Science for our Nation's Energy Future

EFRC, Hub, and CMS
Principal Investigators' Meeting

July 24 -25, 2017
Washington, D.C.

Washington Marriott
Wardman Park

U.S. DEPARTMENT OF ENERGY | Office of Science

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Pre-Meeting

Sunday, July 23, 2017

1:30 – 5:30 PM **ECN Event: Air and Space Museum (all welcome)**

5:00 – 6:30 PM **Early Registration (Mezzanine, outside Thurgood Marshall Ballroom)**

7:00 – 9:00 PM **ECN Event: Dinner near Wardman Park Hotel (all welcome)**

Agenda Day 1

Monday, July 24, 2017
8:30 AM – 6:30 PM

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

Plenary Session

Thurgood Marshall Ballroom
Moderator: Harriet Kung, Director of the DOE Office of Basic Energy Sciences

8:30 – 8:40 AM **Welcome**
Steve Binkley
Acting Director, DOE Office of Science

8:40 – 9:15 AM **With Exascale Looming, this is an Exciting Time for Computational Science**
Doug Kothe
Director of Applications Development, Exascale Computing Project
Deputy Associate Lab Director, Computing and Computational Sciences Directorate
Oak Ridge National Lab

9:15 – 9:50 AM **Emerging Opportunities in Quantum Information Science**
David Awschalom
Director, Chicago Quantum Exchange
University of Chicago & Argonne National Lab

9:50 – 10:20 AM **Break**

10:20 – 10:55 AM **The Role of Philanthropy in Supporting Basic Research**
Marc Kastner
President, Science Philanthropy Alliance
Donner Professor of Physics, Emeritus, MIT

10:55 – 11:30 AM **Announcement of Student & Postdoc Team Science Finalists and Winners of the Intersection of Sound and Science Contest**
Andy Schwartz
EFRC Team Lead

11:30 – 1:00 PM **Lunch (buffet lunch provided)**

11:50 – 12:50 PM **ECN Event: Career Paths for Young Professionals Panel (Lincoln 3/4, all welcome)**

- **Jonathan Ajo-Franklin**, Lawrence Berkeley National Lab
- **Omar Farha**, Northwestern University
- **Gerald Meyer,** University of North Carolina
- **Ashley Predith**, DOE Office of Science

1:00 – 2:30 PM **Parallel Center Highlight Talks**

A/C. Biosciences/Catalysis, *Thurgood Marshall North*
B/G. Carbon Sequestration/Separation Science, *Lincoln 2*
D. Energy Storage, *Thurgood Marshall East*
E. Nuclear Waste and Energy, *Lincoln 5*
F. Quantum Materials, *Lincoln 6*
H. Solar Energy Conversion, *Thurgood Marshall South*
J. Materials and Chemistry by Design, *Thurgood Marshall West*

Invited Talks

1:40 – 2:05 PM **Office of Science Sponsored Undergraduate and Graduate Student Placement Opportunities at DOE Laboratories, *Lincoln 2***

James Glownia
Director, Office of Workforce Development for Teachers and Scientists
DOE Office of Science

2:05 – 2:30 PM **DOE Light Sources: Capabilities, Opportunities, and Access, *Lincoln 6***

Roger Falcone
Director, Advanced Light Source
Lawrence Berkeley National Lab

2:30 – 3:00 PM **Break**

3:00 – 5:00 PM **Parallel Technical Talks Session I**

C. Catalysis, *Thurgood Marshall North*
D. Energy Storage, *Thurgood Marshall East*
E. Nuclear Waste and Energy, *Lincoln 5*
F. Quantum Materials, *Lincoln 6*
H. Solar Energy Conversion, *Thurgood Marshall South*
I. Synthesis Science, *Lincoln 2*
J. Materials and Chemistry by Design, *Thurgood Marshall West*

5:00 – 6:30 PM **Poster Session I (Exhibit Hall C, refreshments provided)**

6:30 PM **Adjourn**

7:00 PM **ECN Event: Board Games with Dinner at The Board Room DC (all welcome)**

Agenda Day 2

Tuesday, July 25, 2017
8:30 AM – 5:00 PM

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

7:30 – 8:20 AM **ECN Event: Diversity in Energy Science Breakfast (Lincoln 3/4, all welcome)**

