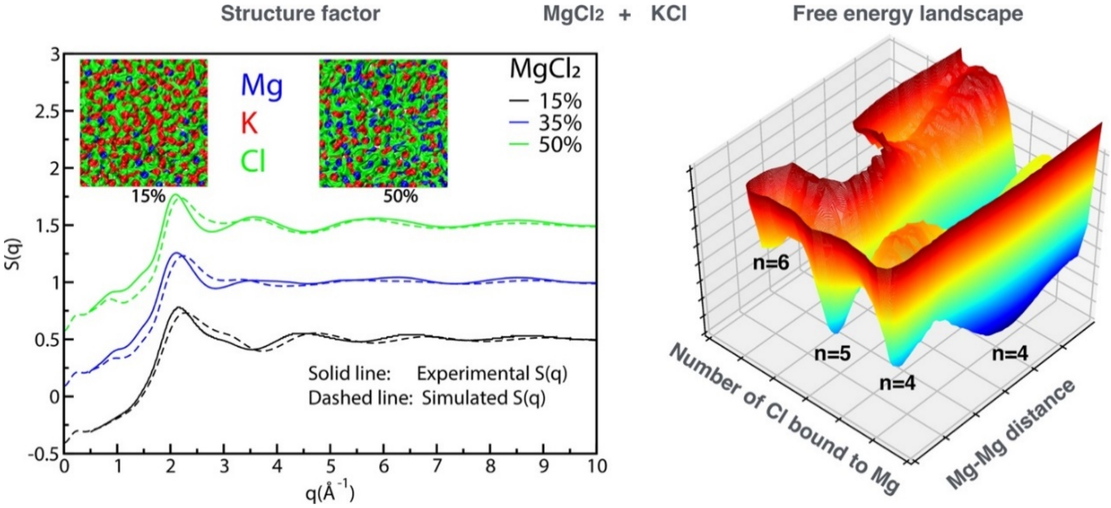
Session III: Tuesday, July 30, 2019; 1:45 – 3:45 PM; Thurgood Marshall West

1:45 PM – Team Science Finalist

F-III-1: Bridging the Gap between Theory and Experiments on the Structure, Dynamics, and Thermodynamics of Molten Salts

[MSEE] Santanu Roy[1], Fei Wu[2], Haimeng Wang[3], Shobha Sharma[2], Yong Zhang[3], Matthew S. Emerson[2], Vyacheslav S. Bryantsev[1], Edward J. Maginn[3], Claudio J. Margulis[2], Alexander S. Ivanov,[1] Shannon M. Mahurin,[1] Phillip Halstenberg,[1] Simerjeet Gill,[4] Mehmet Topsakal,[4] Bobby Layne,[4] Kotaro Sasaki[4]
[1]Oak Ridge National Laboratory; [2]University of Iowa; [3]University of Notre Dame; [4]Brookhaven National Laboratory

A fundamental and predictive understanding of the structure, dynamics, and reactivity of molten salts in the bulk and at interfaces under extreme conditions of temperature and radiation is crucial for the design of a new generation of molten salt nuclear reactors, ensuring their operating efficiency and safety. Achieving the necessary understanding requires significant advances in computational and experimental methods. In our new *Molten Salts in Extreme Environments (MSEE)* EFRC, we apply theory and molecular dynamics (MD) simulation methods at the electronic and classical levels to provide novel atomistic insights into the structure and dynamics of molten salts. These insights permit us to interpret and derive more information from experimental measurements of structure by high-energy X-ray and neutron scattering techniques at high temperature regimes. We focus on a series of molten chloride salts with monovalent, divalent, and trivalent cations, and their mixtures, and we model structural, thermodynamic, and transport properties as functions of temperature. We are breaking new ground in molten salt MD simulations, which requires thorough and rigorous comparison between our experiments and our *ab initio* and classical polarizable and nonpolarizable force field molecular dynamics results. This enables us to assess the quality of our parameterizations, and lays a strong foundation for modeling more complex mixtures including fuel salts, corrosion, and fission products. In this talk, we will discuss our advances so far in understanding properties of molten salts such as structure factors, coordination structure, self-diffusivities, viscosities, ionic conductivities and thermal conductivities, as well as the mechanisms and kinetics of ion-pairing and ion-exchange processes in molten salts.



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Contributions: S.R. analyzed free energy landscapes and rate processes, F.W. analyzed structure factors, and H.W. analyzed dynamical properties such as self-diffusivities, viscosities, and conductivities.

2:05 PM

F-III-2: THE SCIENCE OF ENVIRONMENTAL DEGRADATION OF GLASS MATERIALS

[WastePD] John D. Vienna,[1] Stephane Gin,[2] Jincheng Du,[3] Seong H. Kim,[4] Joseph V. Ryan[1]
[1]Pacific Northwest National Laboratory; [2]Commissariat à l'énergie atomique et aux énergies alternatives (CEA), France; [3]University of North Texas; [4]Pennsylvania State University

The aqueous corrosion of glass materials is being evaluated in a multipronged program. Using coordinated computational, statistical, and mechanistic approaches, new insights into the processes of corrosion have been established. Through these efforts, the impacts of glass composition on various aspects of corrosion behavior are being identified and quantified. We have proven that glass corrosion in dilute systems is not dominated by its starting molecular structure and surface chemistry, as had been commonly thought, but rather by solution feedback effects. Other corrosion behaviors that show strong correlation with composition and structure are being explored. These findings are impacting the design of waste glasses for the Hanford site. The formation, evolution, and impact of the porous alteration layer commonly found on the surfaces of glasses in all but the most dilute conditions are being studied in detail. The mechanisms of formation and corrosion impact remain poorly understood and uncaptured by current glass performance models. We have shown how reorganization impacts transport of water and solutes within the layers, how solution chemistry affects the formation of these layers, and how the whole process can be modeled atomistically. These results were enabled by advances in characterization of the alteration layers and the buried interfaces. Spectroscopic ellipsometry, x-ray photoelectron spectroscopy, and secondary ion mass spectrometry all provide statistically-averaged determination of structural and compositional details. Direct measurement of the region has been made possible with advances using cryogenic atom probe tomography (cryo-APT), which holds promise to characterize water/solid interfaces throughout materials science.

2:25 PM

F-III-3: LIQUID STRUCTURE, ORIENTATION DYNAMICS, AND CHARGE TRANSPORT OF DEEP EUTECTIC SOLVENTS: AN EXPERIMENTAL AND MOLECULAR SIMULATION STUDY

[BEES] Brian Chen[1], Mark Dadmun[2], Burcu Gurkan[1], Luke Heroux[2], Edward Maginn[3], Derrick Poe[3], Joshua Sangoro[2], Stephanie Spittle[2], Henry Squire[1]
[1]Case Western Reserve University; [2]University of Tennessee Knoxville; [3]University of Notre Dame

Deep Eutectic Solvents (DES) are liquids comprised of a hydrogen bond acceptor and a hydrogen bond donor where at certain compositions, the mixture presents a significantly depressed melting point compared to the parent compounds. DES have many superior properties compared to molecular organic solvents including low volatility and high solvation strength, and are therefore promising electrolytes for various electrochemical processes. In this talk, we report the results of molecular simulations and experimental investigations aimed at developing a fundamental understanding of how liquid structure and hydrogen bonding impacts the transport properties of DES, in particular ethaline and glyceline. Broadband dielectric and mechanical relaxation studies reveal that the dynamics of the glycerol networks in glyceline controls the glass transition while the ion transport is coupled to a slow sub-α relaxation. Wide angle neutron scattering studies have documented the local assembly of ethaline, and these results are consistent with molecular dynamics simulations. Ongoing neutron experiments provide similar information for glyceline and the impact of redox active components, such as $ZnCl_2$ and TEMPO, on the liquid structure and hydrogen bonding network in ethaline and glyceline. Simulations of transport properties such as viscosity and ionic conductivity are in excellent agreement with experiments and provide insight into how new DES systems can be designed to optimize performance in electrochemical devices.

2:45 PM

F-III-4: INVESTIGATING CHEMICAL SPECIATION AND THERMODYNAMICS OF METALS IN MOLTEN SALTS USING IN SITU X-RAY ABSORPTION SPECTROSCOPY

[MSEE] Simerjeet K. Gill[1], Kotaro Sasaki[1], Mehmet Topsakal[1], Ruchi Gakhar[2], William C. Phillips[2], Lingfeng He[2], Phillip Halstenberg[3], Shannon Mahurin[3], Lynne Ecker[1], Anatoly I. Frenkel[1]
[1]Brookhaven National Laboratory, [2]Idaho National Laboratory, [3]Oak Ridge National Laboratory

Speciation of dilute metal ions in the environment of molten salts is challenging due to low concentration of ions, changes in their structure, dynamics and electronic properties at different temperatures, concentrations and solvent compositions, and the paucity of most experimental techniques that are capable of detecting these properties in realistic conditions. We applied X-ray Absorption Fine Structure (XAFS) for studies of local coordination environment, bonding dynamics and electronic properties of Ni and Co dopants in single-component $ZnCl_2$ and KCl-$ZnCl_2$ eutectic. For the same concentration (1 wt.%) and temperature range (25 °C to 700 °C), a combination of in situ XAFS and theoretical spectroscopy modeling revealed differences in temperature-dependence of the local structure around Ni and Co. While both types of ions transformed from phase-segregated $NiCl_2$ ($CoCl_2$) regions to single phase, substitutional Ni (Co) in $ZnCl_2$, the phase transition temperature was several hundred degrees higher for Ni. These observations of local structure changes agree with reported lower solubility level of Ni chloride compared with cobalt chloride, and provide information about the changes in the local environment in Ni and Co as a function of temperature. In addition, Einstein temperatures of Ni(Zn)-Cl bonds, and their effective force constants, were obtained. XAFS studies were complemented by optical absorption spectroscopy studies (UV-Vis-near IR range) of molten salts. This will enable a direct correspondence between structural information obtained by UV-Vis absorption and coordination geometry, determined by XAFS.

3:05 PM

F-III-5: ADVANCES IN UNDERSTANDING CONCENTRATED WATER-IN-SALT SOLUTION: STRUCTURE, DYNAMICS AND NUCLEATION MECHANISMS

[IDREAM] Hsiu-Wen Wang[4], David Semrouni[2], Trent R. Graham[1], Katharine L. Page[4], Eugene Mamontov[4], Andrew G. Stack[4], Carolyn I. Pearce[1], Aurora E. Clark [2,1], Sue B. Clark [1,2]
[1]Pacific Northwest National Laboratory, [2]Washington State University, [4]Oak Ridge National Laboratory

The structure and dynamics of salt solutions with low water activity have increasingly important implications for energy storage, radioactive waste remediation and industrial chemical processing. Obtaining a microscopic view of solvent-solute interactions in concentrated water-in-salt solutions allows determination of reactant encounter rates, which influence chemical separation and nucleation processes. The enhanced viscosity in high salt solutions is microscopically related to retardation of ion-water mobilities, and formation of solvent-solute clustering networks. At high concentrations, counterions are no longer innocent charge-balancing/screening species, and instead greatly affect the local coordination responsible for distinct ion-water clustering dynamics. Neutron pair distribution function and quasi-elastic neutron scattering represent experimental tools for probing structure and dynamics of ion-water interactions, providing rigorous and quantitative validation to computational models. Here, we demonstrate the contrasting influence of sodium and potassium countercations on speciation equilibria and stabilization of polynuclear aluminate entities in concentrated solutions. Distinct crystallization mechanisms suggest that different prenucleation cluster dynamics and network packing morphologies can either frustrate (sodium) or promote (potassium) crystallization, as described by non-classical nucleation theory. Characterizing and controlling aluminum speciation in highly concentrated hydroxide solutions is a challenge in the treatment of the nation's high-level legacy radioactive waste

streams. Our studies demonstrate the potential to use ion-specific effects to promote greener, more energy-efficient aluminum processing technologies, as well as chemical strategies for the control of crystallization processes beyond the classical settings. In future work, we will integrate impact of radiation, generated by gamma- and beta-emitting radionuclides in the waste, on reactive species and solution dynamics.

3:25 PM

F-III-6: HIGH ELECTROOSMOTIC COUPLING IN ION CONDUCTANCE OF 1.5 NM DIAMETER CARBON NANOTUBE PORINS

[CENT] Aleksandr Noy[1], Yun-Chiao Yao[1], Amir Taqieddin[3], Narayana R. Aluru[3]
[1]Lawrence Livermore National Laboratory; [2]University of Illinois at Urbana-Champaign

Center for Enhanced Nanofluidic Transport (CENT) is dedicated to studying seven critical knowledge gaps (KGs) that exist in our understanding of fluid transport phenomena on the nanoscale. One such KG involves significant water flow enhancement and unusual ion correlation effects that occur when water and ions undergo extreme confinement in nanometer sized channels. These effects are especially pronounced in vary narrow lumen channels of carbon nanotube porins (CNTPs) that exhibit high slip flow enhancement due to smooth hydrophobic pore walls. We have studied ion transport and ion selectivity in 1.5 nm diameter CNTPs embedded in lipid membranes using single nanopore measurement setup. Our data show that CNTPs are weakly cation-selective at pH=7.5 and become non-selective at pH=3.0 when the negatively charged COO- groups at the CNTP ends become protonated. Remarkably, ion conductance of CNTPs exhibits an unusual 2/3 power law scaling with the ion concentration at both neutral and acidic pH values. This scaling is qualitatively different from the conductance-concentration scaling behaviors reported for most nanopores, including those of larger diameter carbon nanotubes. Coupled Navier-Stokes and Poisson-Nernst-Planck (NS-PNP) simulations and atomistic MD simulations reveal that this experimentally-observed scaling originates from strong coupling between water and ion transport in these channels. These effects could result in development of a new generation of new biomimetic membranes and carbon nanotube-based electroosmotic pumps.

G. Nuclear Energy

Session I: Tuesday, July 30, 2019; 8:00 – 9:40 AM; Thurgood Marshall South

8:00 AM

G-I-1: Simple Methods to Quantitatively Generate Hexavalent Americium

[CAST] Matthew V. Sheridan, Johan R. Gonzalez, Jeffrey R. McLachlan, Christopher J. Dares
Florida International University

In acidic aqueous solutions, americium exists in the trivalent state (Am^{III}). This makes it nearly indistinguishable from the lanthanides which are also trivalent, and have similar radii, and results in one of the most difficult separations to perform. In the hexavalent state, americium exists as $Am^{VI}O_2^{2+}$. While little is known about this ion, we expect that it will feature similar reactivity to other hexavalent actinides, which is distinct from the lanthanides, making it possible to selective separate $An^{VI}O_2^{2+}$ (An = U, Np, Pu, Am) from Ln^{III} in a single step. The extreme $Am^{IV/III}$ redox potential ($E_{1/2}$ = 2.6 V vs. SCE) makes the generation of $Am^{VI}O_2^{2+}$ a challenge. While this has been accomplished using chemical oxidants, we will present here characterization of catalytic methods using semi-conductor metal oxide anodes to quantitatively generate Am(VI) from Am(III) at potentials as low as 1.5 V vs. SCE (1.1 V below the $Am^{IV/III}$ couple). We applied our system to the electrochemical characterization of $Am^{VI}O_2^{2+}$, featuring a quasi-reversible Am(VI/V) couple at ca. 1.60 V vs. SCE in 0.1 M nitric acid.

8:20 AM

G-I-2: Synthesis, Structure and Ion Exchange Potential of New Uranyl Salt Inclusion Phases

[CWHM] Jake Amoroso[1], Theodor Besmann[2], Kyle Brinkman[3], David DiPrete[1], Christian Juillerat[2], Vancho Kocevski[2], Robert J. Koch[4], Scott T. Misture[4], Gregory Morrison[2], Hans-Conrad zur Loye[2]
[1]Savanah River National Laboratory, [2]University of South Carolina, [3]Clemson University, [4]Alfred University

A practical working definition of a hierarchical structure is that of a structural motif contained within a larger structure or framework. Salt Inclusion Materials (SIMs) are a subset of a unique family of crystalline hierarchical structure types that are noteworthy because as a "stuffed" porous material, this type of material is of fundamental interest in the development of new waste forms. These have the general formula $[A_mB_nX][(UO_2)_p(M_qO_r)_t]$ where $[(UO_2)_p(M_qO_r)t]$ is the framework consisting of uranyl, UO_2^{2+}, and M_qO_r units (M = Si, Ge), B_nX is the salt-inclusion, and A are alkali or alkaline earth cations that are separate from the salt-inclusion.

The presentation will focus on the synthesis, crystal growth, structures and potential uses of SIMs, including investigations of the formulations $[Cs_3F][(UO_2)(Si_4O_{10})]$, $[Cs_2Cs_5F][(UO_2)_2(Si_6O_{17})]$, $[Cs_9Cs_6Cl][(UO_2)_7(Si_6O_{17})_2(Si_4O_{12})]$, $[Cs_2Cs_5F][(UO_2)_3(Si_2O_7)_2]$, and several isostructural germanates, such as $[CsCs_6Cl][(UO_2)_3(Ge_2O_7)_2]$ with special emphasis on the overall crystal chemistry of these phases. These, together with the synthesis, structural characterization, and ion exchange potential of a series of novel aluminophosphates having the compositions $[Cs_{13}Cl_5][(UO_2)_3(Al_2P_6O_{25})]$, $[Cs_3[Al_2O_7(PO_2)_3][(UO_2)_3O_2]$, $[Rb_7[Al_2O_7(PO_2)_3][(UO_2)_6(PO_4)_2O_4]$ will be presented.

8:40 AM

G-I-3: ENVIRONMENTS FOR ACTINIDES: SYNTHESIS, STRUCTURE AND ELECTRONIC STATE

[CAST] Ryan E. Baumbach[1,2], W. Lucas Nelson[1,2], Alexander T. Chemey[2], You Lai[1,2], Kaya Wei[1,2], Theo Siegrist[1,2], George S. Nolas[3], and Thomas E. Albrecht-Schmitt[1,2]
[1]National High Magnetic Field Laboratory; [2]Florida State University; [3]University of South Florida

The *f*-electron valence state is a main driver for the behavior of lanthanide- and actinide-based materials and influences properties ranging from the functional (crystal structure/density and melting temperature) to the exotic (unconventional superconductivity and topological electronic protection). Efforts to understand a host of systems, ranging from nuclear fuels (e.g., UO_2 and UN) to novel waste forms (e.g., ultra-hard and stable borides/carbides) depend on basic research in this area. Furthermore, these materials are a deep reservoir for novel phenomena, often because their *f*-electrons have a dual nature with characteristics of both itinerant and localized electrons. I will discuss intermetallics with large unit cells or cage-like structures and focus on examples that crystallize in the (i) $A_6W_4Al_{43}$ and (ii) A/LnT_2X_{20} structures (A = actinide, Ln = lanthanide, T = transition metal, and X = p-block element). Regarding (i), we have uncovered the examples $U_6W_4Al_{43}$ and $Pu_6W_4Al_{43}$, which exhibit weak magnetism, are mainly constructed from inexpensive aluminum, and likely will host many different mixtures of actinide elements making these compounds attractive as waste forms for transuranics. Regarding (ii) we have shown that the Ln = Yb examples exhibit unusually good low temperature thermoelectric properties that originate both from the crystal structure and the hybridization between *f*-electron and conduction electron states. We propose that the wider family of chemical analogues offer a long-desired stage upon which to develop a new generation of thermoelectric materials for low temperature applications.

9:00 AM

G-I-4: RADIATION DRIVEN REACTIVITY AT COMPLEX INTERFACES: ENERGY EXCHANGE AND REACTIONS DURING RADIOLYSIS OF BOEHMITE (γ-ALOOH) NANOPLATES

[IDREAM] Thomas M. Orlando[5], Brant M. Jones[5], Alexandr Aleksandrov[5], Xiaosong Li[3], Xin Zhang[1], Kevin M. Rosso[1], Jay A. La Verne[6], Patricia L. Huestis[6]
[1]Pacific Northwest National Laboratory, [3]University of Washington, [5]Georgia Institute of Technology, [6]University of Notre Dame

Radiation impacts chemical reactivity across multiple length and time scales. Boehmite (γ-AlOOH) is a primary constituent of the aggregated solid components of radioactive waste currently stored in tanks at the Hanford site. Consequently, there have been numerous studies on the radiation stability of boehmite particles in the solid phase and suspended in solutions. Radiolysis of boehmite primarily leads to decomposition of hydroxyl and formation of H and oxygen holes, $>OH^- \rightarrow >O^- + H$. The H are then stabilized within the network of hydroxyls, $>OH^- + H \rightarrow >OH^{-}\cdots H$. These H atoms diffuse and react forming H_2. However, our data demonstrates that some H reacts with neighboring hydroxyl sites, resulting in formation of adsorbed H_2O. Evidence of H_2O formation stems from electron stimulated desorption (ESD) of H_2O^+ and temperature program desorption (TPD) of post-irradiated material. We postulate that ESD of intact H_2O vs. fragment ions is correlated with ultrafast and efficient energy transfer between the valence electrons of the adsorbed H_2O and the aluminum-hole state produced by Auger decay. The surface-localized two-site single-hole states which, when formed, can lead to H_2O^+ ejection via a Coulomb repulsion. This intermolecular Coulomb decay or electron-transfer mediated interfacial energy transfer can be enhanced by the two-dimensional nature of the platelets. In summary, we demonstrate synthesis of H_2O and H_2 during (25-500 eV) electron irradiation of boehmite nanoplates utilizing ESD, TPD and *ab initio* molecular dynamics simulations. These interface reactions and energy exchange events likely contribute to the transformation and aging of radioactive wastes.

9:20 AM

G-I-5: TOWARDS NEW METHODS FOR SEPARATING ACTINIDES AND RELEVANT ANIONS FROM WASTE THROUGH REDOX PROCESSES AND SUPRAMOLECULAR ANION RECOGNITION

[CAST] Thibault Cheisson[1], Jiwen Jian[1], Jing Su[2], Alex McSkimming[1], Conrad Goodwin[2], Teresa M. Eaton[3], Michael R. Gau[1], Patrick J. Carroll[1], Andrew Gaunt[2], Enrique R. Batista[2], Ping Yang[2], John K. Gibson[3], Eric J. Schelter[1]
[1]University of Pennsylvania; [2]Los Alamos National Laboratory; [3]Lawrence Berkeley National Laboratory

Our effort has involved the development of new chemistries of organic hydroxylamines and studies of their solution-, gas phase-, and solid-state chemistries. The Separations team has developed new coordination chemistry of a pyridyl-appended hydroxylamine, 2-(tBuNOH)py, with Ce, Th, U, Np, Pu and Am. The metal-redox couples were probed on these compounds using solution cyclic voltammetry. This work shows how metal redox couples can be altered using strongly donating ligands across the actinide series and may help in identifying reagents that promote the selective separation of minor actinides through complexation/oxidation. In a related application of hydroxylamines, electrospray ionization (ESI) of solutions containing a tripodal ligand, H_3TriNO_x ($[\{(2\text{-tBuNOH})C_6H_4CH_2\}_3N]$), and a hydrogen halide (HX): HCl, HBr, and/or HI, yielded abundant gas-phase anion complexes, $[H_3TriNO_xX]^-$ and $[H_4TriNO_xX_2]^-$. ESI yields and collision induced dissociation pathways of mixed-halide gas-phase complexes, $[H_4TriNO_xX_aX_b]^-$, indicated a highest affinity for I^- and lowest for Cl^-. Structures and energetics computed by DFT were in accord with the gas-phase results and indicated that the gas-phase binding preference is a manifestation of the differing stabilities of the three HX molecules. This demonstrates an exceptional connection between gas and condensed phase chemistry and reveals hydroxylamines as promising candidates for anion recognition. We are evaluating molecular tailored capsules to sequester anionic complexes of *f*-element cations for efficient separations are expected based on molecular recognition.

SESSION II: TUESDAY, JULY 30, 2019; 11:00 – 12:20 PM; THURGOOD MARSHALL SOUTH

11:00 AM

G-II-1: NANOSTRUCTURED HIGH-ENTROPY ALLOYS UNDER EXTREME ENVIRONMENTS

[EDDE] Yanwen Zhang[1], Boopathy Kombaiah[1], Ke Jin[1], Zhe Fan[1], Fuxiang Zhang[1], Chenyang Lu[2], Li Jiang[2], Miguel L. Crespillo[3], Walker L. Boldman[3], Philip D. Rack[1,3], Lumin Wang[2], William J. Weber[3,1]
[1]Oak Ridge National Laboratory; [2] University of Michigan-Ann Arbor; [3]University of Tennessee-Knoxville

The continuous pursuit to develop new metallic alloys has led to considerable increases in structural strength and improved functionality, as well as exciting research developments. In the past 15 years, numerous discoveries of high-entropy alloys (HEAs) with remarkable properties that are unexpected from conventional dilute alloys, have drawn immense attention and opened new frontiers in materials research. Due to their noteworthy composition of five or more elemental species all at high concentrations, HEAs intrinsically have a high atomic-level inhomogeneity (chemical complexity). The equally amazing parallel fields of nanoscience and nanotechnology, with the ability to control individual atoms, have led to many additional breakthroughs and applications. As the size of a structure is reduced to a countable number of atoms, chemical, physical, electrical, optical and magnetic properties become fundamentally different from their bulk counterparts. Combining the advantages of high chemical complexity (to tailor scattering processes through coupled electronic and magnetic interactions and to control atomic motion) and nanoscale manipulation (e.g., the inclusion of low-level substitutional additions, nanoparticles, and grain boundaries), we hypothesize that more advanced structural alloys can be designed to have enhanced radiation tolerance. Here we report significant improvements in radiation performance of nanostructured HEAs through the self-organized formation of coherent nanoprecipitates, the inclusion of dispersed nanooxides, and the engineered high density of grain boundaries. Tuning chemical complexity and controlling microstructural complexity represent powerful tools in the improvement of radiation performance and may also lead to new alloy design criteria to meet application requirements in a variety of related fields.

11:20 AM

G-II-2: UNDERSTANDING THE DEFECT STRUCTURE IN IRRADIATED MATERIALS

[FUTURE] Sahil Agarwal[1], Aaron A. Kohnert[2], Jacob E. Cooper[3], Nan Li[2], Yongqiang Wang[2], Danny J. Edwards[4], Djamel Kaoumi[3], Laurent Capolungo[2], Peter Hosemann[5], Farida A. Selim[1], Blas P. Uberuaga[2]
[1]Bowling Green State University; [2]Los Alamos National Laboratory; [3]North Carolina State University; [4]Pacific Northwest National Laboratory; [5]University of California, Berkeley

FUTURE combines in-situ and ex-situ investigation of ion irradiation induced defects with density functional theory calculations and mesoscale modeling to develop fundamental understanding for defect production and evolution by irradiation and the factors that govern material response in radiation environment.

The in-situ investigation of defect population during ion irradiation examines the production of point defects and their interactions on atomic scale in the early stages of irradiation and monitors their kinetics in real time during irradiation. It requires the development and installation of a positron beam in-line with the ion beam accelerator at LANL, which will take place in the coming months. However our ex-situ studies are underway, employing a range of positron annihilation spectroscopy and electron microscopy techniques. Our early investigations reveal how the original point defects and dislocations in Fe films evolve with irradiation and the impact of alloying and microstructure on their evolution or annihilation. We further illustrate how to characterize the size and structure of vacancy clusters and calculate the density of each defect type and focus on monitoring both the change of defect structure and their electronic structure with irradiation dose and alloying.

11:40 AM

G-II-3: EQUILIBRIUM AND NON-EQUILIBRIUM DEFECT DISORDER IN U-DOPED ThO_2 AND IMPLICATIONS FOR LATTICE THERMAL CONDUCTIVITY

[TETI] Maniesha Singh[1], Anter El-Azab[1], Janelle Wharry[1], Amrita Sen[1], Marat Khafizov[2], Lingfeng He[3], Jian Gan[3], Tiankai Yao[3], Zilong Hua[3], David Hurley[3]
[1]Purdue University, [2]The Ohio State University, [3]Idaho National Laboratory

We investigate the impact of irradiation induced defects on lattice thermal conductivity of U-doped ThO_2. Prior to irradiation, the defect content of this material is tied to off-stoichiometry and hence it is dependent upon the level of U doping, temperature and external oxygen pressure or chemical potential. Under irradiation, non-equilibrium defects are produced by energetic particle bombardment, leading to the formation of nanoscale and sub-nanoscale defect clusters that influence thermal transport in ways that are not fully understood to the community. In this talk we present our modeling results for the equilibrium and non-equilibrium defects in ThO_2 and U-doped ThO_2, combined with preliminary experimental results for ion irradiation-induced defects and their influence on thermal transport. A defect disorder model for the off-stoichiometry of ThO_2 and U-doped ThO_2 in an oxygen environment will be presented. The model shows that, while ThO_2 remains mostly hypo-stoichiometric at relevant thermodynamic conditions, U doping expands the thermodynamics window over which ThO_2 becomes hyper-stoichiometric, thus illustrating the impact of 5*f* electrons introduced by the U doping on defect disorder. We will also present the results of a recent defect clustering model of vacancy and interstitial cluster formation in ThO_2 under ion irradiation, and compare the results with the ion irradiation data. The impact of cluster composition on matrix composition is elucidated, showing that irradiation provides a further mechanism of altering the stoichiometry of the matrix by forming clusters not commensurate with the chemical formula of the crystal. The impact of such defects on phonon scattering will be discussed in connection with our measurements of thermal conductivity of un-irradiated and irradiated ThO_2.

12:00 PM

G-II-4: QUANTIFICATION OF PRESSURE IN HELIUM BUBBLES VIA 4DSTEM AND COMPUTER SIMULATIONS

[FUTURE] Peter Hosemann[1], Laurent Capolungo[2], Aaron A. Khonert[2], Khalid Hattar[3], Claire Chisholm[1], Vasfi B. Özdöl[1], Andrew M. Minor[1]
[1]University of California, Berkeley; [2]Los Alamos National Laboratory; [3]Sandia National Laboratory

Helium is created in materials during neutron irradiation as well as during implantation from alpha decays. The insolubility of Helium in solids leads to the formation of helium bubbles in conjunction with vacancy condensation. Knowing the pressure inside a bubble allows one to account for the Helium present and the relative vacancy to Helium ratio. Furthermore, the local strain around Helium bubbles is an important parameter for understanding the influence of these defects on the mechanical properties of irradiated materials and their propensity as sinks for irradiation-induced defects. Here we apply a novel strain mapping method using electron microscopy to directly quantify the two dimensional strain field around implanted He bubbles. Specifically, nano-beam diffraction strain mapping of a large area at high resolution was carried out using a high frame rate detector. Dark-field inline holography was used to measure the strain field around a bubble at high precision, demonstrating the applicability of this technique to metallic systems with nanoscale defects. Both methods found a peak strain around ~10 nm bubbles that is consistent with loop punching as a pressure limiting mechanism during the formation of the bubbles. Finally, using a combined cluster dynamics-dislocation dynamics capability, the strain around bubbles is modeled. This leads to a reinterpretation of the 4D STEM observations as not measuring the average strain in the sample, but rather the maximum strain around the bubbles through the foil. This new understanding also leads to insight into the mechanisms that led to the bubble formation.

SESSION III: TUESDAY, JULY 30, 2019; 1:45 – 3:45 PM; THURGOOD MARSHALL SOUTH

1:45 PM

G-III-1: T1 - PHONON TRANSPORT IN $TH_{1-x}U_xO_2$ FROM NEUTRON SCATTERING AND FIRST-PRINCIPLES COMPUTATION

[TETI] Michael E. Manley[1], Matthew S. Bryan[1], Chris A. Marianetti[2], Lyuwen Fu[2], Krzysztof Gofryk[3], J. Matthew Mann[4], Zilong Hua[3], Amey Khanolkar[3], David H. Hurley[3]
[1]Oak Ridge National Laboratory, Columbia University, [3]Idaho National Laboratory, [4]Air Force Research Laboratory

We investigate the microscopic origin of thermal transport in advanced oxide nuclear fuels, including thorium dioxide and thorium-uranium dioxides, using inelastic neutron scattering and first-principles calculations, combined with thermal property measurements and temperature dependent elastic property measurements. Neutron scattering measurements performed on large single crystals grown within this program provide a direct measure of the phonon group velocities and lifetimes controlling lattice thermal transport. Neutron scattering measurements on powder samples provide the phonon density of states from which the heat capacity and other thermodynamic quantities are derived. Combined with thermal and elastic property measurements these quantities enable us to deduce mode specific contributions to thermal transport. However, since the phonon scattering processes responsible for lifetime broadening involve anharmonic interactions between multiple branches, a full accounting requires accurate calculations. Density functional theory (DFT) captures the phonon dispersion curves of ThO_2 but breaks down for UO_2. This is due to the relatively narrow bands formed by the 5f-orbitals and their strong on-site Coulomb repulsion. Since $Th_{1-x}U_xO_2$ ($x > 0$) bear 5f-electrons it is critical to deal with these limitations. Dynamical mean-field theory (DMFT) can overcome many of the shortcomings of DFT, and it can be applied to real materials when combined with DFT. While DFT+DMFT is far more computationally expensive than DFT, current algorithms and computing power allow it to be applied to relatively complex crystal structures. The results of these calculations are benchmarked against the inelastic neutron scattering phonon dispersion and linewidth/lifetime measurements as well as thermal transport measurements.

2:05 PM

G-III-2: LOCAL LATTICE DISTORTIONS IN HIGH-ENTROPY ALLOYS

[EDDE] Takeshi Egami[1,2], Yang Tong[2], Shijun Zhao[2], Hongbin Bei[2], Sai Mu[2], Yanwen Zhang[2], Malcolm G. Stocks[2], German D. Samolyuk[2], Fuxiang Zhang[2]
[1]University of Tennessee-Knoxville; [2]Oak Ridge National Laboratory

Because of high degrees of chemical complexity, the crystal lattice in high-entropy alloys (HEAs) or concentrated solid-solution alloys (CSAs) is locally distorted away from the ideal structure. This local distortion is principally responsible for the unusual properties of HEAs, including high strength and high irradiation resistance. We carried out high-energy x-ray diffraction measurements to determine the atomic pair-density function (PDF) and performed the *ab initio* calculation of the electronic states and structure for bcc refractory metal HEAs. We found that the local lattice distortion is particularly significant for alloys containing Zr and Hf for which the nearest neighbor and the second neighbors almost merge. Here we show that the charge transfer resulting from the asymmetric covalent bonding is more prominent for the alloys containing Zr and Hf, and produces strong local lattice distortions. Charge transfer renormalizes the effective atomic size through the atomic-level pressure due to charge transfer. The charge transfer is particularly significant for the partially filled t_{2g} band which is directly pointing to the nearest neighbors, whereas the nearly full e_g band shows no charge transfer. We also discuss how changes in the electronic *d*-band increase the stability of interstitial defects, making the stability comparable to that of vacancies, and resulting in a dramatic decrease in swelling after irradiation. We discuss various spin scattering effects on the electron transport in HEAs with 3*d* spin-polarized transition metal alloys.

2:25 PM

G-III-3: SCIENCE OF ENVIRONMENTAL DEGRADATION OF MATERIALS FOR CORROSION RESISTANT ALLOYS

[WastePD] John R. Scully,[1] Wolfgang Windl,[2] Chris D. Taylor,[2] Jen S. Locke,[2] Pin Lu,[3] Greg B. Olson,[3] Gerald S. Frankel[2]
[1]University of Virginia; [2]Ohio State University; [3]QuesTek Innovations LLC

The WastePD Metals Thrust is focused on the performance prediction and design of corrosion-resistant alloys, which form a protective passive film but are susceptible to localized corrosion such as pits. The framework called Science of Environmental Degradation of Materials (SEDMat) is being used. The current state-of-the-art for prediction of pitting resistance is empirical so it is not useful outside of the composition range used in its determination and has no predictive capability. Modifications of this empirical approach, utilizing additional tools such as Calculation of Phase Diagrams is the approach taken in SEDMat 1.x for metals. Pitting is complex phenomenon that spans the scales of ns and nm to cm and years. Metallurgy, surface science, chemistry, and transport considerations are all critical. Therefore, a fully descriptive and predictive model, the goal of SEDMat 3.x, will require a multi-scale, multi-physics model that links critical events over space and time. SEDMat 2.x, the approach being taken to arrive at that goal, is developing calculable parameters to describe important properties in the passivity and localized corrosion processes, such as metal-metal bond strength, metal-oxygen bond strength, and chloride adsorption tendency. These parameters must be calculated not for pure metals, but for multi-component alloys and oxides. Linking of these calculable parameters to measured properties using machine learning methods represents a major advance that moves the design/performance prediction approach away from pure empiricism and facilitates exploration of unknown regions of alloys compositional space without the need for extensive experimentation.

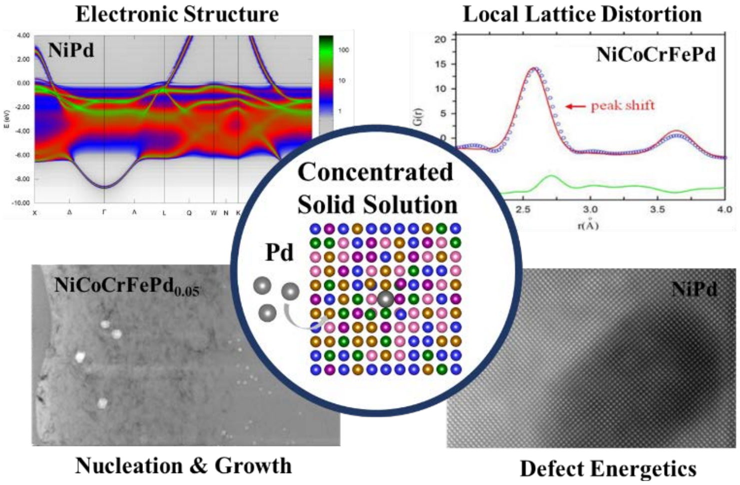
2:45 PM – Team Science Finalist

G-III-4: TUNING LOCAL ATOMIC ENVIRONMENTS TO CONTROL RADIATION DAMAGE

[EDDE] Yang Tong[1], Zhe Fan[1], Xing Wang[1], Sai Mu[1], Shijun Zhao[1], Chenyang Lu[2], Li Jiang[2], Dilpuneet Aidhy[3], Gihan Velisa[1], Lumin Wang[2], Fuxiang Zhang[1], Karren L. More[1], Yanwen Zhang[1]
[1]Oak Ridge National Laboratory; [2]University of Michigan; [3]University of Wyoming

Modifying an alloy's compositional complexity provides a promising pathway for the future implementation of advanced structural materials that intrinsically resist severe radiation damage in nuclear energy applications. The wide selection of alloying elements available for modifying and tuning the chemical landscape of concentrated solid-solution alloys (CSAs) presents us with many opportunities to design novel alloys but also poses a new challenge: how can we efficiently and effectively optimize elements/compositions to create an alloy with the desired, targeted properties? Therefore, understanding and revealing the intricate correlations between elemental composition and radiation damage formation and suppression is timely and of great interest to accelerate the design of radiation-tolerant CSAs.

3*d* transition metal-based CSAs (e.g., Ni, Co, Fe, Cr) have demonstrated superior radiation-tolerance. The EDDE team investigated the effect of adding Pd (a 4*d* transition element) into 3*d* CSAs to further modify a CSA's local atomic environments. In the cases discussed here, we found that their radiation-resistance was enhanced by the addition of Pd. Experimental characterization and theoretical modeling at different length scales revealed the underlying complex mechanisms (see Figure). Transmission electron microcopy studies were conducted to statistically analyze defects in irradiated CSAs. We found that under irradiation, fewer, smaller imperfections and abnormal faceted bubbles or voids formed in the Pd-containing CSAs.[1] Synchrotron X-ray total scattering results showed that alloying with Pd induced both local and long-range lattice distortion.[2] *Ab initio* calculations further revealed that the lattice distortions in Pd-containing-CSAs reduced both the electron conductivity and lattice-mediated thermal conductivity through smearing of both the electron and phonon bands, which served to significantly slow the dissipation of heat and affected defect production and evolution during irradiation. Molecular dynamics simulations demonstrated that radiation-induced defects are preferentially isolated to inhibit their growth. These results provide valuable insights toward the design and deployment of compositionally complex CSAs for nuclear environment applications.



References: [1] Z. Fan, S. Zhao, K. Jin, D. Chen, Y.N. Osetskiy, Y. Wang, H. Bei, K.L. More, Y. Zhang, Acta Mater. 164 (2019) 283-292. [2] Y. Tong, G. Velisa, S. Zhao, W. Guo, T. Yang, K. Jin, C. Lu, H. Bei, J.Y.P. Ko, D.C. Pagan, Y. Zhang, L. Wang, F.X. Zhang, Materialia 2 (2018) 73-81.

Contributions: X.W. and Z.F. performed the transmission electron microscopy characterization, Y.T. conducted the synchrotron X-ray characterization, S.M. conducted the *ab initio* calculations, and D.A. performed the molecular dynamics simulations.

3:05 PM

G-III-5: MULTI-SCALE CHARACTERIZATION OF INTERFACIAL AND CORROSION PROCESSES IN MOLTEN SALT ENVIRONMENTS

[MSEE] Lingfeng He[1], Arthur Ronne[2], Yi Xie[1], Yachun Wang[1], Dmitriy Dolzhnikov[3], Mingyuan Ge[4], Xianghui Xiao[4], Wah-Keat Lee[4], Shannon M. Mahurin[3], Yu-chen Karen Chen-Wiegart[2,4]

[1]Idaho National Laboratory, [2]Stony Brook University, [3]Oak Ridge National Laboratory, [4]Brookhaven National Laboratory

The degradation of material surfaces in chemically active environments can affect the materials performance for structural and energy applications. Molten salts are excellent heat transfer fluids and they are known to order at interfaces due to charge interactions. Their structural interactions are likely to affect dynamics, diffusion and chemical interactions with materials, including corrosion. The Molten Salts in Extreme Environments EFRC aims to understand structure and dynamics of salts near interfaces, and the corrosion behavior of structural materials in salts using multi-scale characterization techniques. In our work, Ni and Ni20Cr microwires were subjected to corrosion in molten KCl-$MgCl_2$l at 800 ˚C for 1-100 hours. Comprehensive X-ray nanotomography and scanning transmission electron microscopy (S/TEM) with spatially resolved energy dispersive X-ray spectroscopy (EDS) and electron energy loss spectroscopy (EELS) were used to study the corrosion of microwires, with a focus on the liquid-solid interface. The three-dimensional morphological structure and chemical composition of microwires and their corrosion products, from atomic to nanometers to micrometers, have been extensively characterized. This multi-scale characterization methodology has proven to be critical in fully understanding interfacial processes leading to corrosion. The inward diffusion of molten salts along the grain boundaries and other defects of the metals appears aggravate the corrosion of metals, resulting in the formation of a porous structure. A planned series of corrosion studies at various temperatures and exposure times, followed by multi-scale characterization of materials, will provide a better understanding of corrosion mechanisms and help build models for predicting materials corrosion behavior under extreme environments.

3:25 PM

G-III-6: NEW METHODS FOR CHARACTERIZING NANOSCALE STRUCTURAL FEATURES: CLEAR LINKS TO PROPERTIES

[CWHM] Deepak Patil[1], Robert J. Koch[1], Shubham Pandey[2], Guangfang Li[3], Douglas A. Blom[3], Hui Wang[3], Simon R. Phillpot[2], Kyle Brinkman[4], Mingyang Zhao[4], and Scott T. Misture[1]
[1]Alfred University, [2]University of Florida, [3]University of South Carolina, [4]Clemson University

Traditional crystallography cannot be used to describe nanoscale ordering, cation clustering, and related local structural features, although we have clear indications from experimental and computational studies that these interesting features are of critical importance to material performance. We are therefore studying tunnel-structured materials including hollandite oxides and salt inclusion oxides, and 3-D porous materials including zeolites and Prussian blue analogs to obtain such properties. Our ongoing work using DFT, calorimetry, EXAFS and X-ray PDF has shown that the ion leach rates from the tunnels for hollandite tunnel-structured materials are controlled by very subtle ion clustering and octahedral distortions around the guest ions. Our related work on zeolites shows that there are unknown mechanisms at play during ion exchange between H^+, Na^+, Cs^+, Ba^{2+} and Sr^{2+}.

In order to extract reliable and robust models of nanoscale order and disorder, we have developed new approaches that are based on X-ray (and neutron) total scattering wherein complex models are obtained and supported by computational results. This new process is computationally efficient and has higher reliability than earlier methods which generally produce non-unique results and/or are statistically unsound values. We demonstrate that these new approaches can be used to study a broad range of materials, including bulk materials with nanoscale order/clustering plus nanoparticle materials.

H. QUANTUM MATERIALS I

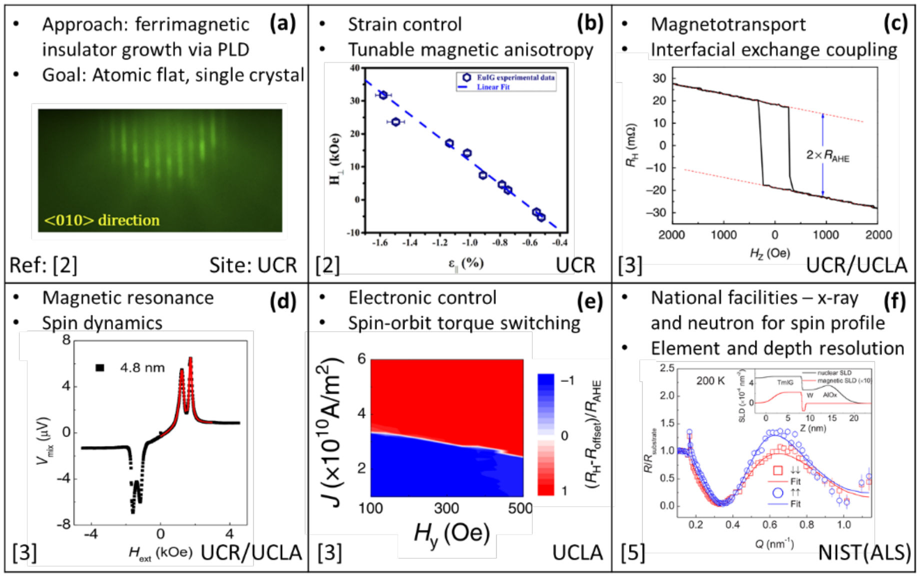
SESSION I: TUESDAY, JULY 30, 2019; 8:00 – 9:40 AM; LINCOLN 3&4

8:00 AM – Team Science Finalist

H-I-1: FERRIMAGNETIC INSULATOR FOR ULTRAFAST AND ULTRALOW-POWER SPINTRONIC DEVICES

[SHINES] Victor H. Ortiz[1], Qiming Shao[2], Mohammed Aldosary[1], Alexander Grutter[3], Junxue Li[1], Guoqiang Yu[2], Yawen Liu[1], Chi Tang[1], Kang L. Wang[2], and Jing Shi[1]
[1]University of California, Riverside; [2]University of California, Los Angeles; [3]NIST

We aim to study the mutual effects of ferrimagnetic insulator and heavy metal with strong spin-orbit coupling by combining the material growth and characterization strength at UCR and spin-orbit torque measurement strength at UCLA. We achieved high-quality rare earth iron garnet film growth and control of the perpendicular magnetic anisotropy (a desirable attribute for memory technology) by tuning the strain in the films (a)(b) [1][2]. We investigated interfacial exchange coupling by performing magnetotransport measurements (b) [1-5] and spin dynamics by using magnetic resonance (c) [3-4]. Extensive spin-orbit torque switching experiments reveal highly efficient switching of the ferrimagnetic garnet (e) in both ferromagnetic and antiferromagnetic regimes [3-4]. We also leveraged external collaborations with NIST and Advanced Light Source (ALS) to perform XMCD and neutron reflectometry experiments to resolve element- and depth-dependent spin profiles [5]. The close collaboration between UCR and UCLA allows us to gain rapid and deep understanding of the interplay between spin, magnon and electron at the atomic scale in the thin film systems, which is an objective of SHINES.



References: [1] C. Tang, et al., Phys. Rev. B, 94, 140403(R) (2016); [2] V. H. Ortiz, et al., APL Mater., 6, 121113 (2018); [3] Q. Shao, et al., Nat. Commun., 9, 3612 (2018); [4] J. Li, et al., Phys. Rev. B, 95, 241305(R) (2017); [5] Q. Shao, et al., Phys. Rev. B, 99, 104401 (2019).

Contributions: Víctor H. Ortiz and the UCR group grew and characterized magnetic garnet thin films. Qiming Shao and the UCLA group performed the current-induced switching measurements. Both groups contributed to the device fabrication and deposition of heavy metal layer, and to magnetotransport and magnetic resonance measurements.

8:20 AM – Team Science Finalist

H-I-2: SYNTHESIS, CHARACTERIZATION AND PREDICTIVE FIRST-PRINCIPLES CALCULATIONS

[M^{2}QM] Jie-Xiang Yu[1], Jonathan Marbey[2], Tuhin Ghosh[1], Ashlyn Hale[1], Dian-Teng Chen[1], Rainier Berkley[3], Hoaming Jin[1], Xiaochen Zhu[1], George Christou[1], Arthur F. Hebard[1], Talat Rahman[3], Stephen Hill[2], and Hai-Ping Cheng

[1]University of Florida, [2]Florida State University, [3]University of Central Florida

We report recent progresses on Mn-based single molecular magnets (SMMs). In particular, we investigated Mn_3 dimers and Mn_{84} molecules. High-frequency EPR measurements demonstrate coherent superposition of the quantum/spin states associated with a pair of covalently linked Mn_3 molecules. Via modifications, we can turn small SMMs (Mn_3, Mn_4) into robust supermolecular oligomers that can have FM or AFM couplings, and which may have applications in mutli-qubit devices. First-principles calculations confirmed the signs of exchange interactions. Furthermore, our calculations predict changes in the spin coupling as a function of applied pressure. For large SMMs (Mn_{70}, Mn_{84}), our goal is to study how large SMMs dope the graphene nano-structure and change its transport characteristics. Studies of these two limits, qubits and novel junctions for spintronic applications, are in line with the center mission: To deepen understanding and optimize control of electron-level physical processes to turn molecular magnets into quantum materials. We tune inter-molecule communication via magnetic interactions in clusters and solids and we design and perfect the underlying materials science for future computers and electronics.

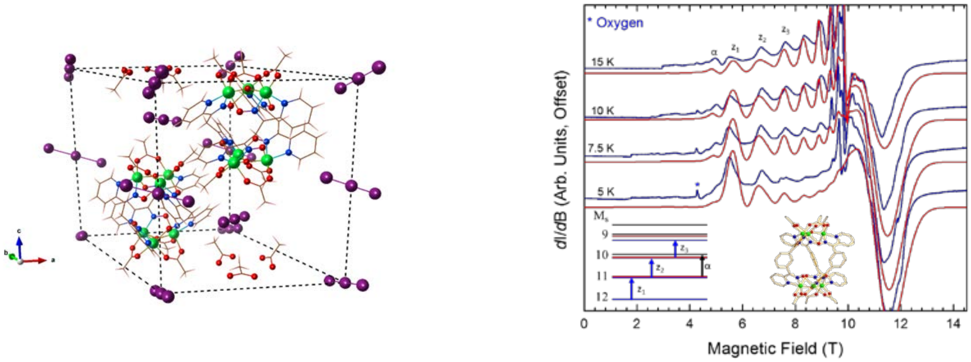


Figure 1. Left pannel: FM Mn_3-dimer in crystalline form; Right panel: EPR measurements.

Author Contributions: J.-X. Yu and H.-P. Cheng, Performed first-principles calculations and analysis of Mn3-dimers in gas phase and in bulk form; T. Ghosh and G. Christou, synthesized Mn_3 dimers; A. Hale and G. Christou synthesize Mn_n (n=70,84), D.-T. Chen and H.-P. Cheng performed first-principles calculations and analysis of Mn_{84}; R. Berkley and T. Rahman performed first-principles calculations of Mn_3-dimer; X.-C. Zhu H.-M. Jin and A. F. Hebard fabricated graphene nano-junction and transport measurements; J. Marbey and S. Hill performed EPR measurements.

8:40 AM

H-I-3: SPIN-HALL EFFECTS IN NOVEL MATERIALS

[Q-MEEN-C] Eric Fullerton[1]
[1]*University of California San Diego*

In order to develop functional magnetic neuromorphic systems, three main components are required: (i) neurons (computation), (ii) synapse (memory), and (iii) learning. Spin-torque magnetic oscillators can provide the neuron functionality but should operate with minimal power, while at the same time provide large signals. This requires a very efficient driving mechanism. Spin-orbit torques have unique advantages addressing these challenges, in that: (a) they are potentially more efficient than spin transfer torques for driving and manipulating oscillations; (b) they enable simple geometries of bilayer systems that enable integration of additional control mechanisms for manipulating magnetic properties; and (c) they enable the assembly of a large number of coupled-oscillators and may allow three-dimensional stacking. Spin-orbit coupling can efficiently generate magnetic torques from charge currents, which in turn has become key to novel applied spintronics devices. We will review recent Q-MEEN-C research on optimized quantum materials and interfacial phenomena (e.g. Au-Si heterostructure, ferrimagnetic CrPt3, FeRh, etc.) to generate high spin-orbit coupling and their integration into spin-torque magnetic oscillators. The experimental research combines non-local magneto-transport, spin-pumping and inverse spin Hall effects, and spin-torque ferromagnetic resonance measurements and compared to theory.

9:00 AM

H-I-4: THERMALLY DRIVEN MAGNON CONDENSATION IN YIG/PY NANOWIRES

[SHINES] B. Arkook[1], R. Rodriguez[1], C. Safranski[2], I. Krivorotov[2], T. Schneider[3], K. Lenz[3], J. Lindner[3], M. Z. Wu[4], I. Barsukov[1]
[1]*University of California, Riverside;* [2]*University of California, Irvine;* [3]*Helmholtz-Zentrum Dresden–Rossendorf;* [4]*Colorado State University*

Injection of a pure spin current into magnetic insulator modifies the chemical potential of magnons and can lead to intriguing phenomena such as long-range spin transport and magnon condensation. We study nanowires fabricated from a bilayer of a metallic ferromagnet and an insulating ferrimagnet. Via interlayer exchange coupling, pure spin current can be thermally transferred from one layer into another. The injected incoherent magnons transfer their angular momentum to the lowest-energy magnon state, thereby reducing its effective damping. Above critical thermal spin current, the magnon system undergoes a phase transition establishing a coherent lowest-energy state. This process corresponds to bosonic condensation of non-equilibrium magnons into a magnon condensate and manifests through microwave emission from the nanowire. The results demonstrate a route towards energy-efficient spintronics devices with sizable spin-charge conversion and advance our understanding of magnon thermodynamics in magnetic heterostructures.

9:20 AM

H-I-5: RECENT PROGRESS ON 3D AXION INSULATORS

[IQM] David Vanderbilt[1], N. Peter Armitage[2]
[1]Rutgers University, [2]Johns Hopkins University

Topological insulators are unique states of matter that – despite an insulating bulk – harbor topologically protected surface states. IQM is attempting to realize a related interacting magnetic state, the axion insulator. This is a theoretically proposed, but heretofore unrealized state of matter that is similar to a topological insulator in that both possess band inversion. However, axion insulators break time reversal symmetry and will exhibit a very large and intrinsic magnetoelectric response. For materials that preserve inversion, the magnetoelectric response is expected to be quantized. Such systems are 3D analogs of the 2D quantum anomalous Hall effect systems and should show a quantized Kerr rotation for the inversion symmetric case and a measurable (and large) dc magnetoelectric response for the inversion symmetry broken state. We have identified a very large class of promising potential materials through ab initio calculations and chemical synthesis considerations. This talk will present current progress in realizing this state of matter as well as related experiments on insulating bulk TI crystals.

SESSION II: TUESDAY, JULY 30, 2019; 11:00 – 12:20 PM; LINCOLN 3&4

11:00 AM

H-II-1: QUANTUM MATERIALS FOR ENERGY EFFICIENT NEUROMORPHIC COMPUTING AND FIRST IMPLEMENTATION OF NEURISTORS AND SYNAPTORS BASED ON CHARGE

[Q-MEEN-C] Javier del Valle[1], Ivan Schuller[1]
[1]University of California San Diego

The QMEENC EFRC is a highly collaborative effort dedicated to the development of energy efficient devices based on quantum materials that will form the basis for neuromorphic computing. This project started by developing two parallel approaches: one based on charge, using highly correlated oxides; and one based on spin, using spin torque oscillators. We are also developing hybrid concepts, which take advantage of the functional properties of both approaches.

In addition to the general description of the QMEENC approach, we will show how correlated oxides can be used to implement neuron and synapse functionalities. We will introduce our recent advances in understanding and controlling the insulator-to-metal transition in vanadium oxides, and how we have used the intrinsic thermal dynamics of these materials to implement an artificial neuron.

11:20 AM

H-II-2: PROGRAMMABLE QUANTUM MATERIALS

[Pro-QM] Ana Asenjo-Garcia[1], Dmitri N. Basov[1], Jiun Haw Chu[2], David Cobden[2], Cory R. Dean[1], Daniel R. Gamelin[2], James Hone[1], Michal Lipson[1], Andrew J. Millis[1], Abhay Pasupathy[1], P. James Schuck[1], Di Xiao[3], Xiaodong Xu, Xiaoyang Zhu[1]
[1]Columbia University, [2]University of Washington, [3]Carnegie Mellon University

The Mission of the Pro-QM Center is to discover, characterize and deploy new forms of quantum matter controllable by gating, magnetic proximity, light and nano-mechanical manipulation, effectively programming their quantum properties. Our team is on track towards fulfilling these ambitious goals. Recent significant accomplishments of the Pro-QM team include: the discovery of topological conducting channels in twisted van der Waals (vdW) heterostructures (*Science 2018*), the discovery of moire excitons in twisted transition metal dichalcogenides bilayers (*Nature 2019*), the first observation of pressure-controlled superconductivity in twisted bilayer graphene (*Science 2019*) and most recent discovery of an electrostatically tuned topological transition is a prototypical vdW semiconductors WSe_2 (*Nature 2019*).

11:40 AM

H-II-3: INTRODUCTION, WITH SELECTED HIGHLIGHTS, TO THE CENTER FOR NOVEL PATHWAYS TO QUANTUM COHERENCE IN MATERIALS

[NPQC] Joel E. Moore[1,2]
[1]Lawrence Berkeley National Laboratory; [2]University of California, Berkeley

This talk starts with an overview of the new NPQC EFRC (Class of 2018), which includes investigators from LBNL/Berkeley, ANL/Chicago, Columbia, and UCSB. The objective of the Center is to dramatically expand our control and understanding of coherence in solids by building on fundamental materials discoveries in recent years. The fundamental importance of the two-level system or qubit was recognized in the early days of quantum mechanics. To fully exploit the potential of quantum-based sensing, communication, and computation, we must find new pathways to protect and use quantum coherence in solid-state environments that are closer to ambient temperatures. Developing the power to manipulate coherence involving many two-level systems, in realistic solid-state environments, requires understanding materials whose basic properties emerge from coherence between spatial regions or from coherent transport at sample boundaries.

We present two initial highlights from the first two thrusts of NPQC. Work in Thrust 1 has clarified the microscopic origin of field and strain sensitivity of the nitrogen-vacancy defect in diamond, one of the most actively pursued quantum sensors. From Thrust 2 we report the observation of superconductivity in gated trilayer graphene, in which a moiré pattern is induced by a hexagonal boron nitride substrate. Results from Thrust 3 will appear in a separate talk by James Analytis.

12:00 PM

H-II-4: SPECTROSCOPIC STUDIES OF MOLECULAR MAGNETIC QUANTUM MATERIALS

[M^{2}QM] Stephen Hill[1,2], Samuel M. Greer[1,2], Johannes McKay[1], Tuhin Ghosh[3], George Christou[3], Kathryn M. Gramigna[4], Christine M. Thomas[4], Stergios Piligkos[5]
[1]National High Magnetic Field Laboratory; [2]Florida State University; [3]University of Florida;4[5]The Ohio State University; [5]University of Copenhagen

The use of magnetic molecules for the development of quantum technologies is attractive because it enables systematic synthetic control of quantum spin (qubit) states via molecular structure, and allows for functionalization of molecules in order to engineer interactions between them. The field has witnessed several important recent breakthroughs, including the demonstration of quantum entanglement between pairs of single-molecule magnets [1], and the implementation of a quantum algorithm in a single magnetic molecule [2]. However, important challenges lie ahead [3], particularly with regards to (i) combining molecular magnetic building blocks into supramolecular architectures that allow for non-trivial quantum logic operations, and (ii) developing the hardware needed to implement such operations with high-fidelity. These are some of the goals of the Center for Molecular Magnetic Quantum Materials (M^{2}QM). This talk will focus on the development of advanced electron spin resonance techniques that impact on both of these goals by enabling precise characterization of the quantum states (i.e. the spin Hamiltonians) of molecular spins and the sophisticated microwave pulse schemes for coherently manipulating them. The talk will also illustrate how these efforts impact synthetic and computational efforts within M^{2}QM.

SESSION III: TUESDAY, JULY 30, 2019; 1:45 – 3:45 PM; LINCOLN 3&4

1:45 PM

H-III-1: PREDICTING OPTICALLY EXCITED PHENOMENA IN QUANTUM MATERIALS

[PTL] Prineha Narang[1], Nicholas Rivera[1], Johannes Flick[1], Christopher J. Ciccarino[1], Fariah Hayee[2], Christina A.C. Garcia[2], Jennifer Dionne[2]
[1]Harvard University; [2]Stanford University

The physics of quantum materials is rich with spectacular excited-state and non-equilibrium effects, but many of these phenomena remain poorly understood and consequently technologically unexplored. Therefore, we focus on understanding how quantum-engineered materials behave, particularly away from equilibrium, and how we can harness these effects to achieve photonic operations at thermodynamic limits. I will present this approach, from a theoretical and computational standpoint. Electron-photon, electron-electron as well as electron-phonon dynamics and far-from-equilibrium transport are critical to describe ultrafast and excited-state interactions in materials. *Ab initio* descriptions of phonons are essential to capture both excitation and loss (decoherence) mechanisms, and are challenging to incorporate directly in calculations due to a large mismatch in energy scales between electrons and phonons. I will discuss a new formalism at the intersection of cavity quantum-electrodynamics and electronic structure methods, quantum-electrodynamical density functional theory (QEDFT), to treat electrons, photons and phonons on the same quantized footing. I will demonstrate how these *ab initio* techniques can guide the search for relevant quantum properties in 2D and 3D materials, including new quantum emitters. In the second part of the talk, I will show recent results using newly developed theoretical methods to evaluate the linear and nonlinear optical properties of low dimensional and heterostructured quantum materials.

2:05 PM

H-III-2: SCAN AND THE CHALLENGE OF CUPRATES AND OTHER COMPLEX MATERIALS

[CCM] Arun Bansil[1], Yubo Zhang[2], Christopher Lane[1], James W. Furness[2], Bernardo Barbiellini[1,3], Iona G Buda[1], Robert S. Markiewicz[1]
[1]Northeastern University, [2]Tulane University, [3]Lappeenranta University of Technology

I will discuss how advanced density functionals are enabling new insights into the electronic structure, phase diagrams and magnetism of a wide variety of materials that have until now been considered to be so strongly correlated as to lie outside the scope of first-principles treatment. A spectacular example is provided by the cuprate high-Tc superconductors in which the density functional theory fails to correctly predict the half-filled parent compounds to be insulators. In sharp contrast, however, the recently constructed SCAN functional [1] not only reproduces the insulating character and magnetism of the half-filled cuprates, but also captures the transition to the metallic state with doping without invoking any free parameters such as the Hubbard U [2,3]. I will also comment on the opportunities for a new generation of predictive modeling in complex materials more generally, including the magnetic structure of α-Mn and cathode battery material $Li_xMn_2O_4$ [4], and the topological phases of quantum matter which are drawing intense current interest [5]. Work supported by the U.S. Department of Energy.

[1] J. Sun, A. Ruzsinszky, J. P. Perdew, *Phys. Rev. Lett.* 115, 036402 (2015). [2] J. W. Furness *et al.*, *Nature Communications Physics* 1, 11 (2018). [3] C. Lane *et al.*, *Phys. Rev. B.* 98, 125140 (2018); Y. Zhang *et al.*, arXiv:1809.08457 (2018). [4] A. Pulkkinen *et al.*, arXiv:1904.10291 (2019). [5] A. Bansil, H. Lin and T. Das, *Reviews of Modern Physics* 88, 021004 (2016).

2:25 PM

H-III-3: COMPUTATIONAL SEARCH FOR MAGNETIC WEYL SEMIMETALS IN EU COMPOUNDS

[CATS] Lin-Lin Wang[1], Na Hyun Jo[2], Brinda Kuthanazhi[2], Yun Wu[2], Ashvin Vishwanath[3], Peter Orth[1,2], Robert J. McQueeney[1,2], Adam Kaminski[1,2], and Paul C. Canfield[1,2]
[1]Ames Laboratory; [2]Iowa State University; [3]Harvard University

Weyl fermions as monopoles of Berry curvature in condensed matter systems are of great interest for both fundamental science and future technology. Weyl points (WPs) in electronic band structure can be realized in compounds with broken inversion and/or time-reversal symmetry. Here we have used high throughput band structure calculations based on density functional theory to search for magnetic Weyl semimetals in Eu compounds. We find that the emergence of WPs depends on the specific magnetic ordering structure. Among several candidates for magnetic Weyl semimetals based on Eu compounds, we show that inducing ferromagnetism in $EuCd_2As_2$ can generate a single pair of WPs caused by the splitting of a single pair of antiferromagnetic Dirac points (DPs). Analysis with a low-energy effective Hamiltonian shows that a single pair of WPs is obtained in $EuCd_2As_2$ because the DPs are very close to the zone center and the ferromagnetic exchange splitting is large enough to push one pair of WPs to merge and annihilate at Γ, while the other pair survives. The interplay of magnetism, crystalline symmetry, and topology provides a mechanism whereby magnetism can be used to control topological states.

2:45 PM

H-III-4: HALF QUANTUM FLUX IN UNCONVENTIONAL SUPERCONDUCTOR β-BI_2PD

[SHINES] Yufan Li and Chia-Ling Chien
Johns Hopkins University

Flux quantization is a distinct hallmark of superconductors. In the classic Little-Parks experiments, the magnetic flux through a superconducting ring made of a singlet superconducting, such as Nb, is without exception always $n\Phi_0$, where Φ_0 = hc/2e is the flux quantum and n = 0, 1, 2, 3… However, in the case of spin triplet superconductor, theory of Geshkenbein, Larkin and Barone (GLB) predicts that one may observe half quantum fluxoid of $(n + ½)\Phi_0$. Recently, we have observed the elusive half quantum flux in thin films of polycrystalline β-Bi_2Pd with (001) texture. We will also discuss the strong indication that β-Bi_2Pd is a spin-triplet superconductor and the potential applications of half-quantum fluxoid in quantum computing.

3:05 PM

H-III-5: TOWARD MONOPOLE SUPERCONDUCTIVITY

[IQM] Yi Li, Tyrel M. McQueen
Johns Hopkins University

IQM is exploring a new topological class of superconductivity which exhibits monopole harmonic symmetry. This so-called monopole superconductivity can be realized in doped Weyl semimetal materials. Generally, when two Fermi surfaces carry different Chern numbers, Cooper pairing between these two Fermi surfaces exhibits a non-trivial Berry phase inherited from band structure topology. The corresponding superconducting gap function exhibits emergent Weyl nodes at zero energy. In contrast to other forms of superconductivity, the total vorticity of gap nodes in momentum space is determined by the monopole charge of the pair Berry phase and is independent of the specific pairing mechanism. Signatures of monopole harmonic superconductivity are proposed and ongoing attempts to realize it in thin film and bulk materials are discussed.

3:25 PM

H-III-6: PROBING ULTRAFAST PHOTOCURRENTS IN THE WEYL SEMIMETAL TAAS USING THZ EMISSION SPECTROSCOPY

[CATS] N. Sirica,[1] R.I. Tobey,[1,2] L.X. Zhao,[3] G.F. Chen,[3] B. Xu,[3] R. Yang,[3] B. Shen,[4] P. Bowlan,[1] S.A. Trugman,[1] P. Orth[6,7], J.-X. Zhu,[1] Y.M. Dai,[1,5] A.K. Azad,[1] N. Ni,[4] X.G. Qiu,[3] A.J. Taylor,[1] R.P. Prasankumar[1], D.A. Yarotski[1]
[1]Los Alamos National Laboratory; [2]University of Groningen; [3]Chinese Academy of Science; [4]University of California-Los Angeles; [5]Nanjing University; [6]Ames Laboratory; [7]Iowa State University

We investigate polarization-dependent ultrafast photocurrents in the Weyl semimetal TaAs using terahertz (THz) emission spectroscopy. Our results reveal that highly directional, transient photocurrents are generated along the non-centrosymmetric c-axis regardless of incident light polarization, while helicity-dependent photocurrents are excited within the ab-plane. This is consistent with static photocurrent experiments, and provides additional insight into their microscopic origin by way of the dynamical information gained from the emitted THz waveform. THz emission spectroscopy is thus a powerful, contact-free approach for distinguishing between injection and shift photocurrents by unraveling the polarization dependence, directionality, and intrinsic timescales that underlie their generation and decay.

I. QUANTUM MATERIALS II

SESSION III: TUESDAY, JULY 30, 2019; 1:45 – 3:45 PM; LINCOLN 2

1:45 PM

I-III-1: CONTROLLING OPTICAL, ELECTRICAL, AND SPIN PROPERTIES WITHIN LEAD-HALIDE INSPIRED HYBRID SEMICONDUCTORS

[CHOISE] Matthew C. Beard[1], Haipeng Lu[1], Xihan Chen[1], Wei You[2], Z. Valy Vardeny[3], Jingying Wang[3], Kai Zhu[1], Joseph J. Berry[1], Xiaolin Zhu[4],Yong Yan[4]
[1]National Renewable Energy Laboratory, [2]University of North Carolina, [3]University of Utah, [4]San Diego State University

Hybrid organic/inorganic semiconductors (HOIS) offer tremendous opportunities to control fundamental properties that underpin energy technologies. While currently there are enormous worldwide efforts exploring, exploiting and improving a narrow class of HOIS (lead-halide perovskites, such as methylammonium lead iodide ($MAPbI_3$)), primarily for photovoltaic (PV) applications, an opportunity exists to transcend this initial focus on PV research and seek deeper understanding and control of their fundamental properties. HOIS exhibit properties that are not solely a juxtaposition of the inorganic and organic sub-units, but are instead truly emergent phenomena, with the concomitant ability to control and design new properties by judicious *choice* of inorganic and organic components. We have studied the carrier and spin-dynamics in single crystals of 2D Ruddlesden-Popper perovskites $PEA_2PbI_4{\cdot}(MAPbI_3)_{n-1}$ (PEA, phenethylammonium; MA, methylammonium; n = 1, 2, 3, 4). Layer thickness dependent charge carrier recombination rates are observed with the fastest rates for n = 1 and the slowest rates for n = 2. Room temperature spin-coherence times also show a nonmonotonic layer thickness dependence with an increasing spin-coherence lifetime with increasing layer thickness from n = 1 to 4, followed by a decrease in lifetime. We are also interested in how organic ligands impact the resulting properties of perovskite based nanocrystals. We show that photon energy can transfer from the NCs to the singlet states of pentacene bound ligands. The singlet states of the pentacene ligands undergo singlet fission yielding long-lived molecular triplet states. Perovskite NCs can act as efficient photocatalyst in organic solvents to promote carbon-carbon bond formation.

2:05 PM

I-III-2: THE LIGHT YEARS: COMBINED OPTICAL AND ENVIRONMENTAL ELECTRON MICROSCOPY TO VISUALIZE PLASMONIC PROCESSES WITH ATOMIC-SCALE RESOLUTION

[PTL] Jennifer A. Dionne[1], Fariah Hayee[1], Leo Yu[1], Christopher Ciccarino[2], Prineha Narang[2], Tony Heinz[1]
[1]Stanford University; [2]Harvard University

Pearl Jam's hit, "The Light Years," declares "We were but stones, light made us stars." Bringing light to the transmission electron microscope (TEM) promises to transform our understanding of materials, enabling both direct observation of light-mediated processes and detection of optical emission with atomic scale resolution. To help achieve this goal, we are developing capabilities for concurrent optical and electron microscopy within an environmental TEM. This presentation will describe our efforts to visualize a variety of photonic processes *in situ* with nanometer-to-atomic scale resolution, including i) plasmon-driven chemical transformations in nanoparticles and ii) quantum light emission from two-dimensional materials. First, we study the photocatalytic dehydrogenation of Au-Pd systems, in which the Au acts as a plasmonic light absorber and Pd serves as the catalyst. We find that plasmons modify the rate of distinct reaction steps differently, increasing the overall rate more than ten-fold. Plasmons also open a new reaction pathway that is not observed without illumination, laying a foundation for site-selective and product-specific photocatalysts. Secondly, we use scanning transmission electron microscopy and cathodoluminescence spectroscopy to investigate color centers in two-dimensional hexagonal boron nitride, a wide bandgap material capable of room-temperature, high-brightness visible quantum emission. We find that sharp, single-photon emission peaks are usually associated with regions of multiple fork dislocations. Additionally, local strain maps indicate that strain is not responsible for the observed broad spectral range, though it can enable spectral tuning of particular emitters. Combined, our results highlight the sensitivity of photochemistry and quantum emission to the surrounding crystallography and provide a foundation for atomic-scale optical characterization.

2:25 PM

I-III-3: TUNABLE INTERNAL QUANTUM WELL ALIGNMENT IN RATIONALLY DESIGNED OLIGOMER-BASED PEROVSKITES

[CHOISE] Wiley A. Dunlap-Shohl1, E. Tomas Barraza1, Andrew Barrette,[2] Seyitliyev Dovletgeldi,[2] Gamze Findik,[2] David J. Dirkes,[1] Chi Liu,[1] Manoj K. Jana,[1] Volker Blum,[1] Wei You,[1] Kenan Gundogdu,[2] Adrienne D. Stiff-Roberts,[1] David B. Mitzi [1]
[1]Duke University, [2]North Carolina State University

Hybrid organic/inorganic semiconductors (HOIS) offer unprecedented opportunity to control fundamental properties related to spin, charge and light. One of the goals of the Center for Hybrid Organic-Inorganic Semiconductors for Energy (CHOISE) is to leverage the distinct attributes of organic and inorganic chemistry, as well as the power of computational sciences and synthetic chemistry, to rationally design/synthesize hybrid perovskites with unique physical phenomena. As one example, hybrid perovskites incorporating conjugated oligothiophene cations have recently been demonstrated and tailored to enable a wide range of quantum well behavior. Selecting a large (small) HOMO-LUMO separation oligothiophene cation and a small (large) band gap lead iodide (chloride) framework, we demonstrate type I quantum well behavior with the lowest energy state for both electrons and holes in the inorganic (organic) layer of the hybrid structure, along with associated luminescence from these components. By contrast, with appropriately selected organic and inorganic components (as guided by DFT theory), type II quantum well structures can also be prepared. Synergistic effects have also been observed for the type II quantum wells, in which excitons transfer from singlet to triplet states, in systems containing organics for which intersystem crossing generally is not allowed. The Resonant infrared matrix-assisted pulsed laser evaporation (RIR-MAPLE) approach will also be discussed as a versatile and uniquely well-suited means of depositing these complex hybrids, since this approach enables gentle and well-controlled deposition of the organic cations, without the need for a common solvent for the organic and inorganic components.