- **Ethan Crumlin**, Lawrence Berkeley National Lab
- **Laura Greene**, Florida State University
- **Jennifer A. Lewis**, Harvard University
- **Krista Walton,** Georgia Institute of Technology

8:30 – 10:10 AM **Parallel Technical Talks Session II**

A. Biosciences, *Lincoln 6*
C. Catalysis, *Thurgood Marshall North*
D. Energy Storage, *Thurgood Marshall East*
E. Nuclear Waste and Energy, *Lincoln 5*
G. Separation Science, *Thurgood Marshall West*
H. Solar Energy Conversion, *Thurgood Marshall South*
I. Synthesis Science, *Lincoln 2*

10:10 – 10:40 AM **Break**

10:40 – 12:00 PM **Parallel Technical Talks Session III**

A. Biosciences, *Lincoln 5*
B. Carbon Sequestration, *Lincoln 2*
C. Catalysis, *Thurgood Marshall North*
D. Energy Storage, *Thurgood Marshall East*
F. Quantum Materials, *Lincoln 6*
H. Solar Energy Conversion, *Thurgood Marshall South*
J. Materials and Chemistry by Design, *Thurgood Marshall West*

12:00 – 1:30 PM **Lunch (buffet lunch provided)**

12:20 – 1:20 PM **ECN Event: Federal R&D Budget Process Panel (Lincoln 3/4, all welcome)**

- **Julie Carruthers,** DOE Office of Science
- **Leland Cogliani**, Lewis-Burke Associates LLC
- **Kei Koizumi**, American Association for the Advancement of Science

1:30 – 3:30 PM	**Parallel Technical Talks Session IV** B. Carbon Sequestration, *Lincoln 2* C. Catalysis, *Thurgood Marshall North* D. Energy Storage, *Thurgood Marshall East* E. Nuclear Waste and Energy, *Lincoln 5* F. Quantum Materials, *Lincoln 6* H. Solar Energy Conversion, *Thurgood Marshall South* J. Materials and Chemistry by Design, *Thurgood Marshall West*
3:30 – 5:00 PM	**Poster Session II (Exhibit Hall C, refreshments provided)**
4:15 PM	**Announce winners of the *Graduate Student and Postdoc Team Science Competition***
5:00 PM	**Adjourn**
7:00 PM – late	**ECN Event: Baseball Game at Nationals Park (all welcome)**

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

PLENARY SPEAKER BIOGRAPHIES

WITH EXASCALE LOOMING, THIS IS AN EXCITING TIME FOR COMPUTATIONAL SCIENCE

Doug Kothe
Director of Applications Development, Exascale Computing Project
Deputy Associate Lab Director, Computing & Computational Sciences Directorate, Oak Ridge National Lab

Dr. Doug Kothe is the Deputy Associate Laboratory Director of the Computing and Computational Sciences Directorate at Oak Ridge National Lab (ORNL) and the Director of Applications Development for the DOE Exascale Computing Project. His previous positions at ORNL include Director of the Consortium for Advanced Simulation of Light Water Reactors, DOE's first Energy Innovation Hub, and Director of Science at the National Center for computational Sciences. Prior to ORNL Dr. Kothe spent 20 years at Los Alamos National Lab, where his research focused on the development and application of modeling and simulation technologies targeting multi-physics phenomena characterized in part by the presence of compressible or incompressible interfacial fluid flow.

EMERGING OPPORTUNITIES IN QUANTUM INFORMATION SCIENCE

David Awschalom
Director, Chicago Quantum Exchange
Univ. of Chicago & Argonne National Lab

Prof. David Awschalom is the Liew Family Professor in Molecular Engineering and Deputy Director of the Institute for Molecular Engineering at the University of Chicago, and he was recently named Director of the Chicago Quantum Exchange, an intellectual hub and partnership for advancing academic and industrial efforts in the science and engineering of quantum information. Previously he was Professor of Physics and of Electrical and Computer Engineering at the University of California-Santa Barbara, where he served as Director of the California NanoSystems Institute and Director of the Center for Spintronics and Quantum Computation. Prof. Awschalom's research involves understanding and controlling the spins of electrons, ions, and nuclei for fundamental studies of quantum systems, as well as potential applications in computing, imaging, and encryption.

THE ROLE OF PHILANTHROPY IN SUPPORTING BASIC RESEARCH

Marc Kastner
President, Science Philanthropy Alliance
Donner Professor of Physics, Emeritus, MIT

Dr. 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.