2:45 PM

I-III-4: SWITCHING 2D MAGNETIC STATES VIA PRESSURE TUNING OF LAYER STACKING

[Pro-QM] Tiancheng Song[1], Zaiyao Fei[1], Matthew Yankowitz[2], Zhong Lin[1], Qianni Jiang[1], Bosong Sun[1], Takashi Taniguchi[3], Kenji Watanabe[3], Michael A. McGuire[4], David Graf[5], Ting Cao[1,6], Jiun-Haw Chu[1], David H. Cobden[1], Cory R. Dean[2], Di Xiao[7] & Xiaodong Xu[1]

[1]University of Washington; [2]Columbia University; [3]National Institute for Materials Science, Japan; [4]Oak Ridge National Laboratory; [5]National High Magnetic Field Laboratory; [6]Stanford University; [7]Carnegie Mellon University

The physical properties of two-dimensional van der Waals (2D vdW) crystals depend sensitively on the interlayer coupling, which is intimately connected to the stacking arrangement and the interlayer spacing. For example, simply changing the twist angle between graphene layers can induce a variety of correlated electronic phases, which can be controlled further in a continuous manner by applying hydrostatic pressure to decrease the interlayer spacing. In the recently discovered 2D magnets, theory suggests that the interlayer exchange coupling strongly depends on layer separation, while the stacking arrangement can even change the sign of the magnetic exchange, thus drastically modifying the ground state. In this talk, we will present our recent demonstration of pressure tuning of magnetic order in the 2D magnet CrI_3. We probe the magnetic states using tunneling and scanning magnetic circular dichroism microscopy measurements. We find that the interlayer magnetic coupling can be more than doubled by hydrostatic pressure. In bilayer CrI_3, pressure induces a transition from layered antiferromagnetic to ferromagnetic phases. In trilayer CrI_3, pressure can create coexisting domains of three phases, one ferromagnetic and two distinct antiferromagnetic phases. The observed changes in magnetic order can be explained by changes in the stacking arrangement. Such coupling between stacking order and magnetism provides ample opportunities for programable magnetic phases and functionalities.

3:05 PM

I-III-5: FRUSTRATION, DISORDER AND COHERENCE IN A NEW CLASS OF ANTIFERROMAGNETIC SPINTRONICS

[NPQC] James G. Analytis[1,2], Eran Maniv[1], Frank Ruta[3], Charlotte Herbig[2], Michael F. Crommie[1,2], Joseph Orenstein[1,2], Joel E. Moore[1,2], Dmitri N. Basov[3]

[1]Lawrence Berkeley National Laboratory; [2]University of California, Berkeley; [3]Columbia University

We report the discovery of a new class of layered materials with electronically switchable magnetic states. A combination of frustration, disorder and symmetry conspire together to direct electrically switchable resistance states with ultra-low power characteristics. We investigate the novel properties of these materials, combining thermodynamic, transport and optical measurements.

3:25 PM

I-III-6: MAGNETOELECTRIC COUPLING IN MOLECULAR MATERIALS

[M^2QM] Vivien Zapf[1*], Vibe Jakobsen[2], Shalinee Chikara[1], Brian Scott[1], Nathan Smythe[1], Emiel Dobbelaar[3], Elizabeth Krenkel[4], Jim Eckert[4], Jie Gu[5], Jie-Xiang Yu[5], Dian-Teng Chen[5], Hai-Ping Cheng[5], Xiaoguang Zhang[5], and Grace Morgan[2]
[1]Los Alamos National Lab; [2]University College Dublin; [3]University of Kaiserslauten; [4]Harvey Mudd College; [5]University of Florida

We are studying molecule-based materials with a view towards applications in traditional and quantum computing. To this end we are exploring coupling mechanisms between magnetic properties and electric states such as electric polarization, conductivity, dielectric constant, etc. With such coupling in place the magnetic state can be interrogated and controlled by electric signals. In particular, coupling between ferroelectricity and magnetism in insulators eliminates electric currents and allows low-power sensing and switching with voltages.

The scientific challenges to creating such coupling are intriguing and varied. We investigate molecules showing spin crossovers, single molecule magnet behavior and other molecule-based systems with antiferromagnetic order. In particular, I will show new results on spin crossover materials that can be switched with record low magnetic fields and couple to the structure and very large electric polarization changes. This is a different route to multiferroic-like behavior. I will present a collaboration among synthesis, structure, magnoelectric coupling measurements, mean field and ab-initio theory.

J. SEPARATION SCIENCE

SESSION I: TUESDAY, JULY 30, 2019; 8:00 – 9:40 AM; THURGOOD MARSHALL NORTH

8:00 AM

J-I-1: COOPERATIVE ADSORPTION AND GAS SEPARATIONS IN METAL–ORGANIC FRAMEWORKS

[CGS] Jeffrey R. Long[1,2]
[1]University of California, Berkeley; [2]Lawrence Berkeley National Laboratory (LBNL)

The chemical and structural versatility accessible with metal–organic frameworks (MOFs) offers the possibility of designing powerful adsorbents that selectively adsorb gas molecules via novel and highly efficient mechanisms. The CGS has developed the first cooperative adsorbents, $(\text{diamine})_2\text{–Mg}_2(\text{dobpdc})$ (dobpdc^{4-} = 4,4′-dioxido-3,3′-biphenyldicarboxylate), which selectively adsorb CO_2 via an unprecedented mechanism wherein initial CO_2 insertion into the metal–amine bonds triggers cascade adsorption at neighboring sites. Notably, these materials can capture CO_2 using much smaller temperature or pressure swings than are required for traditional cooperative adsorbents or state-of-the-art amine-based solvents; exhibit high CO_2 capacities in the presence of water; and are highly versatile for a range of applications, including for the removal of CO_2 from air, flue gases, natural gas, and biogas. The Center has further extended this cooperative mechanism to the selective, reversible capture of CS_2, and is investigating its applicability to other acid gases. The CGS is also applying these insights toward the development of cooperative adsorbents for other toxic and commodity gases. For example, we have shown that a framework with chains of high-spin iron(II) sites (Fe_2Cl_2(bbta); H_2bbta = 1*H*,5*H*-benzo(1,2-*d*:4,5-*d*′)bistriazole) can cooperatively adsorb CO via a spin transition mechanism. This growing class of cooperative adsorbents may enable drastic reductions in the costs associated with key industrial gas separations.

8:20 AM

J-I-2: ACID-GAS INDUCED DEFECTS IN ZEOLITIC IMIDAZOLATE FRAMEWORKS

[UNCAGE-ME] James Collins[3], Kai Cui[1], Akshita Dutta[3], Chu Han[2], Rebecca Han[2], Nina Tymińska[1], Chenyang Zhang[1], Guanghui Zhu[2], Ryan P. Lively[2], David S. Sholl[2], Sergey Vasenkov[3], J. R. Schmidt[1]
[1]University of Wisconsin – Madison; [2]Georgia Institute of Technology; [3]University of Florida

Metal-organic frameworks (MOFs) have attracted considerable attention for their diverse applications ranging from gas adsorption to catalysis. Nonetheless, the long-term stability of MOF materials has received significantly less scrutiny, particularly under "working" conditions that may involve high temperatures and exposure to water and/or acid gases. This talk will discuss recent computational and experimental work that has probed the formation of point defects in zeolitic imidazolate frameworks (ZIFs) under exposure to various acid gases and also examine the energetics and pathways for the subsequent propagation of those defects. In addition, recent quantum chemical "embedding" approaches will be discussed that allow for the calculation of defect formation energies in MOFs with unprecedented accuracy.

8:40 AM

J-I-3: THERMODYNAMICS AND ELECTRONIC PROPERTIES OF HETEROMETALLIC MULTINUCLEAR ACTINIDE-MOFS

[CWHM] Natalia Shustova[1] Otega Ejegbavwo[1], Chuck Jr. Henager[2], Simon Phillpot[3]
[1]University of South Carolina, [2]Pacific Northwest National Laboratory, [3]University of Florida

The stability of actinide-containing architectures and their chemical interactions with the environment have been increasingly studied over the past decades because of their significance for nuclear waste sequestration. Due to their modularity, structural versatility, high porosity, and high tunability, metal-organic frameworks (MOFs) have been utilized as a platform for nuclear waste forms and actinide immobilization, resulting in development of materials with a high actinide content and possessing minimal structural density. However, the field of actinide-based MOFs, unlike the non-actinide-containing counterpart, suffers from the fact that fundamental properties including thermodynamics, electronic, and detailed photophysical have not been investigated. In this talk, the first thermodynamic studies performed for actinide-based MOFs, including several examples containing common organic linkers, will be discussed. In addition, the first example of heterometallic multinuclear actinide-MOF nodes having a coordinated transition metal and the first electronic structure studies determined using density of states and conductivity measurements will be presented. Furthermore, we will demonstrate the established dependence of actinide-MOF stability on the nature of linker connectivity to its secondary building unit.

9:00 AM

J-I-4: HIGH PERFORMANCE MEMBRANES MADE BY LIGAND-INDUCED PERMSELECTIVATION (LIPS)

[CGS] Michael Tsapatsis[1,2]
[1]University of Minnesota; [2]Johns Hopkins University

Zeolitic imidazolate frameworks (ZIFs) are molecular sieves offering exciting opportunities for membrane- and adsorption-based gas separations. We recently developed an all-vapor-phase ligand induced permselectivation (LIPS) method for the fabrication of ZIF nanocomposite membranes with unprecedented high performance for propylene/propane separation (*Science* **2018**, *361*, 1008-1011). The LIPS method consists of a combination of atomic layer deposition of a dense oxide inside the mesopores of a porous support followed by transformation of the dense oxide deposit to ZIF by exposure to sublimated vapors of an imidazolate ligand. It enables the formation of thin (ca. 100 nm) nanocomposite films consisting of ZIF deposited inside pores with diameters smaller than 10 nm. The performance of this confined ZIF deposit is surprisingly superior to that of conventional ZIF membranes consisting of unconfined polycrystalline films deposited mostly on the external surface of porous supports. Specifically, the later exhibit loss of selectivity at industrially relevant high pressures (ca. >5 bar). However, for the confined ZIF membranes made by the LIPS method, the mixture separation factor remained unchanged (ca. 70) as the feed pressure increased from 1 to 7 atm and as the propylene fraction in the 7 atm feed was varied from 10% to 90%.

9:20 AM
Withdrawn

K. SOLAR ENERGY

SESSION I: TUESDAY, JULY 30, 2019; 8:00 – 9:40 AM; LINCOLN 2

8:00 AM – Team Science Finalist

K-I-1: TRANSPARENT CONDUCTING OXIDES AS HIGHLY VERSATILE DYE-SENSITIZED PHOTOELECTRODES

[AMPED] Rachel E. Bangle[1], Jenny Schneider[1], Renato N. Sampaio[2], Ludovic Troian-Gautier[1] and Gerald J. Meyer[1]
[1]UNC Chapel Hill; [2]Brookhaven National Laboratory

Transparent conductive oxides (TCOs) are commercially available materials used for a variety of opto-electronic applications. In recent AMPED research we have found that these materials, when cast as mesoporous thin films of TCO nanocrystallites, are versatile photoelectrode materials with some distinct advantages over semi-conducting oxides. The high doping level of TCOs such as In_2O_3:Sn (ITO) ($N_D > 10^{20}$ cm^{-3}) exhibit metallic properties that include high electron mobility and conduct-ivity while retaining high transparency in the visible region for dye-sensitized catalysis applications.

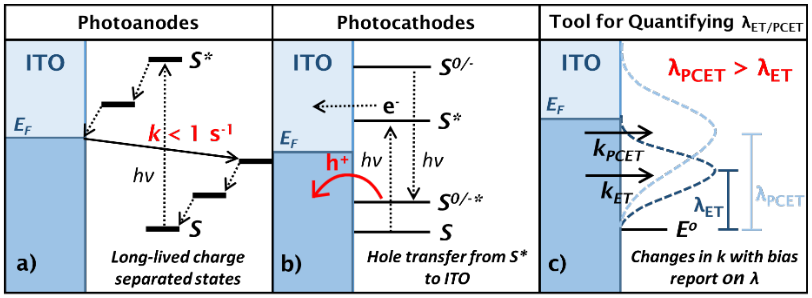


Figure 1: TCOs serve as a (a) photoanode sensitized with a molecular assembly built for sequential electron transfer, (b) photocathode undergoing hole transfer with a sensitizer, and (c) tool for quantifying λ by monitoring changes in rate with applied bias.

We have recently shown that mesoporous ITO electrodes can support long-lived charge separation after dye-sensitized electron transfer. Remarkably the states live for almost a second, and recombination occurs with first-order kinetics (Fig. 1a). The key to success was to spatially position the molecular sensitizer (*S*) distant from the ITO nanocrystalline with an intervening electron acceptor. In unpublished work, we have found that closely related long-lived states with a molecular catalyst are indeed capable of driving multi-electron transfer water oxidation for water splitting applications.

Furthermore, owing to the high concentration of TCO electrons, reductive quenching of sensitizer excited states (*S**), also called hole transfer, has been shown to be operative (Fig. 1b). The acceptor states of ITO overlap with the *S** acceptor levels ($S^{o/-*}$), allowing hole transfer from the sensitizer to ITO. In sharp contrast, the direction for electron transfer was reversed in a semiconducting material such as TiO_2, which exclusively quenches by oxidative electron transfer from *S** to the oxide. This novel photocathodic reactivity of TCOs is discussed in terms of tandem dye-sensitized solar cell applications.

In addition, dye-sensitized TCOs have been successfully applied as a tool to experimentally quantify the reorganization energy for electron transfer λ_{ET} and proton-coupled electron transfer λ_{PCET} (Fig. 1c). The approach required only a TCO, a means to photo-initiate the ET/PCET reaction, and a method to monitor the kinetic rate constant as a function of applied potential. Herewith, the metallic character of ITO allowed the potentiostatic control of the Fermi level (E_F) and thus of the reaction free energy change over a 1 eV range. The reduction of a ruthenium-based water oxidation catalyst from Ru^{III}-OH to Ru^{II}-OH_2 required 0.4 eV higher reorganization energy than did electron transfer without proton involvement, Ru^{III}-OH_2 to Ru^{II}-OH_2. Hence, this study provides quantitative data for parameters controlling interfacial charge transfer processes, a key variable in photoelectrosynthetic cells.

Contributions: REB quantified the kinetics and yields of light-driven hole transfer reactions at dye-ITO interfaces. JS applied Marcus-Gerischer theory to bias dependent kinetic data to extract reorganization energies for PCET reactions that occur with water oxidation catalysts. RNS and LT-G realized long-lived charge separation at ITO interfaces that are competent for water oxidation. GJM directed this research.

8:20 AM

K-I-2: SOFT MATTER AND HYBRID SOLAR CELL INTERFACE SCIENCE AND ENGINEERING

[LEAP] Tobin J. Marks[1,2], R.P.H. Chang[1], Lin X. Chen[1,2], Mark C. Hersam[1], Mercouri Kanatzidis[1], George C. Schatz[1], Michael R. Wasielewski[1]
[1]Northwestern University, [2]Argonne National Lab

Molecularly tailoring interfaces with atomistic precision offers an effective and informative means to selectively modulate charge generation, charge transport, molecular/macromolecular self-assembly, charge recombination, and exciton dynamics at hard matter-hard matter, hard matter-soft matter and soft matter-soft matter interfaces. Such interfaces can act as "filters" to selectively extract "correct charges" while blocking "incorrect charges" at the electrode-active layer and active layer-active layer interfaces in almost all types of solar cells. Such interface engineering can also suppress carrier-trapping defects at interfaces and stabilize such interfaces against physical/thermal de-cohesion and the ingress of oxidants. For soft matter-soft matter interfaces, interfacial tailoring also facilitates exciton scission and photocurrent generation. In this presentation, challenges and opportunities in solar cell interface science are illustrated for five interrelated challenge areas: 1) modulating charge transport across hard matter-soft matter interfaces in bulk heterojunction and perovskite solar cells, 2) controlling charge transport by specific active layer atomistic/microstructural organization within cell active layers and on electrodes, 3) controlling exciton dynamics and carrier generation at active layer donor-acceptor interfaces, 4) extracting maximum performance from non-fullerene acceptors, 5) enhancing solar cell durability It will be seen that rational interface design along with optimized and compatibilized donor-acceptor structures, guided by theoretical/computational analysis and spectroscopy over broad length and time scales, affords exceptional fill factors, power conversion efficiencies, lowers energy loss, and enhances solar cell durability. The symbiosis of green materials creation, computational modeling and simulation, materials characterization, and device fabrication and evaluation, are central to progress in this area.

8:40 AM

K-I-3: CONDUCTIVE OXIDES AS PHOTOELECTRODES THAT SUPPORT LONG-LIVED CHARGE-SEPARATION AND WATER OXIDATION CATALYSIS

[AMPED] Gerald J. Meyer
University of North Carolina at Chapel Hill

The development of oxide materials for dye-sensitized catalysis represents an important thrust in the Alliance for Molecular PhotoElectrode Design (AMPED), with an emphasis on establishing design principles for the photoelectrochemical reduction of CO_2 to fuels and the oxidation of water to dioxygen. This presentation introduces *conductive* electrodes as an alternative to standard semiconductor materials that have historically dominated the photoelectrochemical literature. Ongoing AMPED EFRC research has now shown that through purposeful spatial arrangement of dyes with redox active molecules on conductive tin-doped indium oxide (ITO) it is possible to realize photoelectrodes that effectively harvest sunlight and efficiently store solar energy for time periods that approach one second. Further, sustained

solar water oxidation was achieved by inclusion of a molecular water oxidation catalyst remote to the sensitized ITO electrode. The implications of these findings for solar fuel production will be presented.

9:00 AM

K-I-4: MEDIATED ELECTROLYSIS APPROACHES TO ENERGY CONVERSION

[CME] Yuliya Preger,[1] Sourav Biswas,[1] James B. Gerken,[1] Colin W. Anson,[1] Mathew R. Johnson,[1] Shannon S. Stahl,[1] Thatcher W. Root[1]
[1]*University of Wisconsin–Madison*

Dissolved molecular redox mediators provide an effective means to transport electrons (and protons) between an electrode and catalysts that are not in direct physical contact with an electrode. Effective implementation of this strategy requires the design and synthesis of suitable electron-proton-transfer mediators, development of new catalysts, and integration of these components in an operational system. The initial implementation of this concept was achieved with a novel tetra-substituted quinone mediator that exhibits excellent stability under strongly acidic conditions. Use of this mediator supports electrochemical reduction of O_2 at an off-electrode heterogeneous cobalt catalyst contained within a packed-bed reactor. Efficient oxidation of the hydroquinone by O_2 in the reactor provides the basis for mediator regeneration, and an integrated ‘‘flow-cathode’’ fuel cell system that supports high power densities. These results establish the combination of organic mediators with off-electrode heterogeneous catalysts as a versatile platform for development of new electrode-driven chemical redox transformations. Subsequent studies have begun probing the fundamental relationship between on-electrode and off-electrode catalytic performance

9:20 AM

K-I-5: ACID COMPATIBLE HALIDE PEROVSKITE PHOTOCATHODES: SOLAR-ASSISTED HYDROGEN PRODUCTION ENABLED BY ATOMIC LAYER DEPOSITION

[LEAP] In Soo Kim[1], Dana H. Cao[1], Jonathan D. Emery[2], Omar K. Farha[2], Joseph T. Hupp[2], Michael J. Pellin[1], Mercouri G. Kanatzidis[2], Alex B. F. Martinson[1]
[1]*Argonne National Laboratory;* [2]*Northwestern University*

Although solution-processable halide perovskite semiconductors exhibit optoelectronic performance comparable to the best photoabsorbers for solar fuel production, halide perovskites rapidly decompose in the presence of water or even humid air. We show that a hybrid electron transport layer, a $PC_{61}BM$ + TiO_2 film (18–40 nm thickness) grown over the sensitive absorber by atomic layer deposition, enables photoassisted proton reduction without further encapsulation. These semitransparent photocathodes, when paired with a Pt catalyst, display continuous reduction of H^+ to H_2 for hours under illumination, even while in direct contact with a strongly acidic aqueous electrolyte (0.5 M H_2SO_4). Under 0.5 Sun illumination, a photocurrent density of >10 mA cm^{-2} is observed, and a photovoltage of 0.68 V assists proton reduction, consistent with a structurally related photovoltaic (PV) device. Submersible halide perovskite photoelectrodes point the way to more efficient photo-assisted overall water splitting and other solar fuel generation using solution-processed semiconductors with tunable band gaps. The work lays the foundation for integration of this design into tandem photoelectrochemical (PEC) cells for overall solar-driven water splitting systems. We expect this approach to be directly applicable to other hybrid semiconductors as well as organic photoabsorbers for the PEC production of solar fuels.

L. SUBSURFACE SCIENCE

SESSION II: TUESDAY, JULY 30, 2019; 11:00 – 12:20 PM; LINCOLN 2

11:00 AM

L-II-1: GEO-ARCHITECTURED MATERIAL SYNTHESIS, CHARACTERIZATION AND MODELING

[MUSE] Hassnain Asgar[1], Michael Bartl[2], Hyeyoung Cho[2], Nabankar Dasgupta[3], Milind Deo[2], Greeshma Gadikota[1], Jan Goral[2], Mikalia Hunt[2], Joshua Kane[3], Lani Mckinnon[2], Jules Magda[2], Swomitra Mohanty[2], Murali Muraleedharan[3], Subhash Risbud[5], Viktoriya Semeykina[2], York Smith[2], Adri van Duin[3], Ilya Zharov[1]
[1]University of Wisconsin, [2]University of Utah, [3]Pennsylvania State University, [4]Idaho National Laboratory, [5]University of California Davis

To synthesize geomaterials with repeatable hierarchical heterogeneity for studies of transport and interfacial properties of confined fluids, we prepared hierarchical nanoporous materials using two approaches. In one, non-porous and microporous spherical silica nanoparticles were assembled into close packed arrangements and consolidated using thermal or spark plasma sintering, which allowed controlling porosity by temperature and pressure. The resulting solids contained hierarchical nanopores in 2-100 nm range. In the second approach, microporous silica powders were formed by micelle templating, followed by the consolidation of the powders into the solids with micro- and mesopores using sintering or self-assembly inside microfluidic channels. The internal structure, pore size distribution and porosity of these materials were characterized using BET, SEM, TEM, Nano-CT and FIB-SEM. The processes that occur during sintering were followed by *in-operando* USAXS/SAXS and investigated by varying the pore structure of the building blocks and sintering conditions.

We were able to simulate the formation of mesoporous siliceous materials using ReaxFF reactive molecular dynamics simulations. We used OPLS force field to observe the details of the surfactant self-assembly into micelles and partitioning of the precursors into the micellar interiors and exteriors, followed by co-assembly of these species into liquid crystalline mesophases. We were also able to simulate the sintering events in silica nanoparticles by heating hydroxylated amorphous silica nanoparticles from 298 to 1273 K in the presence of air and evaluated the sintering rates, reaction energy barriers, and particle size-effects on the product to provide guidelines for the synthesis of nanoporous structures.

11:20 AM

L-II-2: MICROFLUIDICS FOR PROBING REACTIVE TRANSPORT IN FRACTURED MEDIA

[CMC-UF] Bowen Ling[1], Ziyan Wang[1], Jennifer L. Druhan[2], Illenia Battiato[1]
[1]Stanford University; [2]Univeristy of Illinois Urbana Champaign

Shales are inherently multiscale systems as their characteristic length-scales can span many orders of magnitude. Petrographic and microscopic studies have shown the existence of micro-fractures networks, furthering the hypothesis that the latter may be a critical component in controlling transport processes. Yet, the topological and chemical complexity of shales, combined with their significant reactivity, has hindered one's ability to isolate the impact that shale network topology may have on transport dynamics. In this study, we designed two micromodels with the same main fracture network but different microfracture topologies and compare passive transport experiments under different flow regimes as quantified by the Peclet number. We then lay out an experimental roadmap to increase the system complexity in such controlled systems to account for both solute reactivity and shale geochemical complexity.

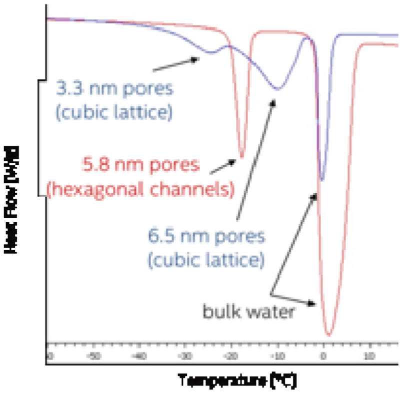
11:40 AM – Team Science Finalist

L-II-3: PROPERTY CHANGES UNDER CONFINEMENT IN ARCHITECTED MATERIALS

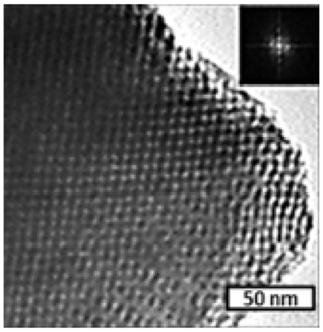
[MUSE] Pranay Asai[1], Hassnain Asgar[2], Michael Bartl[1], Darryl Butt[1], Hyeyoung Cho[1], Milind Deo[1], Greeshma Gadikota[2], Jan Goral[1], Hai Huang[3], Jiaqi Jin[1], Jiaoyan Li[3], Jan Miller[1], Subhash Risbud[4], Viktoriya Semekina[1], Yiping Xia[4], Ilya Zharov[1]
[1]University of Utah; [2]University of Wisconsin [3]Idaho National Laboratory [4]University of California, Davis

The mission of MUSE is to synthesize geomaterials with repeatable hierarchical heterogeneity and develop an understanding of transport and interfacial properties of fluids confined within these materials. There is considerable evidence that the known laws of phase transitions, and flow are affected by the presence of fluids confined in porous materials with nanometer-sized pores. Specially created nanoporous silica powders were architected into discs by using spark plasma sintering. The samples were imaged and characterized for a complete description of porosity using X-ray tomography, scanning electron microscopy and small and wide-angle neutron scattering. Phase transitions (melting and boiling points) and fluid permeabilities were measured in the powders and architected samples using high-pressure differential scanning calorimetry. Phase transition points were significantly different in the nanopores of the architected samples. The entire vapor pressure curve for pure hydrocarbons was below the bulk vapor pressure curve. Gibbs Ensemble Monte Carlo simulations were used to reproduce experimental trends. Permeabilities of polar and non-polar fluids in the architected discs were different indicating a breakdown in Darcy's Law in nanopores. Different permeabilities for the different fluids used showed importance of fluid-solid interactions. Flow in the nanopores of the siliceous matrix was modeled using molecular dynamics. Dissipative particle dynamics was used to molecular dynamics and explore flows in the multiple silica nanopore arrays, considering their packing and length. The models confirmed experimental findings. This paper illustrates the central mission of MUSE of synthesizing and characterizing architected materials, and of measuring and understanding fluid properties inside these materials.

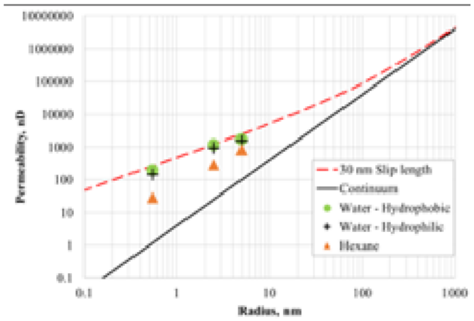
Changes in Phase Transitions



Synthesis and Characterization



Deviations from Darcy's Law



Contributions: Synthesis and Characterization – Asgar, Bartl, Butt, Cho, Gadikota, Goral, Risbud, Semekina, Xia and Zharov; Measurements – Cho, Deo, Jin, Miller and Xia; Modeling – Asai, Jin and Li

12:00 PM

L-II-4: A MULTISCALE, MULTIPHYSICS, AND MULTIDISCIPINARY EFRC TO ACHIEVE CONTROL OF WATER-HYDROCARBON-ROCK INTERACTIONS IN UNCONVENTIONAL AND TIGHT-OIL FORMATIONS

[CMC-UF] Anthony R. Kovscek[1], Vladimir Alvarado[2], Saman Aryana[2], John R. Bargar[3], Illenia Battiato[1], Sally M. Benson[1], Gordon E. Brown Jr.[1,3], Jennifer L. Druhan[4], Matthias Ihme[1], Kristian Jessen[5], Teresa E. Lehmann[2], Hamdi A. Tchelepi[1], Theo T. Tsotsis[5], Mark D. Zoback[1]

[1]Stanford University; [2]University of Wyoming; [3]SLAC National Accelerator Laboratory; [4]Univeristy of Illinois Urbana Champaign; [5]University of Southern California

There are positive and negative impacts of the “shale revolution” on energy supply, energy security, and the environment. The term “shale” is loosely applied to unconventional formations composed of ultrafine-grained rocks including shales, mudstones, marlstones, and chalks. While shale production has profoundly changed energy supply; only about 5% of the original oil and about 25% of the gas in oil/gas shales is recovered. Initial productivity decreases markedly after a few months. Increased fundamental understanding of coupled physical and chemical processes in fractured nanoporous media is needed to realize greater positive and fewer negative impacts. CMC-UF focuses upon interfaces, heterogeneity, disorder, and coupled physical/chemical processes in geological nanoporous media at length scales ranging from nanometers to meters. Because of its availability, water is ubiquitous as a hydraulic fracturing. Carbon dioxide and/or nitrogen are potential substitutes and may have a number of advantages including reduction of stress on water resources, less water to be disposed, and/or less water recycled. Accordingly, examination of CO_2/shale interactions and shale constitutive relations in the presence of CO_2 is one area of focus. Importantly, our fundamental science efforts feature integrated experimental measurements, theory development, computational tools, and scale translation activities. Investigations make use of major DOE and university experimental and computational user facilities as well as specialized experimental equipment to probe pore, microfracture, and fracture-network scales.

M. SYNTHESIS SCIENCE

SESSION II: TUESDAY, JULY 30, 2019; 11:00 – 12:20 PM; LINCOLN 6

11:00 AM

M-II-1: PEPTOID-CONTROLLED SYNTHESIS OF HIERARCHICAL MATERIALS

[CSSAS] Tengyue Jian[1], Peng Mu[1], Madison Monahan[2], Brandi Cossairt[2], Guomin Zhu[1], James J. De Yoreo[1], Alexander Thomas[2], Jinrong Ma[2], François Baneyx[2], Nagesh B. Kolhe[2], Samson A. Jenekhe[2], Janani Sampath[2], Jim Pfaendtner[2], Christopher J. Mundy[1], Mingfei Zhao[3], Andrew Ferguson[3], Chun-Long Chen[1]

[1]Pacific Northwest National Laboratory; [2]University of Washington; [3]University of Chicago

In nature, biominerals (e.g. bones), virus capsids, protein matrices and protein-based machinery, are outstanding examples of hierarchical materials whose assembly and functions are controlled over multiple length scales by high information content biomacromolecules. Inspired by these feats of nature, the ***Center for the Science of Synthesis Across Scales (CSSAS)*** aims at mastering the design of high-information-content macromolecular building blocks that predictively self-assemble into responsive, reconfigurable, self-healing materials, and direct the formation and organization of inorganic components. One of the most advanced classes of sequence-defined protein-mimetics are peptoids, or poly-N-substituted glycines. These molecules offer unique opportunities for the fabrication of complex architectures with tunable functions based solely on sidechain chemistry. In this presentation, three peptoid-based approaches for controlled synthesis of hierarchical materials will be discussed. ***The first*** involves the design and synthesis of amphiphilic peptoids that self-assemble into hierarchical structures, such as nanotubes and nanosheets. ***The second*** involves the conjugation of atomically precise nanoclusters (e.g. POSS and InP), solid-binding proteins, or semiconducting oligomers to self-assembling peptoids for hierarchical self-assembly of hybrid materials with precisely-controlled density and stereochemistry of functional objects. ***The third*** approach uses peptoids as surfacant-like molecules for controlled formation and morphogenesis of inorganic nanomaterials. A combination of *in situ* imaging, molecular simulations and machine learning is being used to elucidate the principles underlying peptoid-controlled synthesis of hierarcial materials with the ultimate goal of enabling predictive materials synthesis across scales.

11:20 AM

M-II-2: COMPLEX METAL OXIDES: MOVING FROM MATERIALS BY DESIGN TO SYNTHESIS BY DESIGN

[CNGMD] Wenhao Sun[1], Feng Wang[2], Bor-Rong Chen[3] Laura Schelhas[3], Jingyang Wang[1], Michael Toney[3], Gerbrand Ceder[1]

[1]Lawrence Berkeley National Laboratory; [2]Brookhaven National Laboratory; [3]SLAC National Accelerator Laboratory

Owing to the broad diversity of crystal structures and materials properties available, transition metal oxides drive the functionality of many energy technologies. However, this broad structural diversity can also lead to a myriad of non-equilibrium crystallization pathways during nucleation and growth, often resulting in poor phase-control. We are combining *ab initio* thermodynamics with *in situ* characterization to build predictive theories for which metastable phases nucleate during synthesis, and under which synthesis conditions. Guided by these calculated *'synthesis maps'*, solid-state chemists can more rationally navigate the thermodynamic and kinetic energy landscape towards the targeted synthesis of desired phases. In the MnO_2 system, we extend Pourbaix (E-pH) diagrams to capture how surface energy and solution alkali chemistry influence the relative nucleation rates of competing polymorphs. Using *in-situ* synchrotron scattering, we monitored the precipitation of metastable MnO_2 intermediates under varying solution chemistries, and demonstrated that our calculated '*synthesis maps'* successfully capture which metastable polymorphs appear, the order of their appearance, and their relative lifetimes. We extended our combined *ab initio* and *in situ* experimental approach to the solid-state synthesis of layered oxides, $LiCoO_2$, $LiNiO_2$, Na_xMnO_2 and Na_xCoO_2, which are the dominant cathode materials for Li- and Na-ion batteries. Structural motifs that arise during low-temperature interfacial reactions are often found to template metastable phase transformations during high-temperature calcination. We show that by engineering which metastable intermediates form during the early stages of crystallization better control can be achieved over the structural polymorphism and defects and hence the associated functional properties.

11:40 AM

M-II-3: ENABLING PRESCRIPTIVE SYNTHESIS OF METASTABLE AND TERNARY OXIDES

[GENESIS] James R. Neilson[1], Paul K. Todd[1], G. Thinh Tran[1], Adam Corrao[2], Iain W. H. Oswald[1], Rebecca D. McAuliffe[3], Matthew McDermont[4], Jonathan Denney[2], Daniel L. Olds[5], Shyam Dwaraknath[4], Kristin A. Persson[4], Peter G. Khalifah[2], Chris J. Wright[6], Chia-Hao Liu[6], S. J. L. Billinge[6], Eric Dooryhée[5]
[1]Colorado State University; [2]Stonybrook University; [3]Oak Ridge National Laboratory, [4]Lawrence Berkeley National Laboratory, [5]Brookhaven National Laboratory, [6]Columbia University

Complex oxides enable a diverse set of electronic properties; however, we do not yet know how to prescriptively synthesize desired compositions or polymorphs of materials, particularly if they are metastable. Metathesis (or double-exchange) reactions are well suited to address synthesis questions pertaining to atomic transport and permit the identification of incipient stages of phase differentiation in solid-state reactions. As an example, the reaction, $A_2CO_3 + Mn_2O_3 + 2\ YCl_3$, where A = Li, Na, or K, yields different Y-Mn-O products (and polymorphs) depending on which spectating alkali is present. From a combination of *in situ* and *ex situ* analysis of myriad synthesis reactions combined with first-principles calculation of thermodynamic parameters, we identify competent intermediates that enable kinetic control of the reaction, such as the phases $LiMnO_2$ and YOCl. By examining the results of multiplexed and multimodal *in situ* reactions, we uncover the role of thermochemistry (e.g., $LiMnO_2$ vs $NaMnO_2$) and reactant crystal structure (e.g., monoclinic vs tetragonal $LiMnO_2$). These results allow us to establish the critical processes in solid-state reaction pathways that enable, or hinder, prescriptive synthesis.

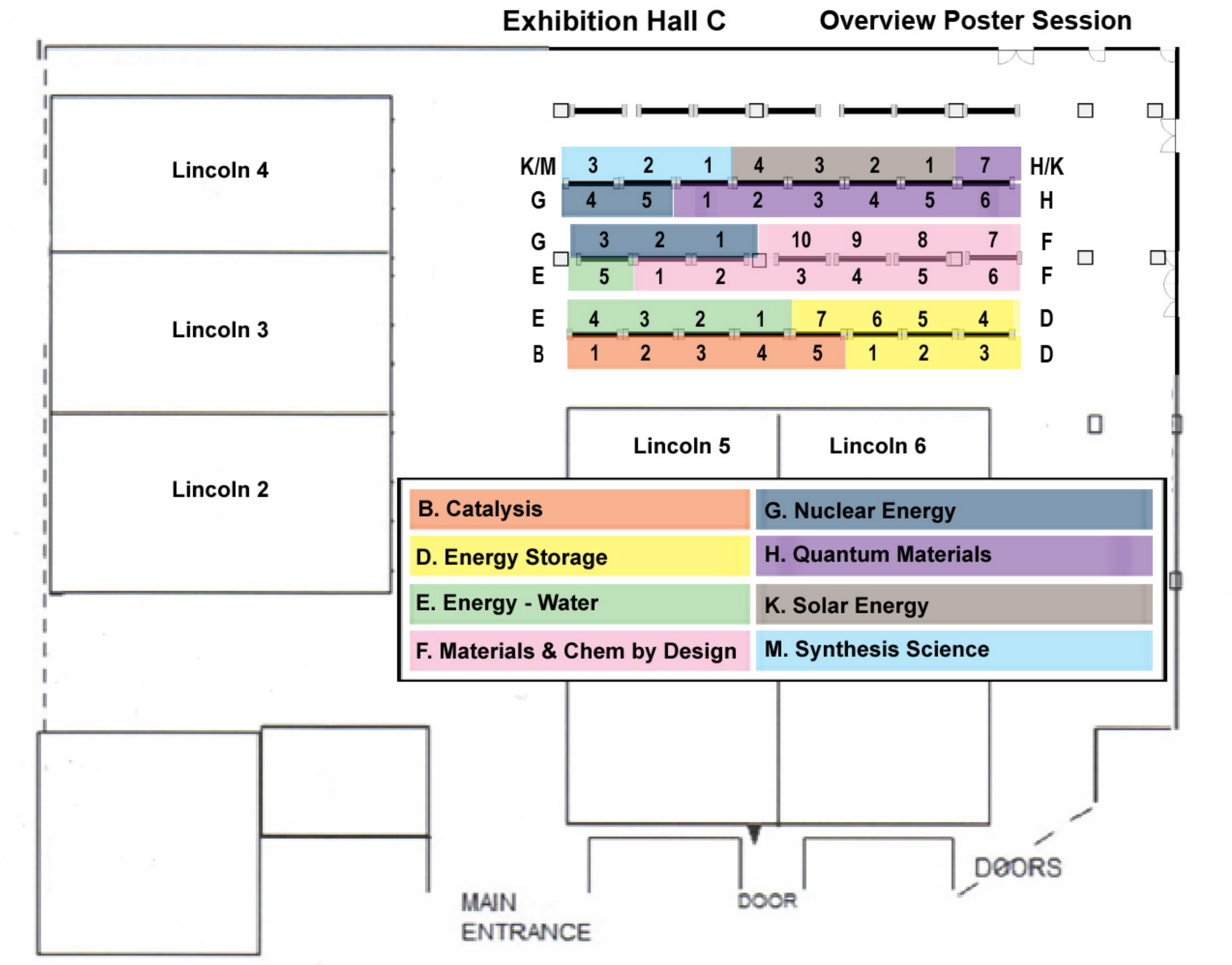
12:00 PM

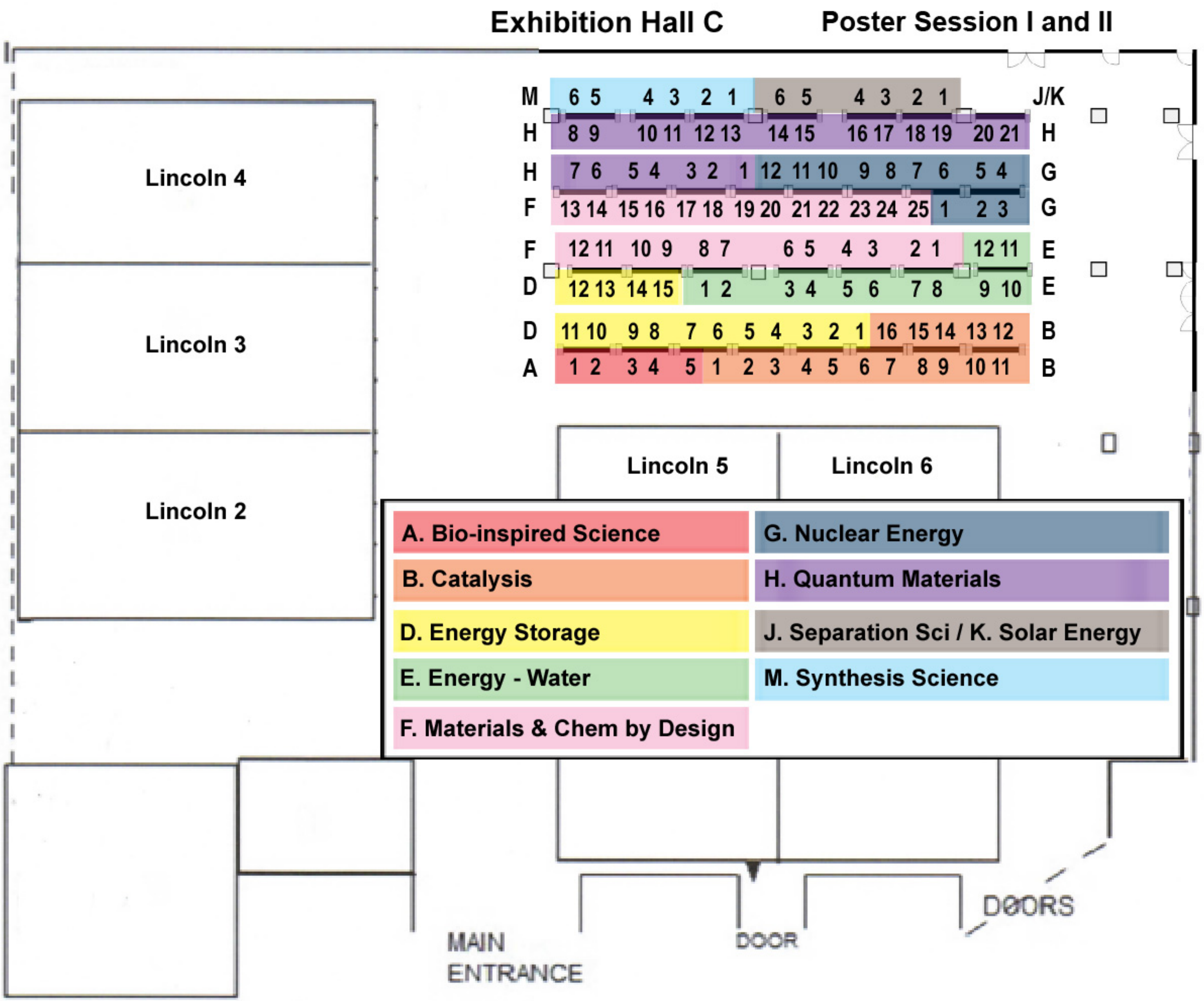
M-II-4: IDENTIFICATION AND FUNCTIONALITY OF NEW POLAR MATERIALS AND INTERFACES

[CNGMD] David Ginley[1], Shyam Dwaraknath[2], Kristin Persson[2], Brian Gorman[3], John Magnum[3], Laura Schelhas[4], Mike Toney[4]
[1]National Renewable Energy Laboratory; [2]Lawrence Berkeley National Laboratory; [3]Colorado School of Mines; [4]SLAC National Accelerator Laboratory

Piezoelectric and ferroelectric materials have increasing technologic importance in a vast array of applications from energy conversion to communications. Many of the materials come from a small set of know materials such as $Ba_{1-x}Sr_xTiO_3$ and $Pb(Zr_xTi_{1-x})O_3$ which have known limitations. We will discuss an effort in the CNGMD EFRC to understand the potential functionality that introducing polarity in bulk and interfacial materials could have on other functionalities such as photovoltaics and multiferroics and how a combination of theory to identify new materials combined with predictive growth can yield new polar materials from metastable polymorphs. We will illustrate the approach by two distinct cases: the observation of ferroelectric behavior in single crystals of methylammonium lead iodide ($MAPbI_3$) and the possible implications of this on the opto-electronic functionality of the material; and the prediction of and realization piezoelectric behavior in $SrHfO_3$, specifically in the non-ground state P_{4mm} structure as compared to its normal high-K applications in the ground state P_{nma} structure. In both cases, theory was used to identify and estimate the degree of polar behavior by calculating the piezoelectric tensor and then to help understand phase behavior to realize the polar phase – i.e. tetragonal for $MAPbI_3$ and P_{4mm} for the $SrHfO_3$. Both targeted materials were realized experimentally and demonstrated to be truly polar. We will discuss the implications of this work toward generating new functional polar materials and the implications of inducing polarity in ostensibly non-polar materials to add or enhance functionality.

2019 EFRC PI MEETING – MAP OF POSTER SESSIONS




Exhibition Hall C
Poster Session I and II
M 6 5 4 3 2 1 6 5 4 3 2 1 J/K
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Lincoln 5
Lincoln 6
A. Bio-inspired Science
B. Catalysis
D. Energy Storage
E. Energy - Water
F. Materials & Chem by Design
G. Nuclear Energy
H. Quantum Materials
J. Separation Sci / K. Solar Energy
M. Synthesis Science
MAIN ENTRANCE
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LIFE AT THE FRONTIERS OF ENERGY RESEARCH VIDEO CONTEST II ENTRIES, *ATTRIUM*

As part of the 2019 Energy Frontier Research Centers (EFRC) Principal Investigators' Meeting, the Department of Energy's Office of Basic Energy Sciences (DOE BES) sponsored a Life at the Frontiers of Energy Research Video Contest II. Following the EFRC 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 EFRCs. After a hiatus of 8 years, the video contest is back! To view all the videos, visit https://www.energyfrontier.us/video-contest-2.

Life at the Frontiers of Energy Research

Center for Lignocellulose Structure and Formation (CLSF)
Creators: Sintu Rongpipi, Dr. Deborah Petrik, and Lynnicia Massenburg

The daily challenges and rewards of performing cell wall biology research is highlighted through interviews with CLSF scientists.

Future of Energy Storage

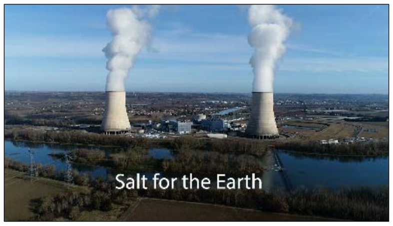
Fluid Interface Reactions, Structures and Transport Center (FIRST)
Creators: Simge Uzun and Bilen Akuzum

A short story of human-centered progress from the challenges of the ancient times to modern day's energy storage sciences.

Collaborating for a Better Future

Inorganometallic Catalyst Design Center (ICDC)
Creator: Lisa Zeeb

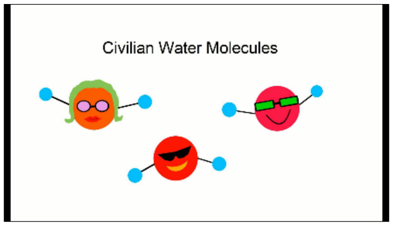
ICDC junior investigators highlight the importance of collaboration between computational and experimental chemists, chemical engineers, and material scientists in the study of metal organic frameworks, catalysts, and chemical reactions relevant to natural gas liquefaction.



Salt for the Earth

Molten Salts in Extreme Environments (MSEE)
Creators: James Wishart, Timothy Kuhn, Diana Murphy, Simon Pimblott, William Phillips, Phillip Halstenberg, Claudio Margulis, Matthew Emerson, Haimeng Wang, and Arthur Ronne

Salt has been key to human survival and now we want to use it to preserve the environment. The mission of the Molten Salts in Extreme Environments Energy Frontier Research Center (EFRC) is to understand the fundamental properties of molten salts for use in a new generation of reactors that will be safer, more efficient and modular. Our success depends on the expertise and teamwork of the institutions participating in this EFRC.



Water in Silica Nanopores – Superman to the Rescue

Multi-Scale Fluid-Solid Interactions in Architected and Natural Materials (MUSE)
Creators: Director & Cartoon: Jiaqi Jin; Editor: Bryce Wilson; Editorial Consultant: Ash Grover; Key Contributors: Hyeyoung Cho, Viktoriya Semeykina, Mikaila Hunt, Jan Goral; Participants: Hassnain Asgar, Siddharth Agrawal, Sohaib J. Mohammed, Jiaoyan Li, and Rajashekhar Marthi; Faculty Advisers: Mark Koopman and Jan Miller. The song "Pressure" is by Matthew Bellamy, the band Muse, and Warner/Chappell Music Inc. (WMG). Copyright permission obtained by e-mail.

The video shows simulations and TEM micrographs of naturally occurring and architected nanoporous materials and their interaction with confined liquids. An animated section to the sound of Pressure by the rock band, Muse, who shares our eponymous EFRC, accompanies the video animation.

Capacity – the Potential and Power for Change

NorthEast Center for Chemical Energy Storage (NECCES)
Creators: Marc Francis Hidalgo, Carrie Kaplan, Yicheng Zhang, and Dongsheng Ji.

Li-ion batteries are a central part of the clean economy, as they enable the utilization of renewables, electric vehicles, and portable devices. This video give a glimpse into how the NorthEast Center for Chemical Energy Storage (NECCES) helps in the push for a more sustainable future through the development of better and longer lasting batteries. At NECCES, we believe that, just like the Li-ion battery, people have the capacity, potential, and power to make a positive change in the world.

Dancing with Heat and Spin

Spins and Heat in Nanoscale Electronic Systems (SHINES)
Creators: Director, shooting and voice: Gen Yin; Animation "Romeo and Juliet": Jiayuan Tian; Editing: Gen Yin and Shuangwei Yan; Music "Funk Interlude" is provided by Dysfunction_AL (license: CC BY-NC 3.0 US). See more details in the final part of the video.

The video describes the basic idea and the social impact of the research projects led by SHINES. It portrays how this EFRC studies heat management and magnetism in devices, and briefly presents the life of young scholars who have been carrying out excellent work in these areas.

Turning Down the Heat

Center for Thermal Energy Transport under Irradiation (TETI)
Creators: Chris Morgan from Idaho National Laboratory, featuring researchers from TETI.

Researchers at the Center for Thermal Energy Transport under Irradiation are working towards uncovering a new paradigm for predicting and ultimately controlling the flow of heat in materials with evolving microstructure. By turning down the heat, their findings can pave the way for the next-generation of efficient, safe and economical nuclear reactors, as well as support new fossil-free clean energy technologies.

Acid Gases in Energy-Related Research

Center for Understanding and Control of Acid Gas-Induced Evolution of Materials for Energy (UNCAGE-ME)
Creator: Tania Evans

We're surrounded by materials. This video explains why the UNCAGE-ME EFRC studies material/acid gas interactions and what it means for energy research.

Nuclear Energy Waste and WastePD

Center for Performance and Design of Nuclear Waste Forms and Containers (WastePD)
Creators: Produced by Zelong Zhang, narrated by Julie Hu.

Nuclear energy is emission free that can mitigate climate change. However, nuclear energy produces radioactive waste which requires durable materials for a safe disposal in environment. WastePD's core mission is to study the science behind the corrosion of nuclear waste materials to improve the safety of nuclear waste management.

CENTER OVERVIEW POSTER SESSION: MONDAY, JULY 29, 2019; 5:00 – 6:30 PM, *EXHIBITION HALL C*

B. CATALYSIS

PO-B-1: BIOLOGICAL ELECTRON TRANSFER AND CATALYSIS ENERGY FRONTIER RESEARCH CENTER (BETCY)

[BETCy] John W. Peters[1], Michael W.W. Adams[2], David N. Beratan[3], Brian Bothner[4], Carrie Harwood[5], Anne K. Jones[6], Shelley C. Minteer[7], and Lance C. Seefeldt[8],
[1]Washington State University (lead institution); [2]University of Georgia; [3]Duke University; [4]Montana State University; [5]University of Washington; [6]Arizona State University; [7]University of Utah; [8]Utah State University

The mission of the BETCy EFRC is to define the molecular mechanisms that control the coupling of electrochemical potential energy to chemical bond formation. During the funding period we have focused on three areas 1) electron bifurcation and the mechanism of combining exergonic and endergonic electron transfer reactions, 2) the mechanisms for controlling directional catalytic rates in electron transfer and oxidation-reduction catalysis, and 3) how biological electron transfer reactions are controlled by conformational changes in macromolecular assemblies.

PO-B-2: BIOINSPIRED LIGHT-ESCALATED CHEMISTRY (BIOLEC)

[BioLEC] Gregory D. Scholes[1], David W. C. MacMillan[1], Robert Knowles[1], Todd Hyster[1], Abigail G. Doyle[1], Barry P. Rand[1], Gabriela Schlau-Cohen[2], Felix Castellano[3], James C. McCusker[4], Ana Moore[5], Tom Moore[5], Matthew Bird[6], Garry Rumbles[7]
[1]Princeton University (lead institution); [2]Massachusetts Institute of Technology, [3]North Carolina State University, [4]Michigan State University, [5]Arizona State University, [6]Brookhaven National Laboratory, [7]National Renewable Energy Laboratory

Our mission is inspired by the way in which photosynthesis combines the energy of two or more photons to perform chemistry that is otherwise strongly uphill at equilibrium. We will employ light harvesting and advances in solar photochemistry to enable unprecedented photoinduced crosscoupling reactions that valorize abundant molecules.

PO-B-3: CATALYSIS CENTER FOR ENERGY INNOVATION (CCEI)

[CCEI] Omar Abdelrahman[11], Eric Bloch[1], Anibal Boscoboinik[6], Stavros Caratzoulas[1], Jingguang Chen[3], Paul Dauenhauer[2], Mark E. Davis[7], Wei Fan[11], Anatoly Frenkel[6], Raymond J. Gorte[8], Song-I Han[9], Marianthi Ierapetritou[4], Yan Jin[1], Dongxia Liu[12], Raul Lobo[1], Christopher Murray[8], Marat Orazov[1], Basudeb Saha[1], , Susannah Scott[9], Dong Su[6], Michael Tsapatsis[5], Ioulia Valla[10], Dionisios G. Vlachos[1], Lynn Walker[13], Donald Watson[1], Bingjun Xu[1]

[1]University of Delaware (lead institution); [2]University of Minnesota; [3]Columbia University; [4]Rutgers, The State University of New Jersey; [5]Johns Hopkins University; [6]Stony Brook University; [7]California Institute of Technology; [8]University of Pennsylvania; [9]University of California-Santa Barbara; [10]University of Connecticut; [11]University of Massachusetts-Amherst; [12]University of Maryland; [13]Carnegie Mellon University

CCEI's mission is to develop innovative heterogeneous catalytic technologies to transform lignocellulosic (non-food-based) biomass materials into fuels, chemicals, and advanced materials. The cornerstone of CCEI research lies in advancing catalysis and its integration into processes that deliver innovative technologies for the conversion of biomass feedstocks, specifically carbohydrates and smaller oxygenated molecules.

PO-B-4: INORGANOMETALLIC CATALYST DESIGN CENTER (ICDC)

[ICDC] Laura Gagliardi[1], Joseph Hupp[5], Aditya Bhan[1], Don Camaioni[7], Karena Chapman[8], Chris Cramer[1], Massimiliano Delferro[2], Omar Farha[5], Bruce Gates[9], Rachel Getman[3], Oliver Gutierrez Tinoco[7], Heather Kulik[4], Johannes Lercher[7], Connie Lu[1], Alex Martinson[2], William Morris[6], Justin Notestein[5], R. Lee Penn[1], and Don Truhlar[1]

[1]University of Minnesota (lead institution); [2]Argonne National Laboratory; [3]Clemson University; [4]Massachusetts Institute of Technology; [5]Northwestern University; [6]NuMat Technologies; [7]Pacific Northwest National Laboratory; [8]Stony Brook University; [9]University of California, Davis

The mission of the Inorganometallic Catalyst Design Center (ICDC) is to computationally guide the discovery of a new class of energy-science-relevant catalytic materials and understand the underlying structure-function relationships that lead to further catalyst discovery. ICDC participants aim to utilize quantum simulations and predictions to aid with synthesis, characterization, and catalysis of new catalytic materials.

PO-B-5: INTEGRATED MESOSCALE ARCHITECTURES FOR SUSTAINABLE CATALYSIS (IMASC)

[IMASC] Joanna Aizenberg[1], Juergen Biener[2], J. Anibal Boscoboinik[3], Maria Flytzani-Stephanopoulos[4], Anatoly I. Frenkel[5], Cynthia M. Friend[1], Boris Kozinsky[1], Robert J. Madix[1], Philippe Sautet[6], Dario J. Stacchiola[3], Eric A. Stach[7], Michail Stamatakis[8], E. Charlie H. Sykes[4], Jason F. Weaver[9]

[1]Harvard University (Lead Institution), [2]Lawrence Livermore National Laboratory, [3]Brookhaven National Laboratory, [4]Tufts University, [5]Stony Brook University, [6]University of California, Los Angeles, [7]University of Pennsylvania, [8]University College London, [9]University of Florida

The mission of IMASC is to develop the ability to improve catalytic selectivity by quantitatively scaling from model studies to catalytic conditions using advanced experiment and theory.

D. ENERGY STORAGE

PO-D-1: CENTER FOR ALKALINE-BASED ENERGY SOLUTIONS (CABES)

[CABES] Héctor Abruña[1], Tomás Arias[1], Joel Brock[1], Peng Chen[1], Geoffrey Coates[1], Francis DiSalvo[1], Robert DiStasio[1], Jiye Fang[2], Emmanuel Giannelis[1], Lena Kourkoutis[1], Tom Mallouk[3], Manos Mavrikakis[4], David Muller[1], Kevin Noonan[5], Piotr Zelenay[6], Bryan Pivovar[7], Sharon Hammes-Schiffer[8], Andrej Singer[1], Jin Suntivich[1]

[1]Cornell University (lead institution), [2]Binghamton University, [3]University of Pennsylvania, [4]University of Wisconsin-Madison, [5]Carnegie Mellon University, [6]Los Alamos National Lab, [7]National Renewable Energy Lab, [8]Yale University

CABES aims to achieve a detailed understanding of the nature, structure, and dynamics of electrocatalysis in alkaline media.

PO-D-2: CENTER FOR ELECTROCHEMICAL ENERGY SCIENCE (CEES)

[CEES] Maria K. Chan[1], Larry Curtiss[1], Jeffrey Elam[1], Paul Fenter[1], Timothy T. Fister[1], Michael Thackeray[1], Andrew Gewirth[2], Ralph Nuzzo[2], Nancy Sottos[2], Michael J. Bedzyk[3], Vinayak Dravid[3], Mark Hersam[3], Christopher Wolverton[3], Jeffrey Greeley[4].

[1]Argonne National Laboratory (lead institution), [2]University of Illinois Urbana-Champaign, [3]Northwestern University, [4]Purdue University

CEES seeks to create a robust fundamental understanding of the phenomena that control the reactivity of electrified oxide interfaces, films and materials relevant to lithium-ion battery chemistries.

PO-D-3: FLUID INTERFACE REACTIONS, STRUCTURES AND TRANSPORT (FIRST)

[FIRST] Sheng Dai,[1] Nina Balke,[1] Stephan Irle,[1] Paul Kent,[1] Shannon Mahurin,[1] Eugene Mamontov,[1] Robert Sacci,[1] Alexei Sokolov,[1] Raymond Unocic,[1] Hsiu-Wen Wang,[1] David Wesolowski,[1] Veronica Augustyn,[2] Peter Cummings,[3] Takeshi Egami,[4] Paul Fenter,[5] Yury Gogotsi,[6] De-en Jiang,[7] Jianzhong Wu,[7] Michael Naguib,[8] Marek Pruski,[9] Adri Van Duin[10]

[1]Oak Ridge National Laboratory, [2]North Carolina State University, [3]Vanderbilt University, [4]University of Tennessee, Knoxville, [5]Argonne National Laboratory, [6]Drexel University, [7]University of California, Riverside, [8]Tulane University, [9]Ames Laboratory, [10]Penn State University

The mission of FIRST is to achieve fundamental understanding and validated, predictive models of the atomistic origins of electrolyte and coupled electron transport under nanoconfinement that will enable transformative advances in capacitive electrical energy storage and other energy-relevant interfacial systems.

PO-D-4: CENTER FOR MESOSCALE TRANSPORT PROPERTIES (M2M/T)

[m2M/t] Esther S. Takeuchi[1], Amy C. Marschilok[1], Lynden A. Archer[2], David C. Bock[3], Yu-chen Karen Chen-Wiegart[1], Marca M. Doeff[4], Ekaterina Pomerantseva[5], Elsa Reichmanis[6], Kenneth J. Takeuchi[1], Feng Wang[3], Lei Wang[3], Stanislaus S. Wong[1], Alan C. West[7], Guihua Yu[8], Yimei Zhu[3]

[1]Stony Brook University (lead institution); [2]Cornell University; [3]Brookhaven National Laboratory; [4]Lawrence Berkeley National Laboratory; [5]Drexel University; [6]Georgia Institute of Technology; [7]Columbia University; [8]University of Texas at Austin

The mission of m2M/t is to build the scientific knowledge to enable creation of scalable electrochemical energy storage systems with high energy, power, and long life, through fundamental understanding of transport properties.

PO-D-5: NORTHEAST CENTER FOR CHEMICAL ENERGY STORAGE (NECCES)

[NECCES] M. Stanley Whittingham[1], Louis Piper[1], Guangwen Zhou[1], Natasha Chernova[1], Karena Chapman[2], Pete Chupas[2], Clare P. Grey[3], Glenn Amatucci[4], Nathalie Pereira[4], Yet Ming Chiang[5], Katsuo Thornton[6], Anton Van der Ven[7], Shirley Meng[8], Shyue-Ping Ong[8]

[1]Binghamton University (lead institution), [2]Stony Brook University, [3]Cambridge University, [4]Rutgers University, [5]MIT, [6]University of Michigan, [7]UC Santa Barbara, [8]UC San Diego.

The mission of NECCES is to develop an understanding of how key electrode reactions occur in cathode materials for Li-based batteries, and how they can be controlled to improve electrochemical performance, from the atomistic level to the macroscopic level through the lifetime of the operating battery. This mission will allow the determination of the ultimate limits of intercalation reactions for chemical energy storage.

PO-D-6: NANOSTRUCTURES FOR ELECTRICAL ENERGY STORAGE (NEES)

[NEES] Gary Rubloff [1], Sang Bok Lee [1], Janice Reutt-Robey [1], A. Alec Talin [2], Bruce Dunn [3], Henry White [4], Yue Qi [5], Kevin Leung [6]

[1]University of Maryland (lead institution), [2]Sandia National Lab Livermore, [3]UCLA, [4]University of Utah, [5]Michigan State University, [6]Sandia National Lab Albuquerque

NEES' mission is to reveal scientific insights and design principles that enable a next-generation electrical energy storage technology based on dense mesoscale architectures of multifunctional nanostructures

PO-D-7: SYNTHETIC CONTROL ACROSS LENGTH-SCALES FOR ADVANCING RECHARGEABLES (SCALAR)

Bradley Chmelka[1], Xiangfeng Duan[2], Bruce S. Dunn[2], Jian Luo[3], Brent C. Melot[4], Thomas F. Miller III[5], Sri R. Narayan[4], Laurent Pilon[2], Philippe Sautet[2], Kimberly A. See[5], Rachel Segalman[1], Ram Seshadri[1], Alex Spokoyny[2], Barry C. Thompson[4], Sarah H. Tolbert[2], Anton Van der Ven[1], and Johanna Nelson Weker[6]
[1]University of California (UC) Santa Barbara; [2]UC Los Angeles (UCLA) "(lead institution)"; [3]UC San Diego; [4]University of Southern California (USC); [5]California Institute of Technology (CalTech); and [6]SLAC National Accelerator Laboratory

SCALAR's mission is to design materials, interfaces, and architectures that revolutionize the performance of energy storage systems by dramatically expanding the range of materials systems and chemistries that can be employed in next generation batteries.

E. ENERGY - WATER

PO-E-1: ADVANCED MATERIALS FOR ENERGY-WATER SYSTEMS (AMEWS)

[AMEWS] Wei Chen[1], Seth Darling[1], Juan de Pablo[1,2], Jeffrey Elam[1], Giulia Galli[1,2], Harold Kung[3], Alex Martinson[1], Karen Mulfort[1], Paul Nealey[1,2], George Schatz[3], Steven Sibener[2], Dmitri Talapin[1,2], David Tiede[1], Matthew Tirrell[1,2], Andrei Tokmakoff[2], Gregory Voth[2], Nestor Zaluzec[1]
[1]Argonne National Laboratory (lead institution); [2]University of Chicago; [3]Northwestern University

The mission of the AMEWS Center is to understand and design water/solid interfaces to enable future advances in materials for efficient water treatment.

PO-E-2: CENTER FOR ENHANCED NANOFLUIDIC TRANSPORT (CENT)

[CENT] Michael Strano[1], YuHuang Wang[2], Aleksand Noy[3], Zuzanna Siwy[4], Mark Reed[5], Narayana Aluru[6], Martin Bazant[1], Daniel Blankschtein[1], John Cumings[2], Menachem Elimelech[5], John T. Fourkas[2], Heather Kulik[1], Arun Majumdar[7], Charles Martin[8], Tuan Anh Pham[3], Eric Schwegler[3].
[1]Massachusetts Institute of Technology (lead institution); [2]University of Maryland; [3]Lawrence Livermore National Laboratory; [4]University of California Irvine; [5]Yale University; [6]University of Illinois at Urbana-Champaign; [7]Stanford University; [8]University of Florida

The mission of CENT is to address emerging and compelling gaps in our knowledge of fluid flow and molecular transport in single digit nanopores (less than 10 nm diameters) and establish the scientific foundation for developing new technologies, from novel membranes for separations and water purification to new gas-permeable materials and energy storage devices.

PO-E-3: Center for Mechanistic Control of water-hydrocarbon-rock interactions in Unconventional Formations (CMC-UF)

[CMC-UF] Anthony R. Kovscek[1], Vladimir Alvarado[2], Saman Aryana[2], John R. Bargar[3], Illenia Battiato[1], Sally M. Benson[1], Gordon E. Brown Jr.[1,3], Jennifer L. Druhan[4], Matthias Ihme[1], Kristian Jessen[5], Teresa E. Lehmann[2], Hamdi A. Tchelepi[1], Theo T. Tsotsis[5], Mark D. Zoback[1]

[1]Stanford University (lead institution); [2]University of Wyoming; [3]SLAC National Accelerator Laboratory; [4]Univeristy of Illinois Urbana Champaign; [5]University of Southern California

The mission of CMC-UF is to seek fundamental understanding of the various nonequilibrium chemical, physical, and mechanistic processes occurring in unconventional formations (i.e., shale resources) to achieve mechanistic control that permits increases in hydrocarbon production while decreasing environmental impacts such as the amount of produced water, contaminants, and the number of wells drilled.

PO-E-4: Multi-scale Fluid-Solid Interactions in Architected and Natural Materials (MUSE)

[MUSE] Michael Bartl[1], Darryl Butt[1], Milind Deo[1], Greeshma Gadikota[2], Michael Hoepfner[1], Hai Huang[3], Joshua Kane[3], John Kaszuba[4], Jules Magda[1], John McLennan[1], Brian McPherson[1], Jan Miller[1], Swomitra Mohanty[1], Pania Newell[1], Bryony Richards[1], Subhash Risbud[5], York Smith[1] James Sutherland[1], Adri van Duin[6], Ilya Zharov[1]

[1]University of Utah (lead institution), [2]University of Wisconsin, [3]Idaho National Laboratory, [4]University of Wyoming, [5]University of California, Davis, [6]Pennsylvania State University

The mission of MUSE is to synthesize geomaterials with repeatable hierarchical heterogeneity and develop an understanding of transport and interfacial properties of fluids confined within these materials.

PO-E-5: The Center for Materials for Water and Energy Systems (M-WET)

[M-WET] Benny Freeman[1], Lynn Katz[1], Rachel Segalman[2], Venkat Ganesan[1], Desmond Lawler[1], Nathaniel Lynd[1], Thomas Truskett[1], Mukul Sharma[1], Michael Webber[1], Mahdi Abu-Omar[2], Christopher Bates[2], Songi Han[2], Craig Hawker[2], Scott Shell[2], Todd Squires[2], Michael Doherty[2], Glenn Fredrickson[2], Ethan Crumlin[3], and Alex Hexemer[3]

University of Texas at Austin (lead institution)[1], University of California at Santa Barbara[2], Lawrence Berkeley National Labs[3]

The mission of the Center for Materials for Water and Energy Systems (M-WET) is to discover and understand the fundamental science critical to designing new membrane materials and develop tools and knowledge to predict new materials' interactions with targeted solutes from recalcitrant water sources in order to provide basic science discoveries to enable new membranes to provide fit for purpose water and recover valuable solutes with less energy.

F. MATERIALS AND CHEMISTRY BY DESIGN

PO-F-1: BREAKTHROUGH ELECTROLYTES FOR ENERGY STORAGE (BEES)

[BEES] Rohan Akolkar[1], Allen Bard[2], Clemens Burda[1], Tessa Calhoun[3], Mark Dadmun[3], Steven Greebaum[4], Burcu Gurkan[1], Douglas Hayes[3], Edward Maginn[5], Ah-Hyung Alissa Park[6], Emily Pentzer[1], Robert Savinell[1], Joshua Sangoro[3], Mark Tuckerman[7], Miomir Vukmirovic[8], Jesse Wainright[1], Thomas Zawodzinski[3]

[1]Case Western Reserve University (lead institution); [2]University of Texan Austin; [3]University of Tennessee at Knoxville; [4]Hunter College; [5]University of Notre Dame; [6]Columbia University; [7]New York University; [8]Brookhaven National Laboratory

BEES research is focused on a central challenge of electrochemical energy storage: how to modulate the movement of ions and charge transfer kinetics for efficient, high-power, high-energy, scalable, and safe storage technologies. Two classes of materials are under study; **develop deep eutectic solvents (DES)** and **soft nanoparticles (SNP)**. The research of **BEES** will also lead to broader scientific impacts by providing new molecular-level model electrolytes that address diverse problems in electrocatalysis, environmental sciences, energy, separations, and sensors.

PO-F-2: CENTER FOR BIO-INSPIRED ENERGY SCIENCE (CBES)

[CBES] Samuel I. Stupp[1], Joanna Aizenberg[2], Anna Balazs[3], Kyle Bishop[4], Paul Chaikin[5], Danna Freedman[1], Sharon Glotzer[6], Erik Luijten[1], Chad Mirkin[1], Monica Olvera de la Cruz[1], John Rogers[1], George Schatz[1], Emily Weiss[1], George Whitesides[2]

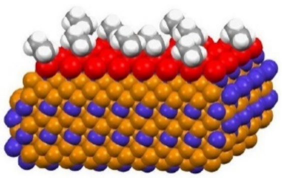
[1]Northwestern University; [2]Harvard University; [3]University of Pittsburgh; [4]Columbia University; [5]New York University; [6]University of Michigan

The mission of the Center for Bio-Inspired Energy Science is to develop the next frontier in soft materials by designing structures that emulate many of the properties we see in biological systems. Our targets to create robotic and photosynthetic soft matter are extremely relevant to future modalities in manufacturing and chemical production, two of the greatest users of energy.

PO-F-3: CENTER FOR COMPLEX MATERIALS FROM FIRST PRINCIPLES (CCM)

[CCM] John P. Perdew[1], Gustavo E. Scuseria[2], Weitao Yang[3], Adrienn Ruzsinszky[1], David J. Srolovitz[4], Arun Bansil[5], Michael L. Klein[1], Xifan Wu[1], Jianwei Sun[6], Qimin Yan[1], Eric Borguet[1], Maria Iavarone[1], Xiaoxing Xi[1], Daniel Strongin[1], Michael J. Zdilla[1], Goran Karapetrov[7], Yimei Zhu[8]

[1]Temple University (lead institution), [2]Rice University, [3]Duke University, [4]University of Pennsylvania, [5]Northeastern University, [6]Tulane University, [7]Drexel University, [8]Brookhaven National Laboratory



The mission of CCM is to develop, test, apply, and experimentally validate improved methods of electronic structure calculation for both simple and complex materials (including quantum materials). Planned tests and applications include the layered and two-dimensional (2D) materials, topological, strongly-correlated, and disordered materials, plus water at interfaces, heterostructures, defects, catalysis, and materials synthesis.

PO-F-4: CENTER FOR GAS SEPARATIONS (CGS)

[CGS] Jeffrey R. Long[1,2], Craig M. Brown[3], Walter S. Drisdell[2], Laura Gagliardi[4], Maciej Haranczyk[2], Brett A. Helms[2], David Hopkinson[5], Jeffrey B. Neaton[1,2], David Prendergast[2], Wendy L. Queen[6], Jeffrey A. Reimer[1,2], Berend Smit[1,6], Simon J. Teat[2], Michael Tsapatsis[4], Stephen Whitelam[2], Ting Xu[1,2], Omar M. Yaghi[1,2], Hong-Cai Zhou[7]

[1]University of California, Berkeley; [2]Lawrence Berkeley National Laboratory (LBNL); [3]National Institute of Standards and Technology (NIST); [4]University of Minnesota; [5]National Energy Technology Laboratory (NETL); [6]Ecole Polytechnique Fédérale de Lausanne (EPFL), Switzerland; [7]Texas A&M University

The mission of the Center for Gas Separations (CGS) is to develop the fundamental science necessary to tailor make new materials that enable the energy-efficient separation of gas mixtures. Particular emphasis is placed on separations that reduce CO_2 emissions from power plants and on energy-intensive gas separations in industry and agriculture. The targeted synthesis of novel metal–organic framework and membrane adsorbents is informed and supported by rigorous *in situ* characterization and computational methods being developed in tandem by the CGS.