EARLY CAREER NETWORK ORGANIZED EVENTS

SOCIAL EVENTS

Open to All

AIR AND SPACE MUSEUM

Sunday, July 23, 2017, 1:30 – 5:30 PM

DINNER NEAR WARDMAN PARK HOTEL

Sunday, July 23, 2017, 7:00 – 9:00 PM

BOARD GAMES WITH DINNER AT THE BOARD ROOM DC

Monday, July 24, 2017, 7:00 PM – Late

BASEBALL GAME AT NATIONALS PARK

Tuesday, July 25, 2017, 6:15 PM – Late

Contacts for each event are listed at https://www.orau.gov/efrc2017/excursions.htm

PANEL DISCUSSIONS

Open to All

CAREER PATHS FOR YOUNG PROFESSIONALS PANEL

Monday, July 24, 2017, 11:50 – 12:50 PM; Lincoln 3/4

- **Jonathan Ajo-Franklin**, Lawrence Berkeley National Lab
- **Omar Farha**, Northwestern University
- **Gerald Meyer,** University of North Carolina
- **Ashley Predith**, DOE Office of Science

DIVERSITY IN ENERGY SCIENCE BREAKFAST

Tuesday, July 25, 2017, 7:30 – 8:20 AM; Lincoln 3/4

- **Ethan Crumlin**, Lawrence Berkeley National Lab
- **Laura Greene**, Florida State University
- **Jennifer A. Lewis**, Harvard University
- **Krista Walton,** Georgia Institute of Technology

FEDERAL R&D BUDGET PROCESS PANEL

Tuesday, July 25, 2017, 12:20 – 1:20 PM; Lincoln 3/4

- **Julie Carruthers,** DOE Office of Science
- **Leland Cogliani**, Lewis-Burke Associates LLC
- **Kei Koizumi**, American Association for the Advancement of Science

EARLY CAREER NETWORK (ECN) REPRESENTATIVES

The Early Career Network (ECN) includes early career scientists from the 36 Energy Frontier Research Centers (EFRC), 5 Computational Materials Sciences Awards (CMS) and 2 Energy Innovation Hubs (Hub). The network promotes interactions among students and postdocs within the programs and provides career development opportunities through ECN organized webinars, meet-ups at national meetings, social events, and panel discussions at the biennial PI meeting.

Name	Institution	Center
Jacob Artz	Washington State University	Center for Biological Electron Transfer and Catalysis (BETCy)
Ankita Bhutani	University of Illinois at Urbana-Champaign	Center for Emergent Superconductivity (CES)
Fernando Castro	Northwestern University	Center for Electrochemical Energy Science (CEES)
Alexander (Sasha) Chemey	Florida State University	Center for Actinide Science & Technology (CAST)
Yu Chen	University of Illinois at Urbana-Champaign	Center for Geologic Storage of CO_2 (GSCO2)
Stacey Chin	Northwestern University	Center for Bio-Inspired Energy Science (CBES)
Joseph Christensen	Northwestern University	Argonne-Northwestern Solar Energy Research Center (ANSER)
Raymond Clay	Sandia National Laboratories	Center for Predictive Simulation of Functional Materials (CPSFM)
Felipe da Jornada	Lawrence Berkeley National Laboratory	Center for Computational Study of Excited-State Phenomena in Energy Materials (C2SEPEM)
Hang Deng	Lawrence Berkeley National Laboratory	Center for Nanoscale Controls on Geologic CO_2 (NCGC)
Carissa Eisler	Lawrence Berkeley National Laboratory	Light-Material Interactions in Energy Conversion (LMI)
Marco Govoni	ANL/ University of Chicago	Midwest Integrated Center for Computational Materials (MICCoM)
Michael Guerette	Carnegie Institution of Washington	Energy Frontier Research in Extreme Environments (EFree)
Mathew Huie	Stony Brook	Center for Mesoscale Transport Properties (m2M)
Kristeen Joseph	University of Minnesota	Catalysis Center for Energy Innovation (CCEI)
Rebecca Key	University of Tennessee	Center for Direct Catalytic Conversion of Biomass to Biofuels (C3Bio)
Sarah Kiemle	Penn State University	Center for Lignocellulose Structure and Formation (CLSF)
Nam Kim	University of Maryland	Nanostructures for Electrical Energy Storage (NEES)
Arny Leroy	MIT	Solid-State Solar-Thermal Energy Conversion Center (S3TEC)