PO-F-5: CENTER FOR HIERARCHICAL WASTE FORM MATERIALS (CHWM)

[CHWM] Jake Amoroso[1], Theodore M. Besmann[2], Kyle Brinkman[3], David DiPrete[1], Agnes Grandjean[4], Charles H. Henager Jr.[5], Shenyang Hu[5], Scott Misture[6], Simon R. Phillpot[7], Natalia Shustova[2], Hans-Conrad zur Loye[2]

[1]Savanah River National Laboratory, [2]University of South Carolina (lead institution), [3]Clemson University, [4]Commissariat à l'Energie Atomique et aux Energies Alternatives, [5]Pacific Northwest National Laboratory, [6]Alfred University, [7]University of Florida

The mission of CHWM is to combine experiment and modeling to develop the chemistry and structure motifs needed to create hierarchical materials that effectively immobilize nuclear waste in persistent architectures.

PO-F-6: CENTER FOR LIGNOCELLULOSE STRUCTURE AND FORMATION (CLSF)

[CLSF] Daniel J. Cosgrove[1], Charles T. Anderson[1], Paul Dupree[2], Enrique Gomez[1], Esther Gomez[1], Ying Gu[1], Candace H. Haigler[3], Mei Hong[4], Seong H. Kim[1], James D. Kubicki[5], Manish Kumar[1], B. Tracy Nixon[1], Hugh O'Neill[6], Alison Roberts[7], Ming Tien[1], Yaroslava Yingling[3], Jochen Zimmer[8]

[1]The Pennsylvania State University (lead institution); [2]University of Cambridge; [3]North Carolina State University; [4]Massachusetts Institute of Technology; [5]University of Texas El Paso; [6]Oak Ridge National Laboratory; [7]University of Rhode Island; [8]University of Virginia

Our mission at the Center for Lignocellulose Structure and Formation (CLSF) is to develop a nano- to meso-scale understanding of cellulosic cell walls, the energy-rich structural material in plants, and the physical mechanisms of wall assembly, forming the foundation for new technologies in sustainable energy and novel biomaterials.

PO-F-7: ENERGY DISSIPATION TO DEFECT EVOLUTION (EDDE)

[EDDE] Karren L. More[1], William J. Weber[2,1], Dilpuneet S. Aidhy[3], Hongbin Bei[1], Magdalena Caro[4], Alfredo Correa[5], Philip D. Edmondson[1], Takeshi Egami[2,1], Yury Osetskiy[1], Ian M. Robertson[6], German D. Samolyuk[1], G. Malcolm Stocks[1], Lumin Wang[7], Eva Zarkadoula[1], Fuxiang Zhang[1], Yanwen Zhang[1]

[1]Oak Ridge National Laboratory (lead institution); [2]University of Tennessee-Knoxville; [3]University of Wyoming; [4]Virginia Tech; [5]Lawrence Livermore National Laboratory; [6]University of Wisconsin-Madison; [7]University of Michigan-Ann Arbor

The scientific mission of the EDDE Energy Frontier Research Center is to understand and exploit extreme chemical complexity to control energy dissipation and defect evolution under equilibrium and non-equilibrium conditions, which will guide the development of radiation-tolerant alloys or alloys with unique magnetic and thermal properties.

PO-F-8: PHOTONICS AT THERMODYNAMIC LIMITS (PTL)

[PTL] Jennifer Dionne[1], Paul Alivisatos[2], Harry Atwater[3], Mark Brongersma[1], Paul Braun[4], Shanhui Fan[1], Naomi Ginsberg[2], Tony Heinz[1], Aaron Lindenberg[1], Prineha Narang[5], Ralph Nuzzo[4], Eran Rabani[2], Alberto Salleo[1], Eli Yablonovitch[2]

[1]Stanford University (lead institution); [2]University of California, Berkeley; [3]California Institute of Technology; [4]University of Illinois at Urbana-Champaign; [5]Harvard University

The Photonics at Thermodynamic Limits Energy Frontier Research Center (PTL-EFRC) strives to achieve photonic operations at thermodynamic limits by controlling the flow of photons, electrons, and phonons in atomically-architected materials, and thereby enable entirely new energy conversion systems.

PO-F-9: THE CENTER FOR UNDERSTANDING AND CONTROL OF ACID GAS-INDUCED EVOLUTION OF MATERIALS FOR ENERGY (UNCAGE-ME)

[UNCAGE-ME] Jonas Baltrusaitis[4], David A. Dixon[7], Sophia E. Hayes[6], Christopher W. Jones[1], Ryan P. Lively[1], Sankar Nair[1], Tina M. Nenoff[3], Katharine Page[2], Rampi Ramprasad[1], Jessica Rimsza[3], J.R. Schmidt[8], David S. Sholl[1], Susan B. Sinnott[5], Bobby G. Sumpter[2], Israel E. Wachs[4], Krista S. Walton[1], Zili Wu[2]

[1]Georgia Institute of Technology (lead institution); [2]Oak Ridge National Laboratory; [3]Sandia National Laboratories; [4]Lehigh University; [5]Pennsylvania State University; [6]Washington University in St. Louis; [7]University of Alabama; [8]University of Wisconsin – Madison.

UNCAGE-ME seeks to develop and harness a deep knowledge base in the characterization, prediction, and control of acid-gas interactions with a broad class of materials to accelerate materials discovery in acid gas separations, conversion, and utilization.

PO-F-10: CENTER FOR PERFORMANCE AND DESIGN OF NUCLEAR WASTE FORMS AND CONTAINERS (WASTEPD)

[WastePD] Gerald S. Frankel,[1] Jincheng Du,[2] Stephane Gin,[3] Seong H. Kim,[4] Jie Lian,[5] Jenifer S. Locke,[1] Gregory B. Olson,[6] Joseph V. Ryan,[7] John R. Scully,[8] Chris D. Taylor,[1] John D. Vienna,[7] Jianwei Wang,[9] Wolfgang Windl[1]
[1]Ohio State University (lead institution); [2]University of North Texas; [3]Commissariat à l'énergie atomique et aux énergies alternatives (CEA), France; [4]Pennsylvania State University; [5]Rensselaer Polytechnic Institute; [6]QuesTek Innovations LLC; [7]Pacific Northwest National Laboratory; [8]University of Virginia; [9]Louisiana State University

The Center for Performance and Design of Nuclear Waste Forms and Containers (WastePD) is an EFRC comprising a focused scientific effort to understand the details of and commonalities in the aqueous corrosion mechanisms of glass, ceramics, and metals. The mission of WastePD is to understand the fundamental mechanisms of waste form degradation, and to apply that understanding to develop approaches for the design of new waste forms with improved performance.

G. NUCLEAR ENERGY

PO-G-1: CENTER FOR ACTINIDE SCIENCE AND TECHNOLOGY (CAST)

[CAST] Susan E. Latturner[1], A. Eugene DePrince III[1], David E. Graf[2], Ryan E. Baumbach[1,2], Kenneth Hanson[1], Eric J. Schelter[3], Stosh Kozimor[4], Andrew J. Gaunt[4], Ping Yang[4], Enrique R. Batista[4], Georg Schreckenbach[5], Jochen Autschbach[6], Christopher J. Dares[7], Konstantinos Kavallieratos[7], Ines Triay[7], Suzanne C. Bart[8], John K. Gibson[9], David E. Hobart[1], Thomas E. Albrecht-Schmitt[1,2]
[1]Florida State University (lead institution); [2]National High Magnetic Field Laboratory; [3]University of Pennsylvania; [4]Los Alamos National Laboratory; [5]University of Manitoba; [6]State University of New York at Buffalo; [7]Florida International University; [8]Purdue University; [9]Lawrence Berkeley National Laboratory

The mission of CAST is to advance our understanding of how electronic structure and bonding influence the chemical and physical properties of heavy elements that lead to the development of game-changing nuclear technologies that improve energy security, environmental remediation, and train the next generation of nuclear scientists.

PO-G-2: FUNDAMENTAL UNDERSTANDING OF TRANSPORT UNDER REACTOR EXTREMES (FUTURE)

[FUTURE] Mark Asta[1], Thak Sang Byun[2], Laurent Capolungo[3], Danny J. Edwards[2], Edward F. Holby[3], Peter Hosemann[1], Djamel Kaoumi[4], Timothy G. Lach[2], Nan Li[3], Digby D. Macdonald[1], Andrew M. Minor[1], Raluca O. Scarlat[1], Daniel K. Schreiber[2], Farida A. Selim[5], John R. Scully[6], Blas P. Uberuaga[3], Yongqiang Wang[3]
[1]University of California, Berkeley; [2]Pacific Northwest National Laboratory; [3]Los Alamos National Laboratory (lead institution); [4]North Carolina State University; [5]Bowling Green State University; [6]University of Virginia

Our mission: 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.

PO-G-3: Interfacial Dynamics in Radioactive Environments and Materials (IDREAM)

[IDREAM] Sue B. Clark[1,2], Aurora E. Clark[2,1], Lawrence A. Anovitz[4], Jaehun Chun[1], James J. De Yoreo[1,3], Kerry W. Hipps[2], Gregory A. Kimmel[1], Jay A. La Verne[6], Xiaosong Li[3], Thomas M. Orlando[5], Katharine L. Page[4], Carolyn I. Pearce[1], Kevin M. Rosso[1], Gregory K. Schenter[1,2], Andrew G. Stack[4], Hsiu-Wen Wang[4]

[1]Pacific Northwest National Laboratory (lead institution), [2]Washington State University, [3]University of Washington, [4]Oak Ridge National Laboratory, [5]Georgia Institute of Technology, [6]University of Notre Dame

The vision of IDREAM is to master molecular–to–mesoscale chemical and physical phenomena at interfaces in complex environments characterized by extremes in alkalinity and low-water activity, and driven far from equilibrium by ionizing (γ,β) radiation.

PO-G-4: Molten Salts in Extreme Environments (MSEE)

[MSEE] James F. Wishart[1], Simon M. Pimblott[2], Shannon M. Mahurin[3], Lynne E. Ecker[1], Yu-chen Karen Chen-Wiegart[1,4], Eric Dooryhee[1], Anatoly I. Frenkel[1,4], Simerjeet K. Gill[1], Benjamin Ocko[1], Kotaro Sasaki[1], Ruchi Gakhar[2], Lingfeng He[2], Gregory Horne[2], Vyacheslav Bryantsev[3], Sheng Dai[3], Xiao-Guang Sun[3], Claudio J. Margulis[5], Jay A. LaVerne[6], Edward. J. Maginn[6]

[1]Brookhaven National Laboratory (lead institution), [2]Idaho National Laboratory, [3]Oak Ridge National Laboratory, [4]Stony Brook University, [5]University of Iowa, [6]University of Notre Dame

MSEE's mission is to provide fundamental and predictive understanding, based in atomistic/molecular level descriptions, of molten salt bulk and interfacial chemistry, including the effects of solutes, impurities and radiation, that will underpin molten salt reactor technology.

PO-G-5: Center for thermal Energy transport under irradiation (TETI)

David Hurley[1], Jian Gan[1], Michael Manley[2], Anter El-Azab[3], Marat Khafizov[4], Krzysztof Gofryk[1], Mukesh Bachlav[1], Jason Harp[1], Lingfeng He[1], Zilong Hua[1], Matthew Mann[5], Chris Marianetti[6], Janelle Wharry[3], Yongfeng Zhang[1]

[1]Idaho National Laboratory (Lead Institution), [2]Oak Ridge National Laboratory, [4]The Ohio State University, [5]Airforce Research Laboratory, [6]Columbia University

The mission of TETI is 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.

H. QUANTUM MATERIALS

PO-H-1: CENTER FOR THE ADVANCEMENT OF TOPOLOGICAL SEMIMETALS (CATS)

[CATS] Anand Bhattacharya[1], Anton Burkov[2], Paul Canfield[3,4], Olle Heinonen[1], Jennifer Hoffman[5], Pablo Jarillo-Herrero[6], Samuel Jiang[1], Adam Kaminski[3,4], Ross McDonald[7], Robert McQueeney[3,4], Peter Orth[3,4], Susanne Stemmer[8], Toni Taylor[7], Ashvin Vishwanath[5], Linlin Wang[3], Dmitry Yarotski[7], Jianxin Zhu[7]
[1]Argonne National Laboratory; [2]University of Waterloo; [3]Ames Laboratory (lead institution); [4]Iowa State University; [5]Harvard University; [6]Massachusetts Institute of Technology; [7]Los Alamos National Laboratory; [8]University of California – Santa Barbara

CATS' mission is to understand and discover new quantum phenomena and functionality in topological semimetals. CATS has three research goals; (1) predict, discover, and understand archetypal magnetic TSMs and new topological states of matter, (2) establish the ability to control transitions between different topological states, and (3) reversibly manipulate the response of topological systems using external fields.

PO-H-2: INSTITUTE FOR QUANTUM MATTER (IQM)

[IQM] Collin L. Broholm[1], N. Peter Armitage[1], Robert J. Cava[2], Natalia Drichko[1], Seyed M. Koohpayeh[1], Yi Li[1], Tyrel M. McQueen[1], Satoru Nakatsuji[1], Predrag Nikolic[1], Brad Ramshaw[3], Nitin Samarth[4], Oleg Tchernyshyov[1], David Vanderbilt[5]
[1]Johns Hopkins University (lead institution), [2]Princeton University, [3]Cornell University, [4]Penn State University, [5]Rutgers University

IQM realizes revolutionary quantum materials and structures where quantum effects such as entanglement and coherence find collective macroscopic manifestations. We expose, understand, and control the corresponding physical properties and explore the potential for energy related applications.

PO-H-3: CENTER FOR MOLECULAR MAGNETIC QUANTUM MATERIALS (M^{2}QM)

[M^{2}QM] Hai-Ping Cheng[1], Garnet Chan[2], George Christou[1], Arthur Hebard[1], Richard Hening[1], Stephen Hill[3], Talat Rahman[4], John Stanton[1], Neil Sullivan[1], Samuel Trickey[1], Vivien Zapf[5], Xiaoguang Zhang[1]
[1]University of Florida (lead institution); [2]California Institute of Technology; [3]Florida State University; [4]University of Central Florida; [5]Los Alamos National Lab

M^{2}QM aims to deepen understanding and optimize control of electron-level physical processes to turn molecular magnets into quantum materials. We tune inter-molecule communication via magnetic interactions in clusters and solids and we design and perfect the underlying materials science for future computers and electronics.

PO-H-4: CENTER FOR NOVEL PATHWAYS TO QUANTUM COHERENCE IN MATERIALS (NPQC)

[NPQC] James G. Analytis[1,2], David D. Awschalom[3,4], Dmitri N. Basov[5], Ania C. Bleszynski Jayich[6], Stefano Cabrini[1], Aashish A. Clerk[3,4], Michael F. Crommie[1,2], Peter Ercius[1], Giulia Galli[3,4], Naomi S. Ginsberg[1,2], Supratik Guha[3,4], F. Joseph Heremans[3], Martin Holt[3], Alessandra Lanzara[1,2], Joel E. Moore[1,2], Jeffrey B. Neaton[1,2], Joseph Orenstein[1,2], Jiwoong Park[3,4], Ramamoorthy Ramesh[1,2], Eli Rotenberg[1], Feng Wang[1,2], Alexander Weber-Bargioni[1], Chao Yang[1], Norman Y. Yao[1,2], Xufeng Zhang[3]

[1]Lawrence Berkeley National Laboratory (lead institution); [2]University of California, Berkeley; [3]Argonne National Laboratory; [4]University of Chicago; [5]Columbia University; [6]University of California, Santa Barbara

The mission of this EFRC is to expand dramatically our understanding and control of coherence in solids by building on recent discoveries in quantum materials along with advances in experimental and computational techniques.

PO-H-5: PROGRAMMABLE QUANTUM MATERIALS (PRO-QM)

[Pro-QM] Ana Asenjo-Garcia[1], Dmitri N. Basov[1], Jiun Haw Chu[2], David Cobden[2], Cory R. Dean[1], Daniel R. Gamelin[2], James Hone[1], Michal Lipson[1], Andrew J. Millis[1], Abhay Pasupathy[1], P. James Schuck[1], Di Xiao[3], Xiaodong Xu, Xiaoyang Zhu[1]

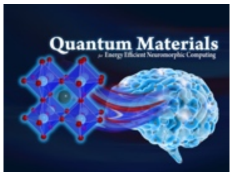
[1]Columbia University (lead institution), [2]University of Washington, [3]Carnegie Mellon University

The Mission of the Pro-QM Center is to discover, characterize and deploy new forms of quantum matter controllable by gating, magnetic proximity, light and nano-mechanical manipulation, effectively programming their quantum properties.

PO-H-6: QUANTUM MATERIALS FOR ENERGY EFFICIENT NEUROMORPHIC COMPUTING (Q-MEEN-C)

[Q-MEEN-C] Amanda Petford-Long[1], Alex Frano[2], Andy Kent[3], Axel Hoffmann[4], Robert Dynes[2], Eric Fullerton[2], Julie Grollier[5], Giulia Galli[6], Ivan K. Schuller[2], Jonathan Schuller[7], Marcelo Rozenberg[6], Mark Stiles[8], Oleg Shpyrko[2], Shriram Ramanathan[9], Shyue Ping-Ong[2], Vitaly Lomakin[2], Yayoi Takamura[10], Yeshaiahu Fainman[2], Yimei Zhu[11]

[1]Northwestern University; [2]University of California San Diego (lead institution); [3]New York University; [4]University of Illinois Urbana-Champaign; [5]Centre National de la Recherche Scientifique; [6]University of Chicago; [7]University of California Santa Barbara; [8]National Institute of Standards and Technology; [9]Purdue University; [10]University of California Davis; [11]Brookhaven National Laboratory



The mission of Q-MEEN-C is to generate the quantum-materials-based foundation for the development of an energy-efficient, fault-tolerant computer that is inspired by the human brain ("neuromorphic"). Q-MEEN-C's approach to achieving this focuses on research in the domains of both Charge- and Spin-related phenomena in quantum materials.

PO-H-7: Spins and Heat in Nanoscale Electronic Systems (SHINES)

[SHINES] Alex Balandin[1], Igor Barsukov[1], Chia-Ling Chien[2], Roger Lake[1], Allan MacDonald[3], Jing Shi[1], and Kang L. Wang[4]

[1]University of California, Riverside (lead institution); [2]Johns Hopkins University; [3] University of Texas at Austin; [4]Univerisity of California, Los Angeles.

SHINES aims at discovering or demonstrating new spintronic phenomena in antiferromagnetic heterostructures, developing an in-depth understanding of these phenomena, and controlling interactions such as magnetic anisotropy, exchange coupling, and spin dynamics.

K. Solar Energy

PO-K-1: Alliance for Molecular PhotoElectrode Design for Solar Fuels (AMPED)

[AMPED] Gerald J. Meyer[1], Alexander J. M. Miller[1], Joanna M. Atkin[1], Maurice S. Brookhart[1], James F. Cahoon[1], Jillian L. Dempsey[1], Yosuke Kanai[1], Thomas J. Meyer[1], John M. Papanikolas[1], John R. Reynolds[2], Kirk S. Schanze[3], Cynthia K. Schauer[1], Joseph L. Templeton[1], M. Kyle Brennaman[1]

[1]University of North Carolina at Chapel Hill (lead institution); [2]Georgia Institute of Technology; [3]University of Texas at San Antonio

The mission of AMPED is to develop the fundamental molecular basis for solar-driven water oxidation and carbon dioxide reduction catalysis.

PO-K-2: Center for Hybrid Organic Inorganic Semiconductors for Energy

[CHOISE] Matthew C. Beard[1], Jinsong Huang[2], Joseph Berry[1], Jeffery L. Blackburn[1], Kai Zhu[1], Joseph M. Luther[1], Giulia Galli[3], Wei You[2], Z. Valy Vardeny[4], Sarah Li[4], Adrienne D. Stiff-Roberts[5], Michael F. Toney[6], Pete Sercel[1], Yanfa Yan[6], Yong Yan[7], Volker Blum[4], David B. Mitzi[4]

[1]National Renewable Energy Laboratory (lead institution), [2]University of North Carolina-Chapel Hill, [3]University of Chicago, [4]University of Utah, [5]Duke University, [6]SLAC National Accelerator *Laboratory, [7]San Diego State University*

The mission of CHOISE is to enable unprecedented control over the emergent phenomena of spin, charge, and light-matter interactions, in tailored organic-inorganic perovskite-inspired systems for energy science.

PO-K-3: CENTER FOR MOLECULAR ELECTROCATALYSIS (CME)

[CME] Aaron M. Appel[1], R. Morris Bullock[1], Brandi M. Cossairt[2], Sharon Hammes-Schiffer[3], James M. Mayer[3], Jeffrey M. Miller[4], Simone Raugei[1], Thatcher Root[5], Shannon Stahl[5], Yogesh Surendranath[6], Eric S. Wiedner[1]

[1]Pacific Northwest National Laboratory (lead institution); [2]University of Washington, Seattle; [3]Yale University; [4]Purdue University; [5]University of Wisconsin–Madison; [6]Massachusetts Institute of Technology

The scientific mission of the Center for Molecular Electrocatalysis (CME) is to establish the fundamental principles needed for efficient interconversion of electrical energy and chemical bonds through precise control of electron and proton transfers.

PO-K-4: CENTER FOR LIGHT ENERGY ACTIVATED REDOX PROCESSES (LEAP)

[LEAP] Victor S. Batista[1], Gary W. Brudvig[1], Lin X. Chen[2,3], Robert Crabtree[1], Omar K. Farha[3], Sharon Hammes-Schiffer[1], Mark C. Hersam[3], Joseph T. Hupp[3], Mercouri G. Kanatzidis[3], Tobin J. Marks[3], Alex B. F. Martinson[2], James M. Mayer[2], Michael J. Pellin[2], George C. Schatz[3], Michael R. Wasielewski[3], Emily A. Weiss[3]

[1]Yale University; [2]Argonne National Lab; [3]Northwestern University (lead institution)

The mission of the Center for Light Energy Activated Redox Processes (LEAP) is to develop the fundamental scientific understanding needed to use efficient light-driven multi-electron redox processes to power energy-demanding chemistry.

M. SYNTHESIS SCIENCE

PO-M-1: CENTER FOR NEXT GENERATION OF MATERIALS DESIGN (CNGMD)

[CNGMD] William Tumas[1], David Ginley[1], Gerbrand Ceder[2], John Perkins[1], Stephan Lany[1], Andriy Zakutayev[1], Kristin Persson[2], Michael Toney[3], Feng Wang[4], Janet Tate[5], Brian Gorman[6], Aaron Holder[7], Daniel Nocera[8]

[1]National Renewable Energy Laboratory (lead institution); [2]Lawrence Berkeley National Laboratory; [3]SLAC National Accelerator Laboratory; [4]Brookhaven National Laboratory; [5]Oregon State University; [6]Colorado School of Mines; [7]University of Colorado; [8]Harvard University

The mission of CNGMD is to dramatically transform the discovery of functional energy materials through multiple-property search, incorporation of metastable materials into predictive design, and the development of theory to guide materials synthesis.

PO-M-2: CENTER FOR THE SCIENCE OF SYNTHESIS ACROSS SCALES (CSSAS)

[CSSAS] François Baneyx[1], James J. De Yoreo[2], Chris Mundy[2], Jim Pfaendtner[1], David Ginger[1], David Baker[1], Chun-Long Chen[2], Brandi Cossairt[1], Andrew Ferguson[3], Samson A. Jenekhe[1], Sergei V. Kalanin[4], F. Akif Tezcan[5]

[1]University of Washington (lead institution); [2]Pacific Northwest National Laboratory; [3]University of Chicago; [4]Oak Ridge National Laboratory; [5]University of California San Diego

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

PO-M-3: A NEXT GENERATION SYNTHESIS CENTER (GENESIS)

[GENESIS] John B. Parise,[1] Karena W. Chapman,[1] Peter Khalifah,[1] Simon L. Billinge,[2] Peter J. Chupas,[1] Kristin A. Persson,[3] Gabriel Veith,[4] Brian Phillips,[1] James R. Neilson,[5] Katsuyo S. Thornton,[6] Line Pouchard,[7] Eric Dooryhee,[7] Ping Liu,[8] Jack Simonson[9]

[1]Stony Brook University (lead institution); [2]Columbia University; [3]Lawrence Berkeley National Laboratory; [4]Oak Ridge National Laboratory; [5]Colorado State University; [6]University of Michigan; [7]Brookhaven National Laboratory; [8]University of California San Diego; [9]Farmingdale State University

GENESIS' mission is develop a new paradigm for synthesis that accelerates the discovery of materials, by understanding how key structural and chemical transformations during synthesis are governed by the synthesis variables.

Poster Session I: Tuesday, July 30, 2019; 9:40 – 11:00 AM, *Exhibition Hall C*

A. Bio-inspired Science

PI-A-1: Characterizing Primary Plant Cell Walls Through Soft X-Ray Scattering and Grazing-Incidence X-Ray Scattering
[CLSF] Sintu Rongpipi, Dan Ye, Sarah Kiemle, William Barnes, Charles Anderson, Daniel J. Cosgrove, Esther Gomez, Enrique Gomez
The Pennsylvania State University

PI-A-2: Reduction potentials of [FeFe]-hydrogenase accessory iron-sulfur clusters provide insights into the energetics of proton reduction catalysis
[BETCy] Jacob H Artz[1,2], David W. Mulder[2], Michael W. Ratzloff[2], Carolyn E. Lubner[2], Oleg A. Zadvornyy[1], Axl X. Levan[3], S. Garrett Williams[4], Michael W. W. Adams[5], Anne K. Jones[4], Paul W. King[2], John W. Peters[1]
[1]Washington State University, [2]National Renewable Energy Laboratory, [3]Montana State University, [4]Arizona State University, [5]University of Georgia

PI-A-3: Cellulose Synthesis Complexes: Structural and Functional Analysis of Protein-Protein Interactions
[CLSF] Arielle M. Chaves[1], Abhishek Singh[2], Mai L. Tran[1], Yaroslava G. Yingling[2], Candace H. Haigler[2], Charlie T. Anderson[3], Ming Tien[3], Alison W. Roberts[1]
[1]University of Rhode Island; [2]North Carolina State University; [3]The Pennsylvania State University

PI-A-4: Mechanisms of gating nucleotide-driven electron transfer in the nitrogenase Fe protein cycle
[BETCy] Natasha Pence[1,2], Monika Tokmina-Lukaszewska[1], Zhi-Yong Yang[3], Rhesa N. Ledbetter[3], Lance C. Seefeldt[3], Brian Bothner[1], John W. Peters[2]
[1]Montana State University, [2]Washington State University, [3]Utah State University

PI-A-5: Heterologously Expressed CesA Isoforms Synthesize Cellulose Microfibrils in Vitro
[CLSF] Pallinti Purushotham[1], Sung Hyun Cho[2], Ruoya Ho[1], Manish Kumar[2], Jochen Zimmer[1], B. Tracy Nixon[2]
[1]University of Virginia; [2]The Pennsylvania State University

B. CATALYSIS

PI-B-1: COMPUTATIONAL STUDIES OF OLEFIN CONVERSION USING METAL ORGANIC FRAMEWORKS

[ICDC] Carlo Alberto Gaggioli[1], Navneet Singh Khetrapal[1], Saumil Chheda[1], Dong Yang[2], Bruce C. Gates[2], Jian Zheng[3], Oliver Y. Gutierrez[3], Donald M. Camaioni[3], Ricardo Bermejo de Val[4], Johannes A. Lercher[3,4], Laura Gagliardi[1]

[1]University of Minnesota; [2]University of California, Davis; [3]Pacific Northwest National Lab; [4]Technische Universität München

PI-B-2: DYNAMICS IN CATALYTIC PROCESSES FROM COMPUTATIONS AND MACHINE LEARNING: BIMETALLIC SURFACE RESTRUCTURING AND ALCOHOL DEHYDROGENATION

[IMASC] Jin Soo Lim[1], Lixin Sun[1], Nicola Molinari[1], Simon Batzner[1], Wei Chen[1], Kaining Duanmu[2], Philippe Sautet[2] Boris Kozinsky[1]

[1]Harvard University, [2]University of California, Los Angeles

PI-B-3: ENHANCED TRANSITION METAL PHOTOCATALYTIC EFFICIENCY USING NATURAL LIGHT-HARVESTING SYSTEMS

[BioLEC] Stephanie M. Hart*[1], Minjung Son* [1], Beryl X. Li* [2] Talia J. Steiman* [2], Abigail G. Doyle [2], David W.C. MacMillan [2], Gabriela S. Schlau-Cohen [1]

*contributed equally

[1]Massachusetts Institute of Technology; [2]Princeton University

PI-B-4: UNDERSTANDING ACIDITY OF MOLTEN SALT HYDRATE MEDIA FOR CELLULOSE HYDROLYSIS BY COMBINING KINETIC STUDIES, ELECTROLYTE SOLUTION MODELING, MOLECULAR DYNAMICS SIMULATIONS AND 13C-NMR EXPERIMENTS

[CCEI] Natalia Rodriquez Quiroz[1], Arul M.D. Padmanathan[2], Samir H. Mushrif[2], Dionisios G. Vlachos[1]

[1]University of Delaware; [2]University of Alberta

PI-B-5: FACILE ELECTROCHEMICAL SYNTHESIS OF DENSELY-FUNCTIONALIZED QUINONES AND THEIR UTILIZATION IN AN ALL-QUINONE ORGANIC REDOX FLOW BATTERY

[CME] James B. Gerken[1], Sung-Eun Suh[1], Alexios Stamoulis[1], Nicholas D. Fischer[1], Colin W. Anson[1], Yuliya Preger[1], Yeon J. Kim[1], Peter G. Symons[3], J. David Genders[2], Yang Qiu[3], Wenzhen Li[3], Thatcher W. Root[1], Shannon S. Stahl[1]

[1]University of Wisconsin–Madison; [2]Electrosynthesis Company, Inc.; [3]Iowa State University

PI-B-6: COPPER COMPLEXES FOR WATER OXIDATION AND PROTON-COUPLED ELECTRON TRANSFER REACTIVITY OF TITANIUM DIOXIDE NANOPARTICLES

[LEAP] Katherine J. Fisher, Jennifer L. Peper, Gary W. Brudvig, Robert H. Crabtree, James M. Mayer

Yale University

PI-B-7: DILUTE PD IN AU ALLOYS FOR SELECTIVE HYDROGENATION REACTIONS: ACHIEVING SYNERGY BY TUNING THE ALLOY SURFACE COMPOSITION

[IMASC] Mathilde Luneau[1], Erjia Guan[2], Nicholas Marcella[2], Wei Chen[1], Alexandre C. Foucher[3], Tanya Shirman[1], Joanna Aizenberg[1], Eric A. Stach[3], Anatoly I. Frenkel[2], Robert J. Madix[1], Cynthia M. Friend[1]

[1]Harvard University, [2]Stony Brook University, [3]University of Pennsylvania

PI-B-8: PCET IN CATALYTIC PROCESSES: SYNTHESIS AND CHARACTERIZATION OF BENZIMIDAZOLE-PHENOL BASED IR-COMPLEXES.

[BioLEC] Emmanuel Odella[2], Hunter H. Ripberger[1], S. Jimena Mora[2], Daniel A. Heredia[2], Ana L. Moore[2], Thomas A. Moore[2], Robert R. Knowles[1]
[1]Princeton University; [2]Arizona State University

PI-B-9: THE REDUCTION OF CO_2 AND FORMATE ESTERS USING RUTHENIUM ELECTROCATALYSTS

[AMPED] Eric Assaf, Sergio Gonell, Alexander J. M. Miller
University of North Carolina at Chapel Hill

PI-B-10: SELF-ASSEMBLED ORGANIC NANOSTRUCTURES FOR PHOTOCATALYTIC CO_2-TO-CH_4 REDUCTION

[CBES] Luka Đorđević[1], Oliver Dumele[1], Hiroaki Sai[1], Adam Dannenhoffer[1], Hussain Sangji[1], Thomas Cotey[1], Liam C. Palmer[1], Samuel I. Stupp[1]
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PI-B-11: STRUCTURE, DYNAMICS, AND REACTIVITY OF FE(II) SITES SITUATED IN THE NODES OF A METAL-ORGANIC FRAMEWORK FOR LIGHT ALKANE OXIDATION

[ICDC] Matthew C. Simons[1], Jenny G. Vitillo[1], Melike Babucci[2], Adam Hoffman[3], Christopher J. Cramer[1], Simon Bare[3], Bruce C. Gates[2], Connie Lu[1], Laura Gagliardi[1], Aditya Bhan[1]
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PI-B-12: FIRST PRINCIPLES STUDIES OF FUNDAMENTAL PROCESSES IN ALKALINE ELECTROCATALYSIS

[CABES] Mariel Tader[1], Zhen (Coraline) Tao[2], Brian Ernst[1], Sharon Hammes-Schiffer[2], Robert DiStasio[1], Tomás Arias[1]
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PI-B-13: COMPUTATIONAL DESIGN OF MOLECULAR COMPLEXES FOR OXIDATION OF NH_3

[CME] Samantha I. Johnson[1], Spencer P. Heins[1], Christina M. Klug[1], Eric S. Wiedner[1], R. Morris Bullock[1], Simone Raugei[1]
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PI-B-14: COMPUTATIONAL CHARACTERIZATION OF HETEROGENEOUS PD(II) CATALYSTS ON ACID FUNCTIONALIZED METAL–ORGANIC FRAMEWORKS

[ICDC] Mukunda Mandal[1], Jingyun Ye[1], Ken-ichi Otake[2], Timur Islamoglu[2], Cassandra T. Buru[2], Joseph T. Hupp[2], Massimiliano Delferro[3], Omar K. Farha[2], Donald G. Truhlar[1], Christopher J. Cramer[1]
[1]University of Minnesota; [2]Northwestern University; [3]Argonne National Laboratory

PI-B-15: REPURPOSING OF FOOD WASTE TO AN INTEGRATED BIOREFINERY

[CCEI] Elvis Ebikade[1], Abhay Athaley[2], Benjamin Fisher[1], Kai Yang[1,3], Changqing Wu[1], Marianthi Ierapetritou[2], Dionisios G. Vlachos[1]
[1]University of Delaware; [2]Rutgers, The State University of New Jersey; [3]Zhejiang University of Technology

PI-B-16: DYNAMIC METAL/METAL OXIDE INTERFACE AFFECTS PDAG REACTIVITY

[IMASC] Christopher R. O'Connor[1], Tobias Egle[1], Matthijs A. van Spronsen[2], Mustafa Karatok[1], Vikram Mehar[3], Jason F. Weaver[3], Robert J. Madix[1], Cynthia M. Friend[1]
[1]Harvard University, [2]Lawrence Berkeley National Laboratory, [3]University of Florida

D. Energy Storage

PI-D-1: Deciphering Potentials across Solid State Battery Cells and Interfaces

[NEES] Michael Swift[1], Yue Qi[1], Kevin Leung[2]
[1]Michigan State University, [2]Sandia National Lab Livermore

PI-D-2: 3D electrode designs enabling high rate and regeneration

[m2M/t] Lei Wang[1], Lisa M. Housel[2], Alison H. McCarthy[2], Jianping Huang[2], Andrea M. Bruck[2], Calvin D. Quilty[2], Alyson Abraham[2], Diana M. Lutz[2], Christopher R. Tang[2], Andrew Kiss[1], Juergen Thieme[1], Kenneth J. Takeuchi[2], Esther S. Takeuchi[2], Amy C. Marschilok[2]
[1]Brookhaven National Laboratory; [2]Stony Brook University

PI-D-3: Ion and Solvent Dynamics in 'Solvent-In-Salt' Electrolytes

[FIRST] Ivan Popov[1], Robert Sacci[1], Nicolette Sanders[1], Naresh Osti[1], Eugene Mamontov[1], Takeshi Kobayashi[2], Marek Pruski[2,3], Ray Matsumoto[4], Peter T. Cummings[4], Alexei P. Sokolov[1,5]
[1]Oak Ridge National Laboratory; [2]U.S. DOE Ames Laboratory; [3]Iowa State University; [4]Vanderbilt University; [5]University of Tennessee

PI-D-4: Experimental and Theoretical Studies of Solid Electrolyte-Electrode Interfaces in Solid State Batteries

[CEES] Jason D. Howard[1], Jae Jin Kim[1], Shane Patel[2], Robert E. Warburton[3], Bruce Buchholtz[2], Jeffrey Greeley[3], Chris Wolverton[2], Timothy T. Fister[1], Larry A. Curtiss[1], Vinayak P. Dravid[2], Paul Fenter[1]
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PI-D-5: Reversible anion redox in lithium metal chalcogenides

[SCALAR] Charles J. Hansen[1], Andrew J. Martinolich[1], Jesse S. Ko[2], Joshua J. Zak[1], Nicholas H. Bashian[3], Brent C. Melot[3], Johanna Nelson Weker[2], Kimberly A. See[1]
[1]California Institute of Technology; [2]SLAC National Accelerator Laboratory; [3]University of Southern California

PI-D-6: Synchrotron radiation techniques for determination of electrochemically induced structural evolution

[m2M/t] David C. Bock[1], Matthew M. Huie[2], Andrea M. Bruck[2], Lei Wang[1], Killian R. Tallman[2], Calvin D. Quilty[2], Lisa M. Housel[2], Kent Jingxu Zheng[3], Qing Zhao[4], Xiaotun Liu[4], Tian Tang[4], Chavis A. Stackhouse[2], Andrew Kiss[1], Juergen Thieme[1], Lynden A. Archer[3], Amy C. Marschilok[2], Kenneth J. Takeuchi[2], Esther S. Takeuchi[2]
[1]Brookhaven National Laboratory; [2]Stony Brook University; [3]Cornell University

PI-D-7: Strategies for Enhancing Safety and Stability of Lithium Metal Batteries

[CEES] Maria A. Philip[1], Xiangbo Meng[2], Joseph A. Libera[2], Lingzi Sang[1], Kimberly L. Bassett[1], Fernando C. Castro[3], Matthias J. Young[2], Lin Chen[2], Patrick T. Sullivan[1], Ruixian Zhang[1], Griffin A. Wooley[1], Stephanie A. Kohn[1], Ken Madsen[1], Rachel Yang[1], Richard T. Haasch[1], Jeffrey W. Elam[2], Vinayak P. Dravid[3], Ralph G. Nuzzo[1], Andrew A. Gewirth[1]
[1]University of Illinois Urbana-Champaign, [2]Argonne National Laboratory, [3]Northwestern University

PI-D-8: Enabling Multielectron Cathode Ɛ-VOPO4 To Reach Theoretical Capacity For Lithium-Ion Batteries

[NECCES] Carrie Siu[1], Hui Zhou[1], Fredrick Omenya[1], Natasha A. Chernova[1], Hanlei Zhang[1], Jatinrana Kumar[1], Mateusz Zuba[1], Louis Piper[1], Guangwen Zhou[1], M. Stanley Whittingham[1], Sylvia Britto[2], Ieuan D. Seymour[2], Clare P. Grey[2] Kamila M. Wiaderek[3], Karena W. Chapman[3,4], Yuh-Chieh Lin[5], Lek-Heng Chu[5], Shyue Ping Ong[5], Bohua Wen[6], Yet Ming Chiang[6]

[1]Binghamton University, [2]Cambridge University, [3]Argonne National Lab., [4]Stony Brook University, [5]UC San Diego, [6]MIT

PI-D-9: DFTB for electrolyte transport/reaction modeling in energy storage systems, and implementation on SUMMIT

[FIRST] [1]Stephan Irle, [1]Van Quan Vuong, [1]Dan Han

[1]Oak Ridge National Laboratory

PI-D-10: High-Performance Ionogel 2.5D Solid-State Batteries: Experiment and Simulation

[NEES] Martin A. Edwards[1], David S. Ashby[2], A. Alec Talin[3], Bruce Dunn[2], Henry S. White[1]

[1]University of Utah, [2]University of California Los Angeles, [3]Sandia National Lab Livermore

PI-D-11: Chemistry of 2D Nanomaterials Gel Electrolyte Interfaces

[CEES] Norman S. Luu[1], Woo Jin Hyun[1], Cesar Villa[1], Carlos G. Torres-Castanedo[1], Jin-Myoung Lim[1], Xiaobing Hu[1], Michael J. Bedzyk[1], Vinayak P. Dravid[1], Mark C. Hersam[1]

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PI-D-12: Understanding lithiation and sodiation mechanisms in volume change anodes for electrochemical energy storage

[SCALAR] Andrew A. Dawson[1], Jesse S. Ko[2], Joseph A. Mazzetti[1], Johanna N. Weker[2], Sarah H. Tolbert[1]

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PI-D-13: Improving electron and ion access: The role of mesoscale electrode chemistry and structure

[m2M/t] Elsa Reichmanis[1], Yo Han Kwon[1], Jung Jin Park[2], Lisa M. Housel[3], Krysten Minnici[1], Guoyan Zhang[1], Sujin R. Lee[1], Seung Woo Lee[1], Zhongming Chen[4], Suguru Noda[4], Esther S. Takeuchi[3], Kenneth J. Takeuchi[3], Amy C. Marschilok[3]

[1]Georgia Institute of Technology; [2]Korea Advanced Institute of Science and Technology (KAIST); [3]Stony Brook University; [4]Waseda University

PI-D-14: Contrasting Oxygen Participation between Conventional and Li-Rich Nmc Layered Oxides

[NECCES] Zachary Lebens-Higgins[1], Antonin Grenier[2], Mateusz Zuba[1], Hyeseung Chung[3], Yixuan Li[3], Y. Shirley Meng[3], Karena Chapmen[2], Louis F. J. Piper[1]

[1]Binghamton University, [2]Stony Brook University, [3]UC San Diego

PI-D-15: Protection Layers for Reactive Electrodes

[NEES] Chuanfu Lin [1], Haotian Wang [1], Yang Wang [1], Sang Bok Lee [1], Gary Rubloff [1]

[1]University of Maryland

E. ENERGY - WATER

PI-E-1: X-RAY SPECTROSCOPY FOR INVESTIGATION OF MEMBRANE CHEMISTRY AND STRUCTURE
[M-WET] Audra DeStefano[1], Thomas Webber[1], Mikayla Barry[1], Pinar Aydogan Gokturk[2], Alex Hexemer[2], Ethan Crumlin[2], Rachel Segalman[1]
University of California at Santa Barbara[1], Lawrence Berkeley National Labs[2]

PI-E-2: A MICROFLUIDIC PLATFORM FOR ASSESSING REACTION AND TRANSPORT IN FRACTURED SHALE MEDIA
[CMC-UF] Bowen Ling[1], Ziyan Wang[1], Jennifer L. Druhan[2], Illenia Battiato[1]
[1]Stanford University;[2]Univeristy of Illinois Urbana Champaign

PI-E-3: – EFFECTS OF CONFINEMENT ON THE HYDRATED PROTON IN MICROPOROUS MATERIALS
[AMEWS] James P. Dombrowski[1], Xinyou Ma[2], Nicholas Lewis[2], Harold H. Kung[1], Gregory Voth[2], Andrei Tokmakoff[2]
[1]Northwestern University; [2]University of Chicago

PI-E-4: COMBINED EXPERIMENTAL, COMPUTATIONAL AND THEORETICAL INVESTIGATION OF PURE FLUIDS AND ELECTROLYTES UNDER CONFINEMENT
[CENT] Samuel Faucher, Rahul Prasanna Misra, Pedro de Souza, Strano, Daniel Blankschtein, Martin Bazant, Michael Strano
Massachusetts Institute of Technology

PI-E-5: UNIVERSAL MEMBRANE PLATFORM TO PROBE FUNDAMENTALS OF MOLECULAR AND MESOSCOPIC SOLUTE-MATERIAL INTERACTIONS
[M-WET] Ségolène Antoine[1], Zhishuai Geng[1], Malgorzata Chwatko[2], Nate Lynd[2], Craig Hawker[1], Rachel Segalman[1]
University of California at Santa Barbara[1], University of Texas at Austin[2]

PI-E-6: VAPOR PRESSURE CURVES OF CONFINED HYDROCARBONS
[MUSE] Hyeyoung Cho[1], Michael Bartl[1], Jiaoyan Li[2], Hai Huang[2], Milind Deo[1]
[1]University of Utah, [2]Idaho National Laboratory

PI-E-7: ION TRANSPORT IN HYDRATED NANOCONFINED POLYELECTROLYTES
[AMEWS] Yu Kambe[1,2], Weiwei Chu[1], Veronica Burnett[1], Juan de Pablo[1,2], Paul Nealey[1,2]
[1]Argonne National Laboratory; [2]University of Chicago

PI-E-8: AN EXPERIMENTAL FRAMEWORK FOR MULTISCALE CHARACTERIZATION OF THE FABRIC OF NANOPOROUS MEDIA
[CMC-UF] Vladimir Alvarado[1], Tony Kovscek[2], Sally Benson[2], Mark Zoback[2], Teresa Lehmann[1]; Timothy I. Anderson[2], Bolivia Vega[2], Arjun Kohli[2]
[1]University of Wyoming; [2]Stanford University

PI-E-9: ION AND WATER TRANSPORT IN HIGHLY SELECTIVE POLYMER MEMBRANES
[M-WET] Rahul Sujanani[1], Marshall Allen[1], Freddy Rivers[1], Samuel Warnock[2], Shou Zhou[2], Christopher Bates[2], Mahdi Abu-Omar[2], Benny Freeman[1]
University of Texas at Austin[1], University of California at Santa Barbara[2]

PI-E-10: FLOW IN MESOSCALE POROUS MEDIA

[MUSE] Pranay Asai[1], Thang Tran[1], James Sutherland[1], Milind Deo[1], Jiaqi JIn[1], Jan Miller[1], Yidong Xia[2], Hai Huang[2]
[1]University of Utah, [2]Idaho National Laboratory

PI-E-11: SEQUENTIAL INFILTRATION SYNTHESIS OF FUNCTIONAL OXIDES: TEMPLATING ISOPOROUS ELECTRODES

[AMEWS] Ruben Waldman[1], Nari Jeon[2], David Tiede[2], Seth Darling[2], Alex Martinson[2]
[1]University of Chicago; [2]Argonne National Laboratory

F. MATERIALS AND CHEMISTRY BY DESIGN

PI-F-1: A PHYSICS-BASED MESOSCALE MODEL OF ION EXCHANGE IN HIERARCHICAL NUCLEAR WASTEFORM MATERIALS

[CHWM] Y.L. Li[1], Ben D. Zeidman[1], Shenyang Hu[1], Charles H. Henager Jr.[1], Theodore M. Besmann[2], Agnes Grandjean[3]
[1]Pacific Northwest National Laboratory, [2]University of South Carolina, [3]Commissariat à l'Energie Atomique et aux Energies Alternatives

PI-F-2: THE CORROSION AND PASSIVE PROPERTIES OF HIGH ENTROPY ALLOYS

[WastePD] Angela Y. Gerard,[1] Stephen J. McDonnell,[1] Keren Freedy,[1] Bi-Cheng Zhou,[1] Kang Wang,[1] Daniel K. Schreiber,[2] Stephane Gin,[3] Pin Lu,[4] James Saal,[4] Gerald S. Frankel,[5] John R. Scully[1]
[1]University of Virginia; [2]Pacific Northwest National Laboratory; [3]Commissariat à l'énergie atomique et aux énergies alternatives (CEA), France; [4]QuesTek Innovations LLC; [5]Ohio State University

PI-F-3: UNDERSTANDING AND EXPLOITING THE INTERACTION OF SOLID-BINDING PROTEINS WITH SILICA

[CSSAS] Brittney Hellner[1], Yundi Zhao[1], Julia Boese[1], Sarah Alamdari[1], Harley Pyles[1], Seong Beom Lee[1], Akshay Subramaniam[1], Kathryn Guye[1], David Ginger[1], Venkat R. Subramanian[1], David Baker[1], Jim Pfaendtner[1], François Baneyx[1]
[1]University of Washington

PI-F-4: REDOX ACTIVE SMALL MOLECULE SALTS IN DEEP EUTECTIC SOLVENTS: SYNTHESIS, CHARACTERIZATION, AND ACTIVITY

[BEES] Sarah Mitchell[1], Maria Escamilla[1], Brian Chen[1], Yun-Yang Lee[1], Burcu Gurkan[1], Emily Pentzer[1]
[1]Case Western Reserve University

PI-F-5: CONTROLLING TRANSPORT IN SOLID-STATE METATHESIS REACTIONS USING MOLECULAR ADDITIVES AND LAYERED HETEROSTRUCTURES

[GENESIS] Paul Todd[1], Rebecca McAuliffe[2], Michelle Beauvais[3], David Montiel,[4] Rhiannon Garrard[3], James R. Neilson[1], Karena W. Chapman[3], Gabriel M. Veith[2], Katsuyo S. Thornton[4]
[1]Colorado State University; [2]Oak Ridge National Laboratory; [3]Stony Brook University; [4]University of Michigan

PI-F-6: PREDICTIVE MODELS ON WATER STABILITY IN METAL ORGANIC FRAMEWORKS USING MACHINE LEARNING

[UNCAGE-ME] Rohit Batra[1], Carmen Chen[1], Krista S. Walton[1], Rampi Ramprasad[1]
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PI-F-7: Heterostructured Electrode Materials for Pseudocapacitive Energy Storage

[FIRST] De-en Jiang[1], Lihua Xu[1], Kaitlyn Prenger[2], Kun Liang[2], Michael Naguib[2], Karthik Ganeshan[3], Yun Kyung Shin[3], Adri van Duin[3], Weiwei Sun[4], Paul Kent[4], Qiang Gao[4], Ray Unocic[4], Nina Balke[4], Sheng Dai[4], Yury Gogotsi[5]

[1]University of California, Riverside; [2]Tulane University; [3]Pennsylvania State University; [4]Oak Ridge National Laboratory; [5]Drexel University

PI-F-8: Characterization of Metal–Organic Frameworks via in Situ Ftir Spectroscopy

[CGS] Henry Z. H. Jiang[1], Julia Oktawiec[1], Rodolfo Torres-Gavosto[1], Eugene Kim[1], Rebecca L. Siegelman[1], Matthew T. Kapelewski[1], Eric Granlund[1], Stephen FitzGerald[2], Jeffrey R. Long[1,3]

[1]University of California, Berkeley; [2]Oberlin College; [3]Lawrence Berkeley National Laboratory

PI-F-9: Light-Activated Magnetoelastic Soft Walker

[CBES] Chuang Li[1], Garrett Lau[1], Hang Yuan[1], Shuangping Liu[1], Victor Lopez Dominguez[1], Aaveg Aggarwal[1], Tyler Pearson[1], Hiroaki Sai[1], Liam C. Palmer[1], Danna Freedman[1], Pedram Khalili[1], Monica Olvera de la Cruz[1], Samuel I. Stupp[1]

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PI-F-10: Photochemical properties of solid-state organic semiconductor photocatalysts

[BioLEC] Xiao Liu[1], Daniela Arias-Rotondo[1], Dave MacMillan[1], Barry P. Rand[1]

[1]Princeton University

PI-F-11: Atomic Layer Deposition of TiO_X and SnO_X on Nanocrystalline, Mesoporous TiO_2 and SnO_2 Thin Films, and the Dye-Metal Oxide Interfacial Dynamics

[AMPED] Michael J. Mortelliti[1], Rachel Bangle[1], Annie N. Wang[1,2], Gerald J. Meyer[1], Jillian L. Dempsey[1]

[1]University of North Carolina at Chapel Hill; [2]North Carolina School of Science and Mathematics

PI-F-12: Stabilization of Formate Dehydrogenase in a Metal-Organic Framework for Bioelectrocatalytic Reduction of CO_2

[LEAP] Yijing Chen, Peng Li, Hyunho Noh, Chung-Wei Kung, Cassandra T. Buru, Xingjie Wang, Xuan Zhang and Omar K. Farha*

Northwestern University

PI-F-13: Scanning Tunneling Spectroscopy of Coherent Atomically-Thin Superlattices

[NPQC] Charlotte Herbig[1], Canxun Zhang[1], Zahra Pedramrazi[1], Fauzia Mujid[2], Saien Xie[3], Jiwoong Park[2,4]; Michael F. Crommie[1,5]

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PI-F-14: Stroboscopic elastic scattering microscopy of 2D transition metal dichalcogenide heterostructures

[PTL] Hannah L. Weaver[1], Milan Delor[1], James K. Utterback[1], Joeson W. Wong[2], Qin (Arky) Yang[2], Cora M. Went[2], Harry A. Atwater[2], Naomi S. Ginsberg[1]

[1]University of California, Berkeley; [2]California Institute of Technology

PI-F-15: HIGH ACCURACY CALCULATIONS OF THE INTERACTIONS OF LEWIS AND BRØNSTED ACID GASES WITH MOF MODELS

[UNCAGE-ME] Zachary Lee[1], Luis Flores[1], Shengjie Zhang[1], Yang Liu[2], David S. Sholl[2], David A. Dixon[1]

[1]University of Alabama; [2]Georgia Institute of Technology

PI-F-16: CONTROLLING PROTEIN ASSEMBLY ON INORGANIC CRYSTALS THROUGH DESIGNED PROTEIN INTERFACES

[CSSAS] Harley Pyles[1], Shuai Zhang[2], Fatima Davila[1], Sarah Alamdari[1], Maxim Ziatdinov[3], James J. De Yoreo[2], Jim Pfaendtner[1], David Baker[1], Christopher J. Mundy[2], Sergei V. Kalanin[3]

[1]University of Washington; [2]Pacific Northwest National Laboratory; [3]Oak Ridge National Laboratory

PI-F-17: DISCOVERY OF NEW TERNARY NITRIDE SEMICONDUCTORS WITH WURTZITE-DERIVED CRYSTAL STRUCTURE

[CNGMD] Sage Bauers[1], Stephan Lany[1], Bor-Rong Chen[2], Wenhao Sun[3], Aaron Holder[4], Christopher Bartel[3], John Mangum[5], Brian Gorman[5], Michael Toney[2], Laura Schelhas[2], John Perkins[1], Gerbrand Ceder[3], William Tumas[1], Andriy Zakutayev[1]

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PI-F-18: THE ELECTRICAL DOUBLE LAYER REVISITED

[CENT] *Amanda Souna[1], Jake Polster[2], Jason Tran[1], Rachel Lucas[2], Narayan Aluru[3], John Fourkas[1], Zuzanna Siwy[2]*

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PI-F-19: ELECTROCHEMISTRY AND NMR STUDIES OF MICROEMULSIONS AND NOHMS

[BEES] Nelly Cantillo-Cuello[1], Adam Imel[1], Jing Peng[1], Gabriel Goenaga[1], Ramez Elgammal[1], K. Mackenzie Nelms[1], Brian Barth[1], Douglas Hayes[1], Thomas A. Zawodzinski[1]

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PI-F-20: ICME DESIGN OF CORROSION RESISTANT HEAS FOR HARSH ENVIRONMENTS

[WastePD] Pin Lu,[1] Greg B. Olson,[1] Tianshu Li,[2] Orion J. Swanson,[2] Gerald S. Frankel,[2] Angela Y. Gerard,[3] Kathleen F. Quiambao,[3] John R. Scully[3]

[1]QuesTek Innovations LLC; [2]Ohio State University; [3]University of Virginia

PI-F-21: ENERGETICS OF MULTIDIMENSIONAL DEFECTS IN NI-BASED CONCENTRATED ALLOYS

[EDDE] Gaurav Arora[1], Anus Manzoor[1], Giovanni Bonny[2], Boopathy Kombaiah[3], Hongbin Bei[3], Phil D. Edmonson[3], Yanwen Zhang[3], Dilpuneet S. Aidhy[1]

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PI-F-22: UNPRECEDENTED STABILITY, FLEXIBILITY, AND STRUCTURAL TUNABILITY OF ACTINIDE-BASED METAL-ORGANIC FRAMEWORKS

[CHWM] Otega A. Ejegbavwo[1], Corey R. Martin[1], Oyindamola A. Olorunfemi[1], Gabrielle A. Leith[1], Richard T. Ly[1], Allison M. Rice[1], Ekaterina Dolgopolova[1], Mark D. Smith[1], Stavros G. Karakalos[1], Nancy Birkner[2], Brian A. Powell[2], Shubham Pandey[3], Robert J. Koch[4], Scott T. Misture[5], Hans-Conrad zur Loye[1], Simon R. Phillpot[3], Kyle S. Brinkman[2], Natalia B. Shustova[1]

[1]University of South Carolina, [2]Clemson University, [3]University of Florida, [4]Brookhaven National Laboratory, [5]Alfred University

PI-F-23: HOMOLEPTIC DITHIOCARBAMATE COMPOUNDS OF THE LANTHANIDES AND MIDDLE ACTINIDES

[CAST] Joseph M. Sperling, Alyssa N. Gaiser, Evan J. Warzecha, Cristain Celis-Barros, Thomas E. Albrecht-Schmitt
Florida State University

PI-F-24: SHAPE-DIRECTED PROPULSION OF LIGHT-RESPONSIVE QUINCKE ROLLERS

[CBES] Yong Dou[1], Zhengyan Zhang[1], Zhiqiang Pei[2], Paul M. Chaikin[3], Samuel I. Stupp[2], Kyle J.M. Bishop[1]
[1]Columbia University; [2]Northwestern University; [3]New York University

PI-F-25: GAS SEPARATIONS VIA BACKBONDING IN A METAL–ORGANIC FRAMEWORK WITH OPEN VANADIUM(II) COORDINATION SITES

[CGS] David E. Jaramillo[1], Douglas A. Reed[1], Henry Z. H. Jiang[1], Julia Oktawiec[1], Alexander C. Forse[1], Valentina Colombo[2], Jeffrey A. Reimer[3,5], Jeffrey R. Long[1,3]
[1]University of California, Berkeley; [2]Università di Milano; [3]Lawrence Berkeley National Laboratory

G. NUCLEAR ENERGY

PI-G-1: DEVELOPMENT OF POSITRON BEAMS FOR IN-SITU SPECTROSCOPY OF IRRADIATION-INDUCED DEFECTS

[FUTURE] Adric C. L. Jones[1], Rasheed Auguste[2], Sahil Agarwal[1], Minhazul Islam[1], Eitenne P. Vermeulen[3], Yongqiang Wang[3], Peter Hosemann[2], Farida A. Selim[1], Blas P. Uberuaga[3]
[1]Bowling Green State University; [2]University of California, Berkeley; [3]Los Alamos National Laboratory

PI-G-2: COUPLING BETWEEN PARTICLE FORCES, AGGREGATION, AND RESPONSE DYNAMICS IMPLEMENTING COMPLEX INTERFACIAL CHEMISTRY/STRUCTURE AND RADIATION

[IDREAM] Elias Nakouzi[1], Anthony J. Krzysko[2], Jaewon Lee[1], Lance E. Edens[2], Sidhant Pednekar[1], Patricia L. Huestis[6], Jennifer A. Soltis[1], Enrique Alvarado[2], Xin Zhang[1], Trent R. Graham[1], Dongsheng Li[1], , Cornelius F. Ivory[2], Kevin M. Rosso[1], Andrew G. Stack[4], Lawrence A. Anovitz[4], Aurora E. Clark[2,1], Greg K. Schenter[1,2], James J. De Yoreo[1,3], Jaehun Chun[1]
[1]Pacific Northwest National Laboratory, [2]Washington State University, [4]Oak Ridge National Laboratory, [6]University of Notre Dame

PI-G-3: RADIATION EFFECTS IN MOLTEN SALTS

[MSEE] Gregory Horne[1], Jay LaVerne[2], Ruchi Gakhar[1], William C. Phillips[1], Kazuhiro Iwamatsu[3], Simon M. Pimblott[1], James Wishart[3]
[1]Idaho National Laboratory, [2]University of Notre Dame, [3]Brookhaven National Laboratory

PI-G-4: PHONON DENSITY OF STATES AND THERMODYNAMIC PROPERTIES ThO_2 AND UO_2

[TETI] Matthew Bryan[1], Lyuwen Fu[2], Krzysztof Gofryk[3], Chris Marianetti[2], Matthew Mann[4], Michael Manley[1]
[1]Oak Ridge National Laboratory, [2]Columbia University, [3]Idaho National Laboratory, [4]Airforce Research Laboratory

PI-G-5: RADIATION EFFECTS IN BOEHMITE

[IDREAM] Patricia L. Huestis[6], Jay LaVerne[6], Brant M. Jones[5], Alexandr Aleksandrov[5], Thomas Orlando[5], Torin Stetina[3], Xiaosong Li[3], Jennifer A. Soltis[1], Xin Zhang[1], Sebastien N. Kerisit[1], Kevin M. Rosso[1]

[1]Pacific Northwest National Laboratory, [3]University of Washington, [5]Georgia Institute of Technology, [6]University of Notre Dame

PI-G-6: ELECTRON-PHONON COUPLING EFFECTS ON ENERGY DISSIPATION AND DAMAGE PRODUCTION IN ION IRRADIATION OF NICKEL AND NICKEL-BASED ALLOYS

[EDDE] Eva Zarkadoula[1], German D. Samoluyk[1], William J. Weber[2,1], Artur Tamm[3], Alfredo Correa[3], Magdalena Caro[4], Alfredo Caro[5], Aleksi Leino[1], Ritesh Sachan[1], Hongbin Bei[1], Yanwen Zhang[1]

[1]*Oak Ridge National Laboratory;* [2]*University of Tennessee-Knoxville;* [3]*Lawrence Livermore National Laboratory;* [4]*Virginia Tech;* [5]*George Washington University*

PI-G-7: MODELING THE FUTURE: TOWARDS A PHYSICS-BASED MODEL OF COUPLED IRRADIATION AND CORROSION

[FUTURE] Mark Asta[1], Amitava Banerjee[2], Laurent Capolungo[2], Edward A. Holby[2], Aaron A. Kohnert[2], Blas P. Uberuaga[2], Nicholas P. Winner[1]

[1]University of California, Berkeley; [2]Los Alamos National Laboratory

PI-G-8: SYNTHESIS AND ULTRAPURIFICATION OF CHLORIDES FOR MOLTEN SALT RESEARCH

[MSEE] Phillip Halstenberg[1], Sheng Dai[1], Shannon Mahurin[1], Alexander Ivanov[1]

[1]Oak Ridge National Laboratory

PI-G-9: IMPACT OF IONIZATION AND DEFECT TRAPPING ON MICROSTRUCTURE EVOLUTION AND THERMAL TRANSPORT IN IRRADIATED FLUORITE OXIDES

[TETI] Marat Khafizov[1], Yuzhou Wang[1], Vinay Chauhan[1], Lingfeng He[2], Tiankai Yao[2], Zilong Hua[2], Amey Khanolkar[2], Matthew Mann[3], Anter El-Azab[4], David Hurley[2]

[1]The Ohio State University, [2]Idaho National Laboratory, [3]Airforce Research Laboratory, [4]Purdue University

PI-G-10: LEVERAGING ISOTOPIC TRACERS TO REVEAL MASS TRANSPORT BEHAVIOR UPON CORROSION AND IRRADIATION

[FUTURE] Sandra D. Taylor[1], Timothy G. Lach[1], Yongqiang Wang[2], Nan Li[2], Daniel K. Schreiber[1], Thak Sang Byun[1]

[1]Pacific Northwest National Laboratory; [2]Los Alamos National Laboratory

PI-G-11: CHARACTERIZATION OF THE STRUCTURE AND DYNAMICS OF HIGH TEMPERATURE MOLTEN SALTS VIA MOLECULAR SIMULATION

[MSEE] Edward J. Maginn[1], Claudio J. Margulis[2], Haimeng Wang[1], Yong Zhang[1], Fei Wu[2], Matthew Emerson[2], Shobha Sharma[2], Santanu Roy[3], Vyacheslav S. Bryantsev[3], Alexander S. Ivanov,[3] Shannon M. Mahurin,[3] Phillip Halstenberg,[3] Simerjeet Gill,[4] Mehmet Topsakal,[4] Bobby Layne,[4] Kotaro Sasaki[4]

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

H. QUANTUM MATERIALS

PI-H-1: STM STUDY OF THE MAGNETIC WEYL SEMIMETAL CANDIDATE CEBI

[CATS] Yu Liu[1], Christian Matt[1], Harris Pirie[1], Nathan Drucker[1], Na Hyun Jo[2], Brinda Kuthanazhi[2], Sergey L. Bud'ko[2,3], Paul Canfield[2,3], Jennifer Hoffman[1]
[1]*Harvard University;* [2]*Iowa State University;* [3]*Ames Laboratory*

PI-H-2: PHASE COEXISTENCE AND EXOTIC QUASIPARTICLES IN $YB_2TI_2O_7$

[IQM] A. Scheie[1], J. Kindervater[1], S. Zhang[1], G. Sala[2], G. Ehlers[2], Xinshu Zhang[1], S. Saubert[3], C. Peiderer[3], N. P. Armitage[1], S.M. Koohpayeh[1], O. Tchernyshyov[1], C. Broholm[1]
[1]*Johns Hopkins University,* [2]*Oak Ridge National Laboratory,* [3]*Tehcnical University of Münich*

PI-H-3: STACKING DEPENDENT MAGNETISM AND PRESSURE INDUCED MAGNETIC PHASE TRANSITION IN CRI_3

[Pro-QM] Di Xiao[1], Matthew Yankowitz[2], Jiun-Haw Chu[3], David H. Cobden[3], Cory R. Dean[2], Xiaodong Xu[3]
[1]*Carnegie Mellon,* [2]*Columbia University,* [3]*University of Washington*

PI-H-4: LANDSCAPE OF COMPETING STRIPES AND MAGNETIC PHASES IN THE SCAN DESCRIPTION OF THE CUPRATES

[CCM] Jianwei Sun[1], Arun Bansil[2], Yubo Zhang[1], Christopher Lane[2], James W. Furness[1,] Bernardo Barbiellini[2,3] , Robert S. Markiewicz[2]
[1]*Tulane University,* [2]*Northeastern University,* [3]*Lappeenranta University of Technology*

PI-H-5: DETECTION AND TUNING OF THE PROPERTIES OF SINGLE-MOLECULE MAGNETS ON TWO-DIMENSIONAL SURFACES

[M^2QM] Rainier Berkley[1], Zahra Hooshmand[1], Talat S. Rahman[1], Art Hebard[2], George Christou[2], Xiaochen Zhu[2], Haoming Jin[2], Ashlyn Hale[2]
[1]*University of Central Florida;* [2]*University of Florida*

PI-H-6: QUANTUM SENSING AT HIGH PRESSURES USING THE NITROGEN-VACANCY CENTER

[NPQC] Satcher Hsieh[1,2], Prabudhya Bhattacharyya[1,2], Chong Zu[2], Thomas Mittiga[2], T. Smart[2], Francisco Machado[2], Bryce Kobrin[2], T. O. Hoehn[2], Nicholas Rui[2], M. Kamrani[3], S. Chatterjee[2], Soonwon Choi[2], Michael Zaletel[2], V. Struzhkin[4], Joel E. Moore[1,2], V. Levitas[3], R. Jeanloz[2], Norman Y. Yao[1,2]
[1]*Lawrence Berkeley National Laboratory;* [2]*University of California, Berkeley;* [3]*Iowa State University;* [4]*Carnegie Institution of Washington*

PI-H-7: TUNING THE OPTICAL PROPERTIES OF 2D MATERIALS FOR ATOMICALLY-THIN PHOTOVOLTAICS

[PTL] Joeson Wong[1], Cora Went[1], Minda Deng[2], Leo Yu[2], Harry Atwater[1], Tony Heinz[2]
[1]*California Institute of Technology;*[2]*Stanford University*

PI-H-8: HYSTERETIC TEMPERATURE DEPENDENT SPIN-WAVE RESPONSE ASSOCIATED WITH THE METAL-INSULATOR TRANSITION IN V_2O_3/NI/NIFE THIN FILMS

[Q-MEEN-C] Yizhang Chen[1], Nicolás Vargas Ayala[2], Pavel Salev[2], Ivan K. Schuller[2], Andrew D. Kent[1]
[1]*New York University;* [2]*University of California San Diego*

PI-H-9: TOPOLOGICAL HALL EFFECT IN A BILAYER COMPOSED OF HEAVY METAL AND FERRIMAGNETIC INSULATOR

[SHINES] Qiming Shao[1], Yawen Liu[2], Guoqiang Yu[1], Se Kwon Kim[1], Xiaoyu Che[1], Chi Tang[2], Qing Lin He[1], Yaroslav Tserkovnyak[1], Jing Shi[2], Kang L. Wang[1]
[1]*University of California, Los Angeles;* [2]*University of California, Riverside*

PI-H-10: TOPOLOGICAL AND MAGNETIC 2D MATERIALS

[Pro-QM] Dmitry Ovchinnikov[1], Zhong Lin[1], Bevin Huang[1], Qianni Jiang[1], Paul Malinowski[1], Zaiyao Fei[1], Jiaqiang Yan[2], Anna Isaeva[3], Jiun-Haw Chu[1], Xiaodong Xu[1]
[1]University of Washington; [2]Oak Ridge National Laboratory; [3]Technische Universitat Dresden

PI-H-11: MBE GROWTH AND CHARACTERIZATION OF MAGNETIC KAGOME METALS

[CATS] Anand Bhattacharya[1], Deshun Hong[1], Samuel Jiang[1], John Pearson[1], Dmitry Yarotski[2], Adam Kaminski[3,4], Jenny Hoffman[5], Christian Matt[5]
[1]Argonne National Laboratory; [2]Los Alamos National Laboratory; [3]Ames Laboratory; [4]Iowa State University; [5]Harvard University

PI-H-12: THE EFFECT OF ATOMIC SCALE STRAIN AND STRAIN RELAXATION MECHANISMS IN MONOLAYER MoS_2

[CCM] Daniel J. Trainer[1], Yuan Zhang[2], Fabrizio Bobba[1,3], Xiaoxing Xi[1], Saw-Wai Hla[2,4], Maria *Iavarone*[1]
[1]Temple University, [2]Argonne National Laboratory, [3]University of Salerno, [4]Ohio University

PI-H-13: TRIMER-BASED FRUSTRATED MOTT INSULATORS

[IQM] Loi T. Nguyen[1], Tom Halloran[2], Weiwei Xie[3], Tai Kong[1], Collin L. Broholm[2], Robert J. Cava[1]
[1]Princeton University, [2]Johns Hopkins University, [3]Louisiana State University

PI-H-14: DESIGN OF HIGHLY COHERENT, INTERACTING SPIN SYSTEMS IN DIAMOND FOR PROBING MANY-BODY QUANTUM PHYSICS

[NPQC] Simon Meynell[1], C. McLellan[1], Chong Zu[2], Thomas Mittiga[2], Norman Y. Yao[2,3], Ania C. Bleszynski Jayich[1]
[1]University of California, Santa Barbara; [2]University of California, Berkeley; [3]Lawrence Berkeley National Laboratory

PI-H-15: COMPOSITE PHOTONIC PLATFORM BASED ON SEMICONDUCTOR MONOLAYERS

[Pro-QM] Ipshita Datta[1], Sang Hoon Chae[1], Gaurang R. Bhatt[1], Mohammad A. Tadayon[1], Baichang Li[1], Yiling Yu[2], Chibeom Park[3], Jiwoong Park[3], Linyou Cao[2], D. N. Basov[1], James Hone[1], Michal Lipson[1]
[1]Columbia University; [2]North Carolina State University; [3]University of Chicago

PI-H-16: RAMAN SPECTROSCOPY AND THERMAL TRANSPORT PROPERTIES OF 2D ANTIFERROMAGNETIC MATERIALS

[SHINES] Subhajit Ghosh, Fariborz Kargar, Tang Su, Richard Wilson, Yongtao Cui, Jing Shi, Alex Balandin
University of California, Riverside

PI-H-17: VISUALIZATION OF ELECTRONIC AND STRUCTURAL PROPERTIES OF HYDROGENATED RARE-EARTH NICKELATE NANOJUNCTIONS WITH SYNAPTIC BEHAVIOR

[Q-MEEN-C] Peter O. Sprau[1], Ivan Zaluzhnyy[1], Sarmistha Das[1], Qi Wang[2], Zhen Zhang[2], Yifei Sun[2], Mathew J. Cherukara[3], Martin V. Holt[3], Evgeny Nazaretski[4], Xiaojing Huang[4], Hanfei Yan[4], Mingyuan Ge[4], Yong Chu[4], Shriram Ramanathan[2], Alex Frano[1], Oleg G. Shpyrko[1]
[1]University of California San Diego; [2]Purdue University; [3]Advanced Photon Source, Argonne National Laboratory; [4]National Synchrotron Light Source II, Brookhaven National Laboratory

PI-H-18: A MICROSCOPIC VIEW OF MAGNETO-ELECTRIC COUPLING IN MN-TAA

[M^2QM] Jie-Xiang Yu[1], Jia Chen[1], Jie Gu[1], Vivien Zapf[2], Xiaoguang Zhang[1], Hai-Ping Cheng[1]
[1]University of Florida; [2]Los Alamos National Lab

PI-H-19: CRYSTAL GROWTH AND PHYSICAL PROPERTIES OF FERROMAGNETIC $EuCd_2As_2$, A SINGLE WEYL PAIR CANDIDATE

[CATS] Na Hyun Jo[1], Brinda Kuthanazhi[1], Sergey L. Bud'ko[1,2], Paul C. Canfield[1,2], Yun Wu[1], Robert J. McQueeney[1,2], Dominic Ryan[3], Benjamin Ueland[2], Adam Kaminski[1,2], Linlin Wang[2]
[1]Iowa State University; [2]Ames Laboratory; [3]McGill University

PI-H-20: SPIN COHERENCE IN METHYLAMMONIUM LEAD HALIDE PEROVSKITES

[CHOISE] Sarah Li[1], Yue Yao[1], Matthew Sheffield[1], Uyen Huynh[1], Ye Liu[1]
Kai Zhu[2], Jinsong Huang[3], Z. Valy Vardeny[1]
[1]University of Utah, [2]National Renewable Energy Laboratory, [2]University of North Carolina-Chapel Hill

PI-H-21: GROWTH AND CHARACTERIZATION OF HYBRID DIRAC SEMIMETAL/SUPERCONDUCTOR/MAGNETIC HETEROSTRUCTURES: A POSSIBLE PATHWAY TO MONOPOLE SUPERCONDUCTIVITY