Name	Institution	Center
Hao Liu	Argonne National Laboratory	NorthEast Center for Chemical Energy Storage (NECCES)
Haylie Lobeck	Notre Dame	Materials Science of Actinides (MSA)
Pin Lu	QuesTek Innovations LLC	Center for Performance and Design of Nuclear Waste Forms and Containers (WastePD)
Robin Knauf	Los Alamos National Laboratory	Center for Advanced Solar Photophysics (CASP)
Ernesto Martinez Baez	Washington State University	Interfacial Dynamics in Radioactive Environments and Materials (IDREAM)
Camille May	University of Minnesota	Inorganometallic Catalyst Design Center (ICDC)
Matthew (Matt) Montemore	Harvard	Integrated Mesoscale Architectures for Sustainable Catalysis (IMASC)
Gregory Morrison	University of South Carolina	Center for Hierarchical Waste Form Materials (CHWM)
Gene Nolis	University of Illinois at Chicago	Joint Center for Energy Storage Research (JCESR)
Demyan Prokopchuk	Pacific Northwest National Laboratory	Center for Molecular Electrocatalysis (CME)
Robert Sacci	Oak Ridge National Laboratory	Fluid Interface Reactions, Structures and Transport Center (FIRST)
Refael Saer	Washington University in St. Louis	Photosynthetic Antenna Research Center (PARC)
Renato Sampaio	UNC Chapel Hill	Center for Solar Fuels (UNC)
Gideon Segev	Lawrence Berkeley National Laboratory	Joint Center for Artificial Photosynthesis (JCAP)
Shi Shi	University of Wisconsin, Madison	Energy Dissipation to Defect Evolution (EDDE)
Wenhao Sun	Lawrence Berkeley National Laboratory	Center for Next Generation of Materials by Design: Incorporating Metastability (CNGMD)
Dan Trainer	Temple University	Center for the Computational Design of Functional Layered Materials (CCDM)
Ian Walton	Georgia Tech	Center for Understanding and Control of Acid Gas-induced Evolution of Materials for Energy (UNCAGE-ME)
Lichun Wang	University of Texas at Austin	Center for Frontiers of Subsurface Energy Security (CFSES)
Mengfei Wu	MIT	Center for Excitonics (CE)
Gen (Jason) Yin	University of California, Los Angeles	Spins and Heat in Nanoscale Electronic Systems (SHINES)
Shuai Yuan	Texas A&M University	Center for Gas Separations Relevant to Clean Energy Technologies (CGS)

NATIONAL AIR AND SPACE MUSEUM, FOLLOWED BY DINNER

SUNDAY, JULY 23, 2017, 1:30 – 5:30PM, 7:00– 9:00PM

Open to All

ECN COMMITTEE MEMBERS

- **Fernando Castro (Chair)**, Northwestern University, CEES
- **Jacob Artz**, Washington State University, BETCy
- **Stacey Chin**, Northwestern University, CBES
- **Marco Govoni**, Argonne National Laboratory/ University of Chicago, MICCoM
- **Michael Guerette**, Carnegie Institution of Washington, EFree
- **Arny Leroy**, MIT, S3TEC
- **Haylie Lobeck**, Notre Dame, MSA
- **Ernesto Martinez Baez**, Washington State University, IDREAM
- **Camille May**, University of Minnesota, ICDC
- **Robert Sacci**, Oak Ridge National Laboratory, FIRST

DESCRIPTION

We will meet in the hotel lobby at 1:30PM and take the train to visit the National Air and Space Museum for the afternoon. We will begin our return to the hotel at 5:30PM and reconvene in the hotel lobby at 7 PM for dinner in the area around the hotel. Latecomers are welcome and should get in contact with the organizers for updates. Admission to the museum is free, but attendees will pay their own transportation fare and dinner costs.

Contacts:

Fernando Castro
fernandocastro2013@u.northwestern.edu

Michael Guerette
mguerette@carnegiescience.edu

BOARD GAMES WITH DINNER

MONDAY, JULY 24, 2017, 7:00PM – late

Open to All

ECN COMMITTEE MEMBERS

- **Stacey Chin (Co-chair),** Northwestern University, CBES
- **Michael Guerette (Co-chair),** Carnegie Institution of Washington, EFree
- **Jacob Artz,** Washington State University, BETCy
- **Fernando