[IQM] Run Xiao[1], Wilson Yanez[1], Michell Tomczyk[1], Yawen Fang[2], Santu Baidya[3], David Vanderbilt[3], Yi Li[4], Tyrel Mcqueen[4], Natalia Drichko[4], Brad Ramshaw[2], Nitin Samarth[1]
[1]Penn State University, [2]Cornell University, [3]Rutgers University, [4]Johns Hopkins University

J. SEPARATION SCIENCE

PI-J-1: A TALE OF PHOTOCHEMICAL SEPARATIONS: FROM TRANSITION METALS TO LANTHANIDES AND ACTINIDES

[CAST] Sahan Salpage, Joseph M. Sperling, Yan Zhou, Ronald C. Lanzetta, Jamie C. Wang, Thomas E. Albrecht-Schmitt, Kenneth Hanson
Florida State University

PI-J-2: EVIDENCE OF MOLECULAR SIEVING OF HEXANE AND CYCLOHEXANE IN CARBON NANOTUBE SINGLE-DIGIT NANOPORES

[CENT] Haoran Qu[1], James Xiaojian Wu[1], Yunfeng Li[1], YuHuang Wang[1], Jeff Fagan[2], Archith Rayabharam[3], Narayana R. Aluru[3]
[1]University of Maryland; [2]NIST; [3]University of Illinois at Urbana-Champaign

PI-J-3: METAL–ORGANIC FRAMEWORK BASED NANOCOMPOSITE MEMBRANES FOR GAS SEPARATION

[CGS] Feng Xue, Meera Shete, Kiwon Eum, Xiaoli Ma, Michael Tsapatsis
University of Minnesota

PI-J-4: SELECTIVE REMOVAL OF HYDROGEN SULFIDE FROM SIMULATED BIOGAS STREAMS USING STERICALLY HINDERED AMINE ADSORBENTS

[UNCAGE-ME] Claudia N. Okonkwo[1], Jason J. Lee[1], Anton De Vylder[2], Yadong Chiang[2], Joris W. Thybaut[2], Christopher W. Jones[1]
[1]Georgia Institute of Technology; [2]Ghent University

PI-J-5: DEVELOPMENT OF NEW EQUATORIAL BONDING MOIETIES FOR URANYL

[CAST] Tyler S. Collins, Diana Perales, Matthias Zeller, Suzanne C. Bart
Purdue University

M. SYNTHESIS SCIENCE

PI-M-1: OBSERVING AND UNDERSTANDING KINETIC PATHWAYS OF FORMING LAYERED OXIDES

[CNGMD] Feng Wang[1], Wenhao Sun[2], Bor-Rong Chen[3] Laura Schelhas[3], Jingyang Wang[2], Michael Toney[3], Gerbrand Ceder[2]
[1]Brookhaven National Laboratory; [2]Lawrence Berkeley National Laboratory; [3]SLAC National Accelerator Laboratory

PI-M-2: DIFFERENTIATION OF CLUSTERS DERIVED FROM OXIDE-HYDROXIDE SOLUTIONS IDENTIFIED THROUGH JOINT NMR SPECTROSCOPY AND X-RAY AND NEUTRON SCATTERING

[GENESIS] John B. Parise[1], Brian L. Phillips[1], Rhiannon Garrard[1], Jack W. Simonson[2], Bingying Xia[2], Karena W. Chapman[1], Peter J. Chupas[1]
[1]Stony Brook University, [2]Farmingdale State University

PI-M-3: DESIGN AND SYNTHESIS OF STABLE, STRONG AND HIGHLY CONDUCTING HYDROXIDE ION EXCHANGE MEMBRANES

[CABES] Wei You[1], Ryan Selhorst[2], Kevin Noonan[2], Geoffrey Coates[1]
[1]Cornell University, [2]Carnegie-Melon University

PI-M-4: ILLUMINATING SINGLE CRYSTAL GROWTH FROM MELTS WITH SYNCHROTRON X-RAY SCATTERING

[GENESIS] Peter G. Khalifah[1,2], Jonathan Denney[1], Yusu Wang[1], Lucas Pressley[3], W. Adam Phelan[3], Katsuyo S. Thornton[4], Simon J.L. Billinge[5], Eric Dooryhée[2], Peter J. Chupas[1], Karena W. Chapman[1]
[1]Stony Brook University, [2]Brookhaven National Laboratory, [3]Johns Hopkins University, [4]University of Michigan, [5]Columbia University

PI-M-5: MECHANISMS FOR HYBRID ORGANIC-INORGANIC FILM FORMATION

[CHOISE] Michael F. Toney[1], Volker Blum[2], Tianyang Li[2], David Mitzi[2]
[1]SLAC National Accelerator Laboratory, [2]Duke University

PI-M-6: UNDERSTANDING CRYSTALLIZATION PATHWAYS LEADING TO MANGANESE OXIDE POLYMORPH FORMATION

[CNGMD] Bor-Rong Chen[1], Wenhao Sun[2], John Mangum[3], David Ginley[4], Brian Gorman[3], Gerbrand Ceder[2], Michael Toney[1], Laura Schelhas[1]
[1]SLAC National Accelerator Laboratory; [2]Lawrence Berkeley National Laboratory; [3]Colorado School of Mines; [4]National Renewable Energy Laboratory

POSTER SESSION II: TUESDAY, JULY 30, 2019; 3:45 – 5:15 AM, *EXHIBITION HALL C*

A. BIO-INSPIRED SCIENCE

PII-A-1: THE CATALYTIC MECHANISM OF BIFURCATING ELECTRON TRANSFER FLAVOPROTEINS INVOLVES INTERMEDIARY SUBSTRATE BINDING AND DOMAIN MOVEMENT

[BETCy] Gerrit J. Schut[1], Xiang Feng[2], Nishya Mohammed-Raseek[3], Monika Tokmina-Lukaszewska[4], David W. Mulder[5], Diep M. Nguyen[1], Gina L. Lipscomb[1], John P. Hoben[3], Angela Patterson[4], Carolyn E. Lubner[5], Paul W. King[5], Brian Bothner[4], Anne-Frances Miller[3], Huilin Li[2], Michael W. W. Adams[1]
[1]University of Georgia, [2]University of Kentucky, [3]Van Andel Research Institute, [4]Montana State University, [5]National Renewable Energy Laboratory

PII-A-2: HEMICELLULOSE-CELLULOSE INTERACTIONS INVESTIGATED WITH NEUTRON SCATTERING AND MOLECULAR SIMULATION

[CLSF] Utsab R. Shrestha[1], Sydney Smith[1], Sai Venkatesh Pingali[1], Hui Yang[2], Mai Zahran[3], Lloyd Breunig[2], Riddhi Shah[1], Mohamadamin Makarem[2], Liza A. Wilson[2], Malgorzata Kowalik[2], Brian H. Davison[1], James D. Kubicki[4], Daniel J. Cosgrove[2], Seong H. Kim[2], Loukas Petridis[1], Hugh O'Neill[1]
[1]Oak Ridge National Laboratory; [2]The Pennsylvania State University; [3]New York City College of Technology; [4]University of Texas El Paso

PII-A-3: INVERTED REDUCTION POTENTIALS FOR ELECTRON BIFURCATION: PHYSICAL ORIGINS TO BIOLOGICAL UTILITY

[BETCy] Jonathon L. Yuly[1], Peng Zhang[1], Carolyn E. Lubner[2], John W. Peters[3], David N. Beratan[1].
[1]Duke University, [2]National Renewable Energy Laboratory, [3]Washington State University

PII-A-4: SUM FREQUENCY GENERATION (SFG) VIBRATIONAL SPECTROSCOPY STUDY OF RELATIONSHIP BETWEEN CELLULOSE MICROFIBRILS ORGANIZATION AND CELL WALL FUNCTION IN PLANTS

[CLSF] Mohamadamin Makarem[1], Sarah N. Kiemle[1], Jason N. Burris[2], Shixin Huang[1], Jongcheol Lee[1], Candace H. Haigler[2], Daniel J. Cosgrove[1], Seong H. Kim[1]
[1]The Pennsylvania State University; [2]North Carolina State University

B. CATALYSIS

PII-B-1: PT-BASED AND NI-BASED BIMETALLIC NANOCRYSTAL CATALYSTS FOR HYDRODEOXYGENATION OF 5-HYDROXYMETHYLFURFURAL AND 2-ACETYLFURAN

[CCEI] Jennifer D. Lee[1], Cong Wang[1], Konstantinos A. Goulas[2], Siyu Yao[3], Yichen Ji[1], Jingguang G. Chen[3,4], Dionisios G. Vlachos[2], Raymond J. Gorte[1], Christopher B. Murray[1]

[1]University of Pennsylvania; [2]University of Delaware; [3]Brookhaven National Laboratory; [4]Columbia University

PII-B-2: ELUCIDATING THE INTERACTIONS OF H2S AND CO2 WITH TRANSITION METAL SULFIDE CATALYSTS FOR NATURAL GAS UPGRADING

[UNCAGE-ME] Lohit Sharma[1], Ronak Upadhyay[1], Zili Wu[2], Srinivas Rangarajan[1], Jonas Baltrusaitis[1]

[1]Lehigh University; [2]Oak Ridge National Laboratory

PII-B-3: PCET-BASED REDOX RELAYS: QUINONE-BIPYRIDINE LIGANDS OF METAL CATALYST FOR HYDROAMINATION AND HYDROAMIDATION REACTIONS.

[BioLEC] Hunter H. Ripberger[1], Walter D. Guerra[2], Ana L. Moore[2], Thomas A. Moore[2], Robert R. Knowles[1]

[1]Princeton University; [2]Arizona State University

PII-B-4: COVALENT FUNCTIONALIZATION OF TRANSITION METAL PHOSPHIDE ELECTROCATALYSTS

[CME] Ian Murphy[1], David Ung[1], Brandi Cossairt[1]

[1]*University of Washington, Seattle*

PII-B-5: DEVELOPING QM/MM METHODS FOR METAL-ORGANIC FRAMEWORKS AND APPLYING THEM FOR INTERPRETING CATALYTIC EXPERIMENTS

[ICDC] Xin-Ping Wu[1], Bo Yang[1], Massimiliano Delferro[2], Omar K. Farha[3], Laura Gagliardi [1], Donald G. Truhlar[1]

[1]University of Minnesota; [2]Argonne National Lab; [3]Northwestern University

PII-B-6: HIGH PERFORMANCE ORR AND HOR ELECTROCATALYSTS FOR ALKALINE MEDIA

[CABES] Yin Xiong[1], Can Li[2], Yao Yang[1], Hongsen Wang[1], Elliot Padgett[1], Pengtao Xu[1], Xi Yin[3], Francis DiSalvo[1], Jiye Fang[2], Jin Suntivich[1], Piotr Zelenay[3], David Muller[1], Héctor Abruña[1]

[1]Cornell University, [2]Binghamton University, [3]Los Alamos National Lab

PII-B-7: A MODULAR DESIGN STRATEGY FOR THE CREATION OF HIGHLY SELECTIVE AND STABLE BIMETALLIC CATALYSTS

[IMASC] Tanya Shirman[1], Mathilde Luneau[1], Youyunqi Wu[1], Amanda Filie[1], David Verbart[1], Robert J Madix[1], Joanna Aizenberg[1], Cynthia M. Friend[1]

[1]Harvard University

PII-B-8: FUNDAMENTAL UNDERSTANDING OF THE INVERSE PT-WOX CATALYST FOR SELECTIVE C-O BOND SCISSION

[CCEI] Shizhong Liu[1], Jiayi Fu[1], Weiqing Zheng[1], Cong Wang[2], Raymond J. Gorte[2], Stavros Catatzoulas[1], Dionisios G. Vlachos[1]

[1]University of Delaware, [2]University of Pennsylvania

PII-B-9: Synergistic Experimental and Computational Investigations of Structure-Activity relationships and Support Effects in Metal-Organic Frameworks-Supported Vanadium Catalysts

[ICDC] Xuan Zhang[1], Xingjie Wang[1], Mukunda Mandal[2], Christopher J. Cramer[2], Laura Gagliardi[2], Omar K. Farha[1]
[1]Northwestern University; [2]University of Minnesota

PII-B-10: Synthesis and Multimodal characterization of 2D Silica-Palladium model catalysts

[IMASC] Nusnin Akter[1], Chen Zhou[1], Samuel Tenney[1], Ashley Head[1], J. Anibal Boscoboinik[1], Dario J. Stacchiola[1]
[1]Brookhaven National Laboratory

PII-B-11: Splitting electron pairs Over a 1V potential range By flavin-based electron bifurcation

[BETCy] Carolyn E. Lubner[1], David P. Jennings[2], David W. Mulder[1], Gerrit J. Schut[3], Oleg A. Zadvornyy[1], John P. Hoben[4], Monika Tokmina-Lukaszewska[5], Luke Berry[5], Diep M. Nguyen[3], Gina L. Lipscomb[3], Anne K. Jones[2], Anne-Frances Miller[4], Paul W. King[1], Michael W. W. Adams[3], John W. Peters[1]
[1]Washington State University, [2]Arizona State University, [3]University of Georgia, [4]University of Kentucky, [5]Montana State University

PII-B-12: Merging Photoredox Catalysis and Photochemical Upconversion

[BioLEC] Daniela M. Arias-Rotondo[1], Artem Tsymbal[1], David W. C. MacMillan[1]
[1]Princeton University

PII-B-13: A Local Short Circuit Model for Quantitative Analysis of Redox-Mediator-Driven Heterogeneous Catalysis

[CME] William C. Howland III[1], James B. Gerken[2], Sourav Biswas[2], Shannon S. Stahl[2], Yogesh Surendranath[1]
[1]Massachusetts Institute of Technology; [2]University of Wisconsin–Madison

PII-B-14: Hierarchical *Operando* Characterization of Electrocatalytic Systems in Alkaline Media

[CABES] Elliott Padgett, Daniel Weinstock, David Muller, Andrej Singer
Cornell University

PII-B-15: Mechanistic insights into the dehydra-decyclization of tetrahydrofuran in zeolites.

[CCEI] Sha Li[1], Omar A. Abdelrahman[3], Gaurav Kumar[2], Michael Tsapatsis[4], Dionisios G. Vlachos[1], Stavros Caratzoulas[1], Paul J. Dauenhauer[2]
[1]University of Delaware; [2]University of Minnesota; [3]University of Massachusetts Amherst; [4]Johns Hopkins University

PII-B-16: Oxidation of Ammonia by Hydrogen Atom Abstractions with Molecular Mediators

[CME] Brian J. Cook[1], Samantha I. Johnson[1], Peter L. Dunn[1], Eric S. Wiedner[1], Werner Kaminsky[2], R. Morris Bullock[1]
[1]Pacific Northwest National Laboratory; [2]University of Washington, Seattle

D. ENERGY STORAGE

PII-D-1: KINETICALLY-LIMITED LITHIUM REINSERTION IN LAYERED TRANSITION-METAL OXIDE POSITIVE ELECTRODES

[NECCES] Antonin Grenier[1,2], Hao Liu[1,3], Kamila M. Wiaderek[1], Philip J. Reeves[4], Ieuan D. Seymour[4], Clare P. Grey[4], Peter J. Chupas[1,2], Karena W. Chapman[1,2]

[1]Argonne National Laboratory, [2]Stony Brook University, [3]Binghamton University, [4]University of Cambridge

PII-D-2: TOWARD INCREASING ELECTRONIC AND IONIC TRANSPORT IN TRANSITION METAL OXIDE ELECTRODE MATERIALS

[SCALAR] Molleigh B. Preefer[1], JoAnna Milam-Guerrero[2], Qiulong Wei[3], Sanjeev Kolli[1], Muna Saber[1], Kira E. Wyckoff[1], Nicholas H. Bashian[2], Johanna Nelson Weker[4], Anton Van der Ven[1], Brent C. Melot[2], Bruce S. Dunn[3], Ram Seshadri[1]

[1]University of California, Santa Barbara; [2]University of Southern California; [3]University of California, Los Angeles; [4]SLAC National Accelerator Laboratory

PII-D-3: CHEMO-MECHANICAL STRAINS IN SOLID-STATE BATTERIES

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PII-D-4: CATALYTIC POLYMERIZATION OF 1,3-DIOXOLANE (DOL) IN MG BATTERY SYSTEM

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PII-D-5: DEVELOPMENT OF POLYTHIOPHENE-BASED MIXED ION/ELECTRON CONDUCTING POLYMERS FOR CATHODE BINDERS

[SCALAR] Qiulong Wei[1], Liwei Ye[2], Pratyusha Das[2], Dongwook Lee[3], Charlene Z. Salamat[1], Billal Zayat[2], Rodrigo Elizalde-Segovia[2], Ahamed I. Maniyanganam[2], Stephen A. Munoz[4], Ioan-Bogdon Magdau[4], Ram Seshadri[3], Sarah H. Tolbert[1], Thomas F. Miller[4], Sri R. Narayan[2], Bruce S. Dunn[1], Rachel A. Segalman[3], Barry C. Thompson[2]

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PII-D-6: CHARGE-TRANSFER KINETICS OF REDOX REACTIONS IN DEEP EUTECTIC SOLVENTS: ROLE OF COMPLEXATION

[BEES] Dai Shen[1], Katherine Steinberg[1], Nora Shaheen[1], Charles Kolodziej[1], Clemens Burda[1], Miomir Vukmirovic[2], Robert Savinell[1], Rohan Akolkar[1]

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PII-D-7: IONS/SOLVENTS DYNAMICS AND STRUCTURE IN CONFINEMENT BETWEEN TWO-DIMENSIONAL LAYERS OF TRANSITION METAL CARBIDES

[FIRST] Michael Naguib[1], Nina Balke[2], Alexander Brady[2], Qiang Gao[2], Yury Gogotsi[3], Ilia N. Ivanov[2], De-en Jiang[4], Nadine Kabengi,[5] Poorandokht I. Kashkouli[5], Paul Kent[2], Alexander I. Kolesnikov[2], Eugene Mamontov[2], Eric S. Muckley[2], Naresh Osti[2], Kaitlyn Prenger[1], Robert L. Sacci[2], Weiwei Sun[2], Yangyunli Sun[4], Ray Unocic[2], Adri van Duin[6], Hsiu-Wan Wang[2]

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PII-D-8: UNDERSTANDING MULTI-ELECTRON TRANSFER VIA LOCAL AND BULK CHARACTERIZATION

[m2M/t] Feng Wang[1], Wei Zhang[1], Yan Li[2], Lijun Wu[1], Yandong Duan[1], Kim Kisslinger[1], Chulin Chen[3], David C. Bock[1], Feng Pan[4], Yimei Zhu[1], Amy C. Marschilok[5], Esther S. Takeuchi[5], Kenneth J. Takeuchi[5]

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PII-D-9: IMPLICATIONS OF TRANSITION METAL IDENTITY FOR INTERLAYER MIGRATION IN LAYERED CATHODE MATERIALS

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PII-D-10: EXPLORING THE FLUORIDE INTERCALATION REACTION THROUGH MODEL ELECTRODE MATERIALS

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PII-D-11: SURFACE STABILIZATION AND FUNCTIONALIZATION STRATEGIES FOR LITHIUM MANGANESE OXIDE CATHODES

[CEES] Siddharth Deshpande[1], Robert Warburton[1], Hakim Iddir[2], Larry Curtiss[2], Donghyeon Kim[2], Lin Chen[2], Matthias Young[2], Jeffrey Elam[2], Christopher Johnson[2], Wesley Dose[2], Kimberly Bassett[3], Andrew Gewirth[3], Jeffrey Greeley[1]

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PII-D-12: NONPLANAR ARCHITECTURES FOR HIGH CAPACITY BATTERIES: PREPARATION AND CHARACTERIZATION

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PII-D-13: EFFECT OF PARTICLE SIZE AND MORPHOLOGY ON THE PROPERTIES OF ANIONIC REDOX CATHODE MATERIALS

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PII-D-14: SYNTHESIS AND ELECTROCHEMISTRY OF 3D NANOPORE STRUCTURES TOWARD SOLID STATE BATTERIES ON SI
[NEES] Nam Kim[1], Keith Gregorczyk[1], Miles Mowbray[1], John Hayden[1], Emily Sahadeo[1], Chanyuan Liu[1], Olivia Rose[1], Gary Rubloff[1], Sang Bok Lee[1]
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PII-D-15: CATION MOLECULAR STRUCTURE: INFLUENCE ON MOBILITY AND TRANSPORT IN POROUS CARBONS
[FIRST] Jianzhong Wu,[1] Alejandro Gallegos,[1] Naresh Osti,[2] Boris Dyatkin,[3] David Voneshen,[4] Jong Keum,[2] Ken Littrell,[2] Pengfei Zhang,[2] Sheng Dai,[2] Yury Gogotsi,[3] Eugene Mamontov[2]
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E. ENERGY - WATER

PII-E-1: SYNCHROTRON X-RAY IMAGING OF REACTIVE TRANSPORT IN SHALE
[CMC-UF] Vincent Noel[1], Wenjia Fan[1], Jennifer L. Druhan[2], Adam D. Jew[1], Anthony R. Kovscek[3], Gordon E. Brown Jr.[1,3], John R. Bargar[1]
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PII-E-2: CARBONYL VIBRATIONAL PROBES OF LOCAL ELECTRIC FIELDS IN AQUEOUS ELECTROLYTES: CALIBRATING TRANSIENT VIBRATIONAL SPECTROSCOPY AND MOLECULAR DYNAMICS SIMULATIONS TOWARDS IN SITU MEASUREMENTS AT THE ELECTRODE-ELECTROLYTE INTERFACE
[AMEWS] Nicholas Lewis[1], Aysenur Iscen[2], Bogdan Dereka[1], Alanna Felts[2], Jeff Elam[3], George Schatz[2], Andrei Tokmakoff[1]
[1]University of Chicago; [2]Northwestern University; [3]Argonne National Laboratory

PII-E-3: ADVANCING UNDERSTANDING OF FLUID INDUCED REACTIVITY IN CONFINEMENT USING *IN-OPERANDO* MEASUREMENTS AND MOLECULAR SIMULATIONS
[MUSE] Hassnain Asgar[1], Nabankar Dasgupta[2], Greeshma Gadikota[1], Murali Muraleedharan[2], Adri van Duin[2], John Kaszuba[3]
[1]University of Wisconsin,[2]Pennsylvania State University, [3]University of Wyoming

PII-E-4: INTERACTIVE MODEL FLUID PLATFORM SOLUTE DATABASE
[M-WET] Lauren Nalley[1], Matthew Landsman[1], Dylan McReynolds[2], Carolyn Cooper[1], Harinarayan Krishan[2], Alex Hexemer[2], Lynn Katz[1]
University of Texas at Austin[1], Lawrence Berkeley National Labs[2]

PII-E-5: ELECTROCHEMICAL STUDIES OF SOLUTIONS CONFINED WITHIN NANOPORES
[CENT] Stevie Walters[1], Charles R. Martin[1], *Jake Polster[2], Zuzanna Siwy[2]*
[1]University of Florida; *[2]University of California Irvine*

PII-E-6: SYNTHESIS, CHARACTERIZATION, AND MODELING OF SELECTIVE ADSORPTION SITES FOR AQUEOUS ENVIRONMENTS PREPARED USING SELF-LIMITING SURFACE CHEMISTRY
[AMEWS] Jeffrey Elam[1], Vepa Rozyyev[2], Edward Barry[1], Li Tang[2], Nicholas Lewis[2], George Schatz[3], Andrei Tokmakoff[2]
[1]Argonne National Laboratory; [2]University of Chicago; [3]Northwestern University

PII-E-7: Atomistic-scale simulations of CO_2 and capillary condensation in nano porosity

[CMC-UF] Alireza Ostandhossein[1], Matthias Ihme[1], Filip Simeski[1], Arnout Boelens[1], Hamdi Tchelepi[1], Jiyue Wu[2], Lin Sun[2], Kristian Jessen[2],Theo Tsotsis[2]
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PII-E-8: Micro-Scale Strength and Deformation Measurements and Complementary Geomechanical Modeling

[MUSE] Will Nguyen[1], Thang Tran[1], Cedric Shaskey[1], Truong Vo[1], Pania Newell[1], Keunhan Park[1], John McLennan[1], Darryl Butt[1]
[1]University of Utah

PII-E-9: Controlling Hydration Water Behavior and Solute Affinity Via Chemical Patterning of Molecules and Surfaces

[M-WET] Sally Jiao[1], Jacob Monroe[1], Dennis Robinson-Brown[1], Nicholas Sherck[1], Audra DeStefano[1], Mikayla Barry[1], Thomas Webber[1], Timothy Keller[1], Rachel Segalman[1], Songi Han[1], Lynn Katz[2], Glenn Fredrickson[1], M. Scott Shell[1]
University of California at Santa Barbara[1], University of Texas at Austin[2]

PII-E-10: Advanced Imaging to Enable Studies of Confined Fluids

[CENT], Ze Zhang[1], Joel Martis[1], Kyle Sendgikoski[2], Joy Chao[2], Zoey Warecki[2], Arun Majumdar[1], John Cumings[2]
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PII-E-11: SCAN and the Water/Alumina Interface

[CCM] Eric Borguet[1], Michael L. Klein[1], Mark J. Dellostritto[1], Stefan M. Piontek[1], Ruiyu Wang[1], Richard C. Remsing[1], Vincenzo Carnevale[1]
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PII-E-12: Mass Transfer in Fractured Nanoporous Materials

[CMC-UF] Shadi Torabi[1], Kristian Jessen[1], Theo T. Tsotsis[1], Saman Aryana[2], Vladimir Alvarado[2], Sally M. Benson[1], Anthony R. Kovscek[1]
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F. Materials and Chemistry by Design

PII-F-1: Rigorous assessment of nanoscale order using total scattering

[CHWM] Deepak Patil[1], Robert J. Koch[1], Shubham Pandey[2], Guangfang Li[3], Douglas A. Blom[3], Hui Wang[3], Simon R. Phillpot[2], Kyle Brinkman[4], Mingyang Zhao[4], Scott T. Misture[1]
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PII-F-2: Spectroscopic Study of Formation and Stability of Thin Films on Glass and Metal Surfaces during Corrosion in Aqueous Solutions

[WastePD] Dien Ngo,[1] Huseyin Kaya,[1] Hongshen Liu,[1] Seong H. Kim,[1] Stéphane Gin,[2] Kathleen F. Quiambao,[3] Angela Y. Gerard,[3] John R. Scully[3]
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PII-F-3: SYNTHESIS AND CHARACTERIZATION OF REDOX-ACTIVE *f*-ELEMENT COMPLEXES AND SUPRAMOLECULAR RECOGNITION OF ANIONS

[CAST] Thibault Cheisson[1], Alex McSkimming[1], Jing Su[2], Jiwen Jian[3], Enrique R. Batista[2], Ping Yang[2], John K. Gibson[3], Andrew J. Gaunt[2], Eric J. Schelter[1]

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PII-F-4: CONTROLLING BROADBAND EMISSION VIA TIN ALLOYING IN RUDDLESDEN-POPPER HYBRID LEAD IODIDE PEROVSKITES

[CHOISE] Tianyang Li[1], Xiaoming Wang[2], Xihan Chen[3], Matthew C. Beard[3], Yanfa Yan[2], David B. Mitzi[1]

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PII-F-5: DEVELOPING A SIMULATION-BASED FRAMEWORK TO PREDICT HIERARCHICAL SELF-ASSEMBLY IN BIO-INSPIRED MATERIALS

[CSSAS] Janani Sampath[1], Mingfei Zhao[2], Sarah Alamdari[1], Jesse Prelesnik[1], Orion Dollar[1], Andrew Ferguson[2], Christopher J. Mundy[3], Jim Pfaendtner[1]

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PII-F-6: AUTOMATING INTERPRETATION OF IN-SITU SCATTERING DATA OBTAINED DURING SYNTHESIS REACTIONS

[GENESIS] Simon J.L. Billinge[1], Matthew McDermott[2], Chia Hao Liu[1], Kristin A. Persson[2], Jonathan Denney[3], Peter G. Khalifah[3]

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PII-F-7: THEORETICAL DESCRIPTION OF ELECTRON/PHONON, ELECTRON/PHOTON, AND PHOTON/PHONON DYNAMICS IN NANOPARTICLES AND 2D MATERIALS

[PTL] Wenjie Dou[1], Johannes Flick[2], Nicholas Rivera[2], Christopher J. Ciccarino[2], Eran Rabani[1], Prineha Narang[2]

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PII-F-8: UNDERSTANDING THE ROLE OF SURFACE SITES AND INTER-FACIAL DYNAMICS FOR PHOTOCATHODES IN DYE-SENSITIZED PHOTOELECTROSYNTHESIS CELLS

[AMPED] Aaron D. Taggart[1], Jake E. Evans[1], Lenzi J. Williams[1], Linda Nhon[2], Lesheng Li[1], Katherine J. Lee[1], Bing Shan[1], Christina M. Klug[3], R. Morris Bullock[3], Thomas J. Meyer[1], Jillian L. Dempsey[1], Yosuke Kanai[1], John R. Reynolds[2], John M. Papanikolas[1], James F. Cahoon[1]

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PII-F-9: MOTIONS OF MAGNETOELASTIC MATERIALS AT THE NANOSCALE

[CBES] Chase Brisbois[1], Hang Yuan[1], Mykola Tasinkevych[1], Monica Olvera de la Cruz[1]

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PII-F-10: GRAPH THEORETIC CONSTRUCTION OF CRYSTAL SURFACES AND ITS PREDICTION OF 2D ZEOLITES

[CGS] Matthew D. Witman[1], Sanliang Ling[2], Peter Boyd[3], Senja Barthel[3], Maciej Haranczyk[4,5], Ben Slater[2], Berend Smit[1,3]

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PII-F-11: Towards a holistic understanding of protein self-assembly at mineral interfaces: A hybrid experimental/computational approach

[CSSAS] Robert G. Alberstein[1], Shuai Zhang[2], James J. De Yoreo[2], F. Akif Tezcan[1]
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PII-F-12: The Effect of Cesium Substitution on the Structure and Thermodynamic Stability of Hollandite Waste Forms

[CHWM] Mingyang Zhao[1], Jake Amoroso[2], Theodore Besmann[3], Scott Misture[4], Kyle Brinkman[1]
[1]Clemson University; [2]Savannah River National Laboratory; [3]University of South Carolina; [4]Alfred University

PII-F-13: Nano-Architected Materials by Self-Assembly and Rapid Consolidation Techniques

[MUSE] Michael Bartl[1], Darryl Butt[1], Hyeyoung Cho[1], Milind Deo[1], Mikalia Hunt[1], Viktoriya Semeykina[1], Subhash Risbud[2], Yiqing Xia[2], Ilya Zharov[1]
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PII-F-14: The investigation of unique transport behaviors based on hierarchical structures of nano-scale binary fluids

[BEES] Sara Triana Hamilton[1], Anthony Feric[1], Nelly Cantillo-Cuello[2], Jing Peng[2], Gabriel Goenaga[2], Carla Cecilia Fraenza[3], Steven Greenbaum[3], Thomas A. Zawodzinski[2], Ah-Hyung Alissa Park[1]
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PII-F-15: Effect of Local Lattice distortion on Radiation-defect Growth in Concentrated Alloys

[EDDE] Yang Tong[1], Shijun Zhao[1], Chenyang Lu[2], Takeshi Egami[1], Fuxiang Zhang[1], Lumin Wang[2], Yanwen Zhang[1]
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PII-F-16: Direct Monitoring of Electron-Phonon Coupling in Colloidal Nanocrystals

[PTL] Burak Guzelturk[1], Benjamin L. Cotts[1], Brent K. Koscher[2], David A. Hanifi[1], Stefan Fischer[1], Arunima D. Balan[2], Jennifer A. Dionne[1], Eran Rabani[2], Alberto Salleo[1], A. Paul Alivisatos[2], Aaron M. Lindenberg[1]
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PII-F-17: Dissolution of Pyrochlore-based Waste Forms: Microstructure and Composition Effects

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PII-F-18: Thermodynamics and Electronic Structure Properties of Actinide based Metal-Organic Frameworks (MOFs): An Integrated Computational and Experimental Investigation

[CHWM] Shubham Pandey[1], Zhilin Jia[1], Ximeng Wang[1], Brian Demaske[2], Otega Ejegbavwo[3], Wahyu Setyawan[4], Chuck Jr. Henager[4], Natalia Shustova[3], Simon Phillpot[4]
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PII-F-19: DNA-Mediated Assembly of Low symmetry Colloidal Crystals

[CBES] Haixin Lin[1], Sangmin Lee[2], Sharon C. Glotzer[2], Chad A. Mirkin[1]
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PII-F-20 Machine Learning the Periodic Table

[CCM] Qimin Yan[1], Quan Zhou[2], Peizhe Tang[2], Shexiu Liu[2], Jinbo Pan[1], Shou-Cheng Zhang[2.3]
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PII-F-21: Neutron Studies of Liquid Structure and Assembly near surfaces of Microemulsions and Deep Eutectic Solvents: Correlating Structure to Performance

[BEES] Luke Heroux[1], Yong Zhang[2], Derrick Poe[2], Adam Imel[1], Brian Barth[1], Nelly Cantillo-Cuello[1], Stephanie Spittle[1], Joshua Sangoro[1], Edward Maginn[2], Mark Dadmun[1], Thomas A. Zawodzinski[1], Doug Hayes[1]
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PII-F-22: Sorbent structure and acid gas exposure: unique insights from solid-state NMR

[UNCAGE-ME] Erika L. Sesti[1], Chia-Hsin Chen[1], Robert M Marti[1], Jason J. Lee[2], Claudia Okonkwo[2], Jayraj N. Joshi[2], Colton M. Moran[2], Christopher W. Jones[2], Krista S. Walton[2], Sophia E. Hayes[1]
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PII-F-23: Self-accelerated Corrosion of Nuclear Waste Forms at Material Interfaces

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PII-F-24: Deep machine learning analysis of protein assembly from dynamic SPM data

[CSSAS] Maxim Ziatdinov[1], Xin Li[1], Shuai Zhang[2], Harley Pyles[3], David Baker[3], James J. De Yoreo[2], Sergei V. Kalanin[1]
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PII-F-25: Tailoring Pore Environment of Metal–Organic Frameworks for CO_2 Capture, Separation and Conversion

[CGS] Liang Feng[1], Kunyu Wang[1], Shuai Yuan[1], Hao Li[1], Feng Xue[2], Michael Tsapatsis[2], Hong-Cai Zhou[1]
[1]Texas A&M University; [2]University of Minnesota

G. NUCLEAR ENERGY

PII-G-1: THEORY, MODELING, AND SIMULATION OF EXTREME ENVIRONMENTS

[IDREAM] Greg K. Schenter[1,2], Enrique Alvarado[1], Jaehun Chun[1], Rafal M. Gorniak[2], Trent R. Graham[1], Sebastien Kerisit[1], Nitesh Kumar[2], Ernesto Martinez-Baez[2], Daniel J. Pope[2], Maxime J. Pouvreau[2], Micah Prange[1], Zhizhang Shen[1], William T. Smith[2], Andrew G. Stack[4], Torin Stetina[3], Andrew P. Wildman[3], Xiaoning Yang[2], Tiecheng Zhou[2], Xiaosong Li[3], Aurora E. Clark[2,1]

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PII-G-2: THE ORIGIN OF SELECTIVITY OF A TRIAZINYL LIGAND FOR Am(III) OVER Ln(III)

[CAST] Cristian Celis-Barros, David Dan, Frankie D. White, Joseph M. Sperling, Thomas E. Albrecht-Schmitt

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PII-G-3: UNDERSTANDING THE INTERACTION OF PASSIVATING AND NON-PASSIVATING ENVIRONMENTS WITH MODEL ALLOY SURFACES VIA SPECTROSCOPY TECHNIQUES

[FUTURE] Jie Qiu[1], Marlene Wartenberg[2], Franziska Schmidt[1], Junsoo Han[2], John R. Scully[2], Peter Hosemann[1]

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PII-G-4: VISUALIZATION OF MOLTEN SALT INTERACTION WITH NI AND NI-20CR ALLOY VIA MULTISCALE IMAGING

[MSEE] Arthur Ronne[1], Lingfeng He[2], Dmitriy Dolzhnikov[3], Mingyuan Ge[4], Yi Xie[2], Kotaro Sasaki[4], Xianghui Xiao[4], Wah-Keat Lee[4], Shannon M. Mahurin[3], Yu-chen Karen Chen-Wiegart[1,4]

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PII-G-5: EFFECTS OF COMPOSITION AND RADIATION PARAMETERS ON DEFECT EVOLUTION IN CONCENTRATED SOLID-SOLUTION ALLOYS: A COMPREHENSIVE TEM STUDY

[EDDE] Li Jiang[1], Pengyuan Xiu[1], Chenyang Lu[1], Gihan Velisa[2], Yufan Zhou[2], Zhe Fan[2], Hongbin Bei[2], Yury Osetskiy[2], William J. Weber[3,2], Lumin Wang[1]

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PII-G-6: ATOM PROBE TOMOGRAPHY OF HIGH BANDGAP ThO_2

[TETI] Janelle Wharry[1], Amrita Sen[1], Vinay Chauhan[2], Maniesha Singh[1], Brian Gorman[3], Marat Khafizov[2], Mukesh Bachhav[4]

[1]Purdue University, [2]The Ohio State University, [3]Colorado School of Mines, [4]Mukesh Bachhav

PII-G-7: RELATING STRUCTURE TO SPECTROSCOPIC SIGNATURES: EXPERIMENTAL ANALYSIS AND THEORETICAL INTERPRETATION OF DIFFERENT ALUMINUM COORDINATION ENVIRONMENTS

[IDREAM] Andrew P. Wildman[3], Mateusz Dembowski[1], Trent R. Graham[1], Ernesto Martinez Baez[2], Rafal M. Gorniak[2], Maxime J. Pouvreau[2], Micah Prange[1], Anthony J. Krzysko[2], Xin Zhang[1], David Semrouni[2], Hsiu-Wen Wang[4], Xiaosong Li[3], Gregory K. Schenter[1,2], Kevin M. Rosso[1], Carolyn I. Pearce[1], Aurora E. Clark[2,1], Sue B. Clark[1,2]

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PII-G-8: THIN FILMS OF MODEL MATERIALS FOR THE FUTURE
[FUTURE] Jon K. Baldwin[1], Jacob E. Cooper[2], Benjamin Derby[1], Danny J. Edwards[3], Djamel Kaoumi[2], Timothy G. Lach[3], Nan Li[1], Daniel K. Schreiber[3]
[1]Los Alamos National Laboratory; [2]North Carolina State University; [3]Pacific Northwest National Laboratory

PII-G-9: METAL SPECIATION AND COORDINATION ENVIRONMENTS IN MOLTEN SALTS: INVESTIGATIONS USING X-RAY AND OPTICAL ABSORPTION TECHNIQUES
[MSEE] Ruchi Gakhar[1], William C. Phillips[1], Simerjeet K. Gill[2], Kotaro Sasaki[2], Mehmet Topsakal[2], Lingfeng He[1], Phillip Halstenberg[3], Shannon Mahurin[3], Lynne Ecker[2], Anatoly I. Frenkel[2]
[1]Idaho National Laboratory, [2]Brookhaven National Laboratory, [3]Oak Ridge National Laboratory

PII-G-10: ELECTRONIC AND THERMODYNAMIC PROPERTIES OF UZR_2 AND THO_2
[TETI] Krzysztof Gofryk[1], Xianxin Ding[1], Narayan Poudel[1], Tiankai Yao[1], Matthew Mann[2], Jason Harp[1], Madhab Neupane[3], Firoza Kabir[3], Chris Marianetti[4]
[1]Idaho National Laboratory, [2]Airforce Research Laboratory, [3]University of Central Florida, [4]Columbia University

PII-G-11: UNDERSTANDING FUNDAMENTAL INTERACTIONS OF METAL SUBSTITUENTS DEFINING THE PROPERTIES OF ALUMINUM OXYHYDROXIDES IN EXTREME ENVIRONMENTS
[IDREAM] Xin Zhang[1], Daniel J. Pope[2], Wenwen Cui[1], Micah Prange[1], Carolyn I. Pearce[1], Ying Chen[1], Shuai Zhang[1], Wen Liu[1], Mark H. Engelhard[1], Libor Kovarik[1], Meirong Zong[1], Hailin Zhang[1], Eric D. Walter[1], Zihua Zhu[1], James J. De Yoreo[1,3], Zheming Wang[1], Kevin M. Rosso[1], Aurora E. Clark[2,1], Sue B. Clark[1,2]
[1]Pacific Northwest National Laboratory, [2]Washington State University

PII-G-12: MICROSCOPY CHARACTERIZATION OF DEFECT EVOLUTION IN CONCENTRATED ALLOYS
[EDDE] Zhe Fan[1], Xing Wang[1], Taini Yang[2], Shijun Zhao[1], Chenyang Lu[2], Ke Jin[1], Yongqiang Wang[3], Hongbin Bei[1], Lumin Wang[2], William J. Weber[4,1], Karren L. More[1], Yanwen Zhang[1]
[1]Oak Ridge National Laboratory; [2]University of Michigan-Ann Arbor; [3]Los Alamos National Laboratory; [4]University of Tennessee-Knoxville

H. QUANTUM MATERIALS

PII-H-1: MICROMAGNETIC SIMULATIONS OF MAGNON THERMODYNAMICS IN YIG-BASED NANOSTRUCTURES
[SHINES] R. Rodriguez, M.R. Akanda, R. Lake, I. Barsukov
University of California, Riverside

PII-H-2: PROBING THE ELECTRONIC STATES OF A PROTOTYPE 3D DIRAC SEMIMETAL
[CATS] Timo Schumann[1], Anton A. Burkov[2], Jianxin Zhu[3], Shulei Zhang[4], Olle Heinonen[4], Ross McDonald[3], Susanne Stemmer[1]
[1]University of California – Santa Barbara; [2]University of Waterloo; [3]Los Alamos National Laboratory; [4]Argonne National Laboratory

PII-H-3: BENCHMARKING DIMER EXCHANGE COUPLINGS ACROSS A WIDE VARIETY OF COMPUTATIONAL METHODS
[M^2QM] Henry Schurkus[1], Garnet Chan[1], Hai-Ping Cheng[2], John Stanton[2]
[1]Cal Tech; [2]University of Florida

PII-H-4: TOPOTACTIC TRANSFORMATIONS IN COBALTITE FILMS FOR NEUROMORPHIC FUNCTIONALITIES

[Q-MEEN-C] I-Ting Chiu[1], Minhan Lee[2], Zhen Zhang[3], Shriram Ramanathan[3], Ivan Schuller[2], Yayoi Takamura[1]

[1]University of California Davis; [2]University of California San Diego; [3]Purdue University

PII-H-5: OBSERVATION OF FLAT MINIBAND AT THE FERMI LEVEL OF TWISTED BILAYER GRAPHENE NEAR THE MAGIC ANGLE TWIST

[NPQC] M. Iqbal B. Utama[1,2], Roland J. Koch[1], Kyunghoon Lee[1,2], Hongyuan Li[2], Sihan Zhao[2], Jiayi Zhu[2], Kenji Watanabe[1], Takashi Taniguchi[1], Paul D. Ashby[1], Alexander Weber-Bargioni[1], Alex Zettl[1,2], Chris Jozwiak[1], Aaron Bostwick[1], Eli Rotenberg[1], Feng Wang[1,2]

[1]Lawrence Berkeley National Laboratory; [2]University of California, Berkeley

PII-H-6: CONTROLLING SPIN, CHARGE AND LIGHT/MATTER INTERACTIONS IN LOW DIMENSIONAL PEROVSKITE MATERIALS

[CHOISE] Haipeng Lu[1], Xihan Chen[1], Jingying Wang[2], Kai Zhu[1], Wei You[4], Joseph J. Berry[1], Manoj K. Jana[3], David B. Mitzi[3], Z. Valy Vardeny[2], Matthew C. Beard[1]

[1]National Renewable Energy Laboratory, [2]University of Utah, [3]Duke University, [4]University of North Carolina

PII-H-7: MEASUREMENT AND CALCULATION OF ELECTRONIC AND TRANSPORT PROPERTIES OF 2D MATERIALS OVERLAYED WITH MOLECULAR MAGNETS

[M^{2}QM] Xiaochen Zhu[1], Haoming Jin[1], Ashlyn Hale[1], Andrew Brooks[1], Dmitry Skachkov[1], Art Hebard[1], George Christou[1], Hai-Ping Cheng[1], Richard Hennig[1], Xiaoguang Zhang[1]

[1]University of Florida

PII-H-8: ATOMIC SCALE STRUCTURE AND ELECTRONIC PROPERTIES IN TWISTED GRAPHENE HETEROSTRUCTURES

[Pro-QM] Carmen Rubio-Verdú[1], Alexander Kerelsky[1], Leo McGilly[1], Dante M. Kennes[2], Lede Xian[3], Lei Wang[1], Matthew Yankowitz[1], Shaowen Chen[1], Kenji Watanabe[4], Takashi Taniguchi[5], James Hone[1], Cory Dean[1], Angel Rubio[3,5], Abhay N. Pasupathy[1]

[1]Columbia University; [2]Freie Universität Berlin; [3]Max Planck Institute for the Structure and Dynamics of Matter; [4]National Institute for Materials Science, Japan; [5]The Flatiron Institute

PII-H-9: SPIN CURRENT TRANSMISSION THROUGH ANTIFERROMAGNETIC LAYERS

[SHINES] Victor Ortiz, Junxue Li, Bassim Arkook, Weiwei Lin, Igor Barsukov, Chia-Ling Chien, Jing Shi

[1]University of California, Riverside; [2]Johns Hopkins University

PII-H-10: FIRST-PRINCIPLES STUDY OF MECHANICAL AND ELECTRONIC PROPERTIES OF BENT TRANSITION-METAL DICHALCOGENIDES

[CCM] Adrienn Ruzsinszky[1], Qimin Yan[1], Niraj K. Nepal[1], Liping Yu[2]

[1]Temple University, [2]University of Maine

PII-H-11: MICROMAGNETIC SIMULATION OF THZ SIGNALS IN ANTIFERROMAGNETIC FERH BY SUB-PICOSECOND THERMAL PULSES

[Q-MEEN-C] Marco Menarini[1], Rajasekhar Medapalli[1], Eric E. Fullerton[1], Vitaliy Lomakin[1]

[1]University of California San Diego

PII-H-12: SPIN-TO-CHARGE CONVERSION IN A NORMAL METAL-MAGNETIC WEYL HETEROSTRUCTURE

[CATS] [1]Shulei Zhang, [1]Ivar Martin, [2]Anton A. Burkov, [1]Olle Heinonen

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

PII-H-13: DIRAC FERMIONS AND WEAK ANTILOCALIZATION IN LACUSB$_2$

[IQM] J. R. Chamorro[1], A. Topp[2,3], Y. Fang[4], M. J. Winiarski[1,5], C. R. Ast[2], M. Krivenkov[6], A. Varykhalov[6] B. J. Ramshaw[4], L. M. Schoop[2,3], T. M. McQueen[1]
[1]Johns Hopkins University, [2]Max Planck Institute, [3]Princeton University, [4]Cornell University, [5]Gdansk University, [6]Helmholtz-Zentrum Berlin

PII-H-14: OXIDATION OF A MOLECULE BY THE BIEXCITONIC STATE OF A CDS QUANTUM DOT

[LEAP] Shichen Lian, Joseph A. Christensen, Mohamad S. Kodaimati, Cameron R. Rogers, Michael R. Wasielewski, Emily A. Weiss
Northwestern University

PII-H-15: CORRELATIONS AND SUPERCONDUCTIVITY IN TWISTED GRAPHENE HETEROSTRUCTURES

[Pro-QM] Matthew Yankowitz[1], Shaowen Chen[1], Hryhoriy Polshyn[2], Yuxuan Zhang[2], K. Watanabe[3], T. Taniguchi[3], Andrea F. Young[2], Cory R. Dean[1]
[1]Columbia University; [2]University of California, Santa Barbara; [3]National Institute for Materials Science, Japan

PII-H-16: FIRST-PRINCIPLES STUDIES OF SPIN-ORBIT TORQUE IN FE-INTERCALATED NBS$_2$

[NPQC] Sophie Weber[1,2,], Eran Maniv[1], James G. Analytis[1,2], Jeffrey B. Neaton[1,2]
[1]Lawrence Berkeley National Laboratory; [2]University of California, Berkeley

PII-H-17: QUANTUM SUPERPOSITION AND ENTANGLEMENT IN SUPRAMOLECULAR AGGREGATES OF SINGLE-MOLECULE MAGNETS

[M^{2}QM] George Christou[1], Tuhin Ghosh[1], Jonathan Marbey[3], Khoa Dang[1], Wolfgang Wernsdorfer[2], Steve Hill[3]
[1]University of Florida; [2]Karlsruhe Institute of Technology; [3]Florida State University

PII-H-18: LOW-FREQUENCY NOISE IN MAGNETIC TUNNEL JUNCTIONS

[SHINES] A. Etesamirad[1], D. Nelson[2], I. Krivorotov[2], J. A. Katine[3], I. Barsukov[1]
[1]University of California, Riverside; [2]University of California, Irvine; [3]West Digital Corporation

PII-H-19: NUMERICAL SIMULATIONS OF STRONGLY CORRELATED ELECTRONIC MATERIALS FOR NEUROMORPHIC FUNCTIONALITIES

[Q-MEEN-C] Marcelo Rozenberg[1], Alberto Camjayi[2], Federico Tesler[2], Javier del Valle[3], Yoav Kalcheim[3], J. Trastoy[1], Pavel Salev[3], Ivan K. Schuller[3]
[1]CNRS, Université Paris-Saclay; [2]Ciudad Universitaria, Argentina; [3]University of California San Diego

PII-H-20: ANOMALOUS TRANSPORT AND MAGNETISM OF THE TOPOLOGICAL SEMI-METALS MN$_3$GE AND MN$_3$SN

[IQM] Jonathan Gaudet[1], Youzhe Chen[1], Guy G. Marcus[1], Lin Jiao[2], M. B. Stone[2], Y. Zhao[3], W. C. Chen[3], T. Higo[4], D. Qu[4], Y. Li[1], C. L. Chien[1], Y. Otani[4], S. Nakatsuji[1,4], C. Broholm[1]
[1]Johns Hopkins University, [2]Oak Ridge National Laboratory, [3]NIST Center for Neutron Research, [4]Institute for Solid State Physics, University of Tokyo

K. SOLAR ENERGY

PII-K-1: COMPUTATIONAL STUDIES ON LIGHT INDUCED ELECTRON TRANSFER AND CHEMICAL REACTIONS
[LEAP] Subhajyoti Chaudhuri[1], Ke R Yang[1], Nathan T La Porte[2], Jose F Martinez[2], Yang Yang[1], Gary Brudvig[1], Sharon Hammes-Schiffer[1], Michael R Wasielewski[2], Victor S Batista[1]
[1]*Yale University,* [2]*Northwestern University*

PII-K-2: TRANSPARENT CONDUCTIVE OXIDES FOR STUDIES ON DRIVING FORCE DEPENDENCE OF THE CHARGE CARRIER KINETICS
[AMPED] Jenny Schneider, Rachel E. Bangle, Gerald J. Meyer
University of North Carolina at Chapel Hill

PII-K-3: MODULATION OF OPTOELECTRONIC PROPERTIES OF LOW-DIMENSIONAL HYBRID PEROVSKITES BY CHEMICAL DOPING
[CHOISE] Evan Lafalce[1], Tianyang Li[2], Joseph M. Luther[3], Ashley Gaulding[3], Byron Larson[3], Z. Valy Vardeny[1], David Mitzi[2], Jeffery L. Blackburn[3]
[1]*University of Utah,* [2]*Duke University,* [3]*National Renewable Energy Laboratory*

PII-K-4: DETERMINING THE REORGANIZATION ENERGY OF TRIPHENYLAMINE DERIVATIVES USING TRANSPARENT CONDUCTING OXIDES
[AMPED] Rachel E. Bangle, Jenny Schneider, Ludovic Troian-Gautier, Gerald J. Meyer
University of North Carolina at Chapel Hill

PII-K-5: PHOTONIC THERMODYNAMIC SYSTEMS
[PTL] Bo Zhao[1], Zunaid Omar[2], Siddharth Buddhiraju[1], Parthiban Santhanam[1], Kaifeng Chen[1], Luis M. Pazos-Outon[2], Jae Jin Bang[3], Maggie Potter[3,4], Ralph Nuzzo[3], Harry Atwater[4], Eli Yablonovitch[2], Shanhui Fan[1]
[1]*Stanford University;* [2]*University of California, Berkeley;* [3]*University of Illinois at Urbana-Champaign;* [4]*California Institute of Technology*

PII-K-6: THEORETICAL STUDIES OF A NEW GENERATION OF DONOR-ACCEPTOR STRUCTURES FOR OPV SOLAR CELLS
[LEAP] Leighton O. Jones, Micaela Matta, Kevin L. Kohlstedt, George C. Schatz, Tobin J. Marks.
Northwestern University

M. SYNTHESIS SCIENCE

PII-M-1: TARGETED SYNTHESIS OF BROOKITE TiO_2, A METASTABLE POLYMORPH

[CNGMD] John Mangum[1], Okan Agirseven[2], John Perkins[3], Laura Schelhas[4], David Ginley[3], Michael Toney[4], Janet Tate[2], Brian Gorman[1]

[1]Colorado School of Mines; [2]Oregon State University; [3]National Renewable Energy Laboratory; [4]SLAC National Accelerator Laboratory

PII-M-2: SINGLE CRYSTAL SYNTHESIS OF ADVANCED NUCLEAR FUELS ($U_xTh_{1-x}O_2$ AND UZr_{2-x}): FIRST STEP TO DEVELOP A FIRST PRINCIPLE UNDERSTANDING OF THERMAL TRANSPORT UNDER IRRADIATION

[TETI] Matthew Mann[1], David Turner[1], Karl Richert[1], Jason Harp[2], Tiankai Yao[2], Lingfeng He[2], Jian Gan[2], Michael Benson[2]

[1]Airforce Research Laboratory, [2]Idaho National Laboratory

PII-M-3: COMBINING MULTI-MODAL IN-SITU CHARACTERIZATION AND MULTIVARIATE DATA ANALYSES TO DECOUPLE THE ROLES OF CHEMISTRY AND LOCAL GEOMETRY IN NANOPARTICLE SYNTHESIS

[GENESIS] Karena W. Chapman[1], Peter J. Chupas[1], Soham Banerjee[2], Antonin Grenier[1], Zhihengyu Chen,[1] Simon J.L. Billinge[2], Haiyan Zhao[3], Tina M. Nenoff[4]

[1]Stony Brook University; [2]Columbia University; [3]Argonne National Laboratory; [4]Sandia National Laboratories

PII-M-4: PHYSICAL DESCRIPTOR FOR THE GIBBS ENERGY OF INORGANIC CRYSTALLINE SOLIDS AND TEMPERATURE DEPENDENT MATERIALS CHEMISTRY

[CNGMD] Christopher Bartel[1], William Tumas[2], Stephan Lany[2], Aaron Holder[3]

[1]Lawrence Berkeley National Laboratory; [2]National Renewable Energy Laboratory; [3]University of Colorado

PII-M-5: CARBONS AND CONDUCTIVE METAL OXIDES AS SUPPORTS FOR ALKALINE HYDROGEN OXIDATION

[CABES] Jeremy Hitt[1], Apostolos Enotiadis[2], Zhifei Yan[1], Linxi Xu[1], Emmanuel Giannelis[2], Tom Mallouk[1]

[1]University of Pennsylvania, [2]Cornell University

GRADUATE STUDENT AND POSTDOCTORAL TEAM SCIENCE CONTEST

(From left) Rachel Bangle and Jenny Schneider

K-I-1: TRANSPARENT CONDUCTING OXIDES AS HIGHLY VERSATILE DYE-SENSITIZED PHOTOELECTRODES

[AMPED] Rachel E. Bangle[1], Jenny Schneider[1], Renato N. Sampaio[2], Ludovic Troian-Gautier[1] and Gerald J. Meyer[1]

[1]UNC Chapel Hill; [2]Brookhaven National Laboratory

(Standing, from left) Xin Gao, Bryan Kudisch, Andrew Miechan, and Daniel Oblinsky. (Sitting, from left) Simon Cooper, Kyle Biegasiewicz, and Michael Black.

A-I-4: DISCOVERY OF A NEW PHOTOBIOCATALYST PLATFORM: NON-NATURAL RADICAL PHOTOCHEMISTRY ENABLED BY FLAVOPROTEINS

[BioLEC] Kyle F. Biegasiewicz[1], Bryan Kudisch[1], Simon J. Cooper`, Xin Gao[1], Michael Black[1], JiHye Kim[1], Daniel Oblinsky[1], Braddock A. Sandoval[1], Andrew Meichan[1], Samuel E. Garfinkle[1], Gregory D. Scholes[1], and Todd K. Hyster[1]

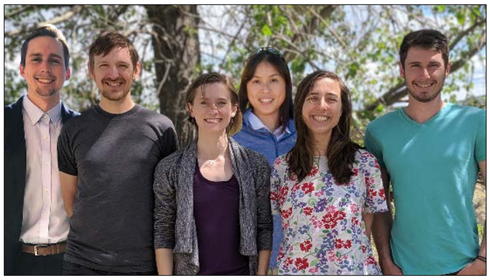
[1]Princeton University

(From left) Daniel Martin and Samantha Johnson

B-I-5: THE EFFECT OF ELECTROSTATICS ON SMALL MOLECULE BINDING AND CATALYSIS USING A POLYCATIONIC IRON PORPHYRIN

[CME] Daniel J. Martin[1], Samantha I. Johnson[2], James M. Mayer[1], Simone Raugei[2]

[1]Yale University, [2]Pacific Northwest National Laboratory (PNNL)

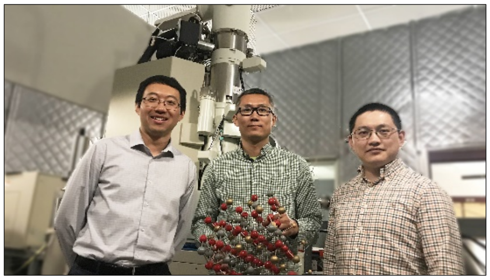


(From left) Chris Bartel, Sage Bauers, Karen Heinselman, Bor-Rong Chen, Rachel Woods-Robinson, John Mangum, and Elisabetta Arca (not shown).

F-I-3: DESIGNING NEW NITRIDE SEMICONDUCTORS: FROM COMPUTATIONAL DISCOVERY TO EXPERIMENTAL REALIZATION

[CNGMD] S.R. Bauers[1], C.J. Bartel[2], R. Woods-Robinson[3], J.S. Mangum[4], B.R. Chen[5], K. Heinselman[1], E. Arca[1], W. Sun[6], A.M. Holder[2], A. Zakutayev[1], S. Lany[1], G. Ceder[3, 6], L. Schelhas[5], M. Toney[5]

[1]National Renewable Energy Laboratory, [2]University of Colorado Boulder, [3]University of California, Berkeley, [4]Colorado School of Mines, [5]SLAC National Laboratory, [6]Lawrence Berkeley National Laboratory



(From left) Xing Wang, Zhe Fan, and Yang Tong

G-III-4: TUNING LOCAL ATOMIC ENVIRONMENTS TO CONTROL RADIATION DAMAGE

[EDDE] Yang Tong[1], Zhe Fan[1], Xing Wang[1], Sai Mu[1], Shijun Zhao[1], Chenyang Lu[2], Li Jiang[2], Dilpuneet Aidhy[3], Gihan Velisa[1], Lumin Wang[2], Fuxiang Zhang[1], Karren L. More[1], Yanwen Zhang[1]

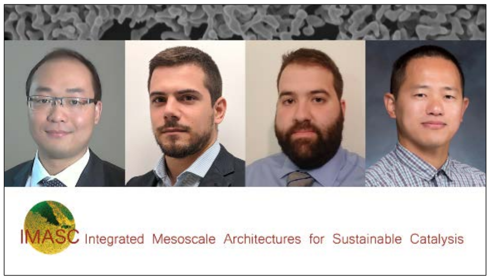
[1]Oak Ridge National Laboratory; [2]University of Michigan; [3]University of Wyoming

(From left) Tyler Mathis, Xuehang Wang, Nicolette Sanders, Ray Matsumoto, Lukas Vlcek, and Matt Thompson

D-II-4: DYNAMICS OF ELECTROLYTES UNDER CONFINEMENT IN NEXT GENERATION (PSEUDO)CAPACITIVE MATERIALS

[FIRST] X. Wang[1], L. Vlcek[2], M.W. Thompson[3], T.S. Mathis[1], R. Matsumoto[3], N.C. Sanders[4]

[1]Drexel University, [2]Oak Ridge National Laboratory/University of Tennessee, [3]Vanderbilt University, [4]Oak Ridge National Laboratory

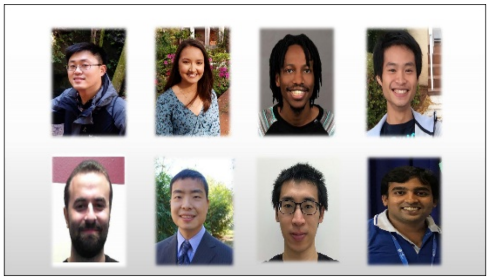


(From left) Kaining Duanmu, Georgios Giannakakis, Paul Kress, and Zhen Qi

B-II-2: MECHANISTIC STUDIES OF NON-OXIDATIVE ETHANOL DEHYDROGENATION ON NIAU SINGLE ATOM ALLOYS

[IMASC] Georgios Giannakakis[1]; Kaining Duanmu[2]; Paul Kress[1]; Zhen Qi[4]; Jurgen Biener[3]; Simon R. Bare[4]; Charles Sykes[1]; Philippe Sautet[2]; Maria Flytzani-Stephanopoulos[1]

[1]Tufts University, [2]University of California, Los Angeles, [3] Lawrence Livermore National Laboratory, [4] SLAC National Accelerator Laboratory

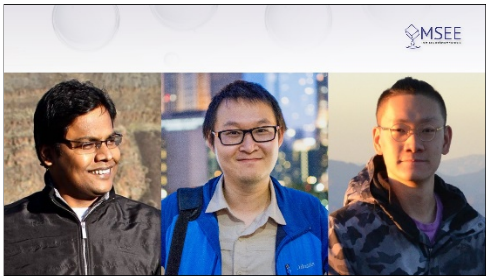


(Top row from left) Jie-Xiang Yu, Ashlyn Hale, Rainier Berkley, and Dian-Teng Chen
(Bottom row from left) Jonathan Marbey, Haoming Jin, Xiaochen Zhu, and Tuhin Ghosh

H-I-2: SYNTHESIS, CHARACTERIZATION AND PREDICTIVE FIRST-PRINCIPLES CALCULATIONS

[M^{2}QM] Jie-Xiang Yu[1], Jonathan Marbey[2], Tuhin Ghosh[1], Ashlyn Hale[1], Dian-Teng Chen[1], Rainier Berkley[3], Hoaming Jin[1], Xiaochen Zhu[1], George Christou[1], Arthur F. Hebard[1], Talat Rahman[3], Stephen Hill[2], and
Hai-Ping Cheng

[1]University of Florida, [2]Florida State University, [3]University of Central Florida



(From left) Santanu Roy, Fei Wu and Haimeng Wang

F-III-1: Bridging the Gap between Theory and Experiments on the Structure, Dynamics, and Thermodynamics of Molten Salts

[MSEE] Santanu Roy[1], Fei Wu[2], Haimeng Wang[3], Shobha Sharma[2], Yong Zhang[3], Matthew S. Emerson[2], Vyacheslav S. Bryantsev[1], Edward J. Maginn[3], Claudio J. Margulis[2], Alexander S. Ivanov,[1] Shannon M. Mahurin,[1] Phillip Halstenberg,[1] Simerjeet Gill,[4] Mehmet Topsakal,[4] Bobby Layne,[4] Kotaro Sasaki[4]

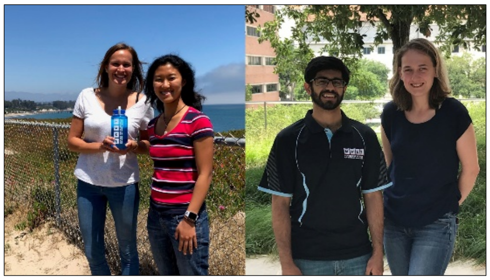
[1]Oak Ridge National Laboratory; [2]University of Iowa; [3]University of Notre Dame; [4]Brookhaven National Laboratory

(From left) Hyeyoung Cho, Jiaoyan Li, Jiaqi Jin and Hassnain Asgar

L-II-3: Property changes under confinement in architected materials

[MUSE] Pranay Asai[1], Hassnain Asgar[2], Michael Bartl[1], Darryl Butt[1], Hyeyoung Cho[1], Milind Deo[1], Greeshma Gadikota[2], Jan Goral[1], Hai Huang[3], Jiaqi Jin[1], Jiaoyan Li[3], Jan Miller[1], Subhash Risbud[4], Viktoriya Semekina[1], Yiping Xia[4], Ilya Zharov[1]

[1]University of Utah; [2]University of Wisconsin [3]Idaho National Laboratory [4]University of California, Davis

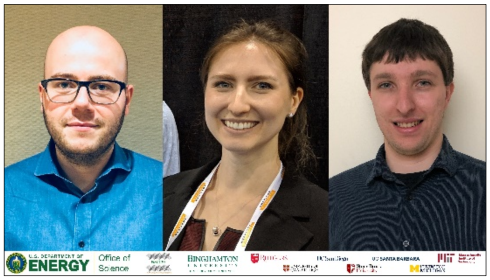


(From left) Segolene Antoine, Sally Jiao, Rahul Sujanani, and Malgorzata Chwatko

E-II-1: Understanding the Impact of Mesoscale Membrane Architecture on Water Transport

[M-WET] Segolene Antoine[1], Malgorzata Chwatko[2], Dipak Aryal[2], Rahul Sujanani[2], Sally Jiao[1], Venkat Ganesan[2], Nathaniel Lynd[2], Rachel Segalman[1], Lynn Katz[2], Benny Freeman[2]

[1]University of California, Santa Barbara; [2]The University of Texas at Austin



(From left) Antonin Grenier, Julija Vinckeviciute, and Zachary Lebens-Higgins

D-I-4: From Cation to Anion Redox: Pushing the ultimate limit of layered oxides

[NECCES] Zachary W. Lebens-Higgins[1], Antonin Grenier[2], Julija Vinckeviciute[3], Anton Van der Ven[3], Karena Chapman[2], Louis F. J. Piper[1]

[1]Binghamton University; [2]Stony Brook University; [3] University of California, Santa Barbara

(From left) Nicholas H. Bashian, Andrew Dawson, Rebecca Kubena, and Josh Zak

D-I-5: Investigating the Redox Activity and Lithiation of Icosahedral Boron Clusters in the Solid State

[SCALAR] Rebecca M. Kubena[1], Dahee Jung[1], Zeeshan Parvez[1], Jonathan C. Axtell[1], Nicholas H. Bashian[2], Andrew Dawson[1], Josh Zak[3], Anton Van der Ven[4]*, Brent C. Melot[2]*, Kimberly A. See[3]*, Sarah H. Tolbert[1]* & Alexander M. Spokoyny[1]*

[1] University of California, Los Angeles; [2]University of Southern California; [3]Caltech; [4] University of California, Santa Barbara

(From left) Qiming Shao and Víctor H. Ortiz

H-I-1: FERRIMAGNETIC INSULATOR FOR ULTRAFAST AND ULTRALOW-POWER SPINTRONIC DEVICES

[SHINES] Victor H. Ortiz[1], Qiming Shao[2], Mohammed Aldosary[1], Alexander Grutter[3], Junxue Li[1], Guoqiang Yu[2], Yawen Liu[1], Chi Tang[1], Kang L. Wang[2], and Jing Shi[1]

[1]University of California, Riverside; [2]University of California, Los Angeles; [3]National Institute of Standards and Technology

Talk ID: **Letter of Technical Session – Session Block – Number**
(e.g. D-I-1 is an Energy-Water talk on Tuesday at 8:00 am)
Poster ID: **P Session Block – Letter of Technical Session – Number**
(e.g. PII-B-1 is a Catalysis poster on Tue at 3:45 – 5:15 pm)

ENERGY FRONTIER RESEARCH CENTERS

[AMEWS] Advanced Materials for Energy-Water Systems
Seth Darling, Argonne National Laboratory
Class: 2018 – 2022

[AMPED] Alliance for Molecular PhotoElectrode Design for Solar Fuels
Gerald Meyer, University of North Carolina
Class: 2009 – 2020

[BEES] Breakthrough Electrolytes for Energy Storage
Robert Savinell, Case Western Reserve University
Class: 2018 – 2022

[BETCy] Biological Electron Transfer and Catalysis Center
John Peters, Washington State University
Class: 2014 – 2020

[BioLEC] Bioinspired Light-Escalated Chemistry
Gregory Scholes, Princeton University
Class: 2018 – 2022

[CABES] Center for Alkaline-Based Energy Solutions
Héctor Abruña, Cornell University
Class: 2018 – 2022

[CAST] Center for Actinide Science and Technology
Thomas Albrecht-Schmitt, Florida State University
Class: 2016 – 2020

[CATS] Center for the Advancement of Topological Semimetals
Robert McQueeney, Ames Laboratory
Class: 2018 – 2022

[CBES] Center for Bio-Inspired Energy Science
Samuel Stupp, Northwestern University
Class: 2009 – 2022

[CCM] Center for Complex Materials from First Principles
John Perdew, Temple University
Class: 2014 – 2020

[CCEI] Catalysis Center for Energy Innovation
Dionisios Vlachos, University of Delaware
Class: 2009 – 2022

[CEES] Center for Electrochemical Energy Science
Paul Fenter, Argonne National Laboratory
Class: 2009 – 2020

[CENT] Center for Enhanced Nanofluidic Transport
Michael Strano, Massachusetts Institute of Technology
Class: 2018 – 2022

[CGS] Center for Gas Separations Relevant to Clean Energy Technologies
Jeffrey Long, University of California, Berkeley
Class: 2009 – 2020

[CHOISE] Center for Hybrid Organic Inorganic Semiconductors for Energy
Matthew Beard, National Renewable Energy Laboratory
Class: 2018 – 2022

[CHWM] Center for Hierarchical Wasteform Materials
Hans-Conrad zur Loye, University of South Carolina
Class: 2016 – 2020

[CLSF] Center for Lignocellulose Structure and Formation
Daniel Cosgrove, Pennsylvania State University
Class: 2009 – 2022

[CMC-UF] Center for Mechanistic Control of Water-Hydrocarbon-Rock Interactions in Unconventional and Tight Oil Formations
Anthony Kovscek, Stanford University
Class: 2018 – 2022

[CME] Center for Molecular Electrocatalysis
R. Morris Bullock, Pacific Northwest National Laboratory
Class: 2009 – 2022

[CNGMD] Center for Next Generation of Materials by Design: Incorporating Metastability
William Tumas, National Renewable Energy Laboratory
Class: 2014 – 2020

[CSSAS] Center for the Science of Synthesis Across Scales
François Baneyx, University of Washington
Class: 2018 – 2022

[EDDE] Energy Dissipation to Defect Evolution
Yanwen Zhang, Oak Ridge National Laboratory
Class: 2014 – 2020

[FIRST] Fluid Interface Reactions, Structures and Transport Center
Sheng Dai, Oak Ridge National Laboratory
Class: 2009 – 2022

[FUTURE] Fundamental Understanding of Transport Under Reactor Extremes
Blas Uberuaga, Los Alamos National Laboratory
Class: 2018 – 2022

[GENESIS] A Next Generation Synthesis Center
John Parise, Stony Brook University
Class: 2018 – 2022

[ICDC] Inorganometallic Catalyst Design Center
Laura Gagliardi, University of Minnesota
Class: 2014 – 2022

[IDREAM] Interfacial Dynamics in Radioactive Environments and Materials
Sue Clark, Pacific Northwest National Laboratory
Class: 2016 – 2020

[IMASC] Integrated Mesoscale Architectures for Sustainable Catalysis
Cynthia Friend, Harvard University
Class: 2014 – 2022

[IQM] Institute for Quantum Matter
Collin Broholm, Johns Hopkins University
Class: 2018 – 2022

[LEAP] Center for Light Energy Activated Redox Processes
Michael Wasielewski, Northwestern University
Class: 2009 – 2020

[m2M/t] Center for Mesoscale Transport Properties
Esther Takeuchi, Stony Brook University
Class: 2014 – 2022

[M^{2}QM] Center for Molecular Magnetic Quantum Materials
Hai-Ping Cheng, University of Florida
Class: 2018 – 2022

[MSEE] Molten Salts in Extreme Environments
James Wishart, Brookhaven National Laboratory
Class: 2018 – 2022

[MUSE] Multi-Scale Fluid-Solid Interactions in Architected and Natural Materials
Darryl Butt, University of Utah
Class: 2018 – 2022

[M-WET] Center for Materials for Water and Energy Systems
Benny Freeman, University of Texas at Austin
Class: 2018 – 2022

[NECCES] NorthEast Center for Chemical Energy Storage
M. Stanley Whittingham, Binghamton University
Class: 2009 – 2020

[NEES] Nanostructures for Electrical Energy Storage
Gary Rubloff, University of Maryland
Class: 2009 – 2020

[NPQC] Center for Novel Pathways to Quantum Coherence in Materials
Joel Moore, Lawrence Berkeley National Laboratory
Class: 2018 – 2022

[Pro-QM] Programmable Quantum Materials
Dmitri Basov, Columbia University
Class: 2018 – 2022

[PTL] Photonics at Thermodynamic Limits
Jennifer Dionne, Stanford University
Class: 2018 – 2022

[Q-MEEN-C] Quantum Materials for Energy Efficient Neuromorphic Computing
Ivan Schuller, University of California, San Diego
Class: 2018 – 2022

[SCALAR] Center for Synthetic Control Across Length-scales for Advancing Rechargeables
Sarah Tolbert, University of California, Los Angeles
Class: 2018 – 2022

[SHINES] Spins and Heat in Nanoscale Electronic Systems
Jing Shi, University of California, Riverside
Class: 2014 – 2020

[TETI] Center for Thermal Energy Transport under Irradiation
David Hurley, Idaho National Laboratory
Class: 2018 – 2022

[UNCAGE-ME] Center for Understanding and Control of Acid Gas-induced Evolution of Materials for Energy
Krista Walton, Georgia Institute of Technology
Class: 2014 – 2022

[WastePD] Center for Performance and Design of Nuclear Waste Forms and Containers
Gerald. Frankel, Ohio State University
Class: 2016 – 2020

U.S. NATIONAL LABORATORIES

ANL	Argonne National Laboratory
BNL	Brookhaven National Laboratory
LBNL	Lawrence Berkeley National Laboratory
LLNL	Lawrence Livermore National Laboratory
LANL	Los Alamos National Laboratory
NETL	National Energy Technology 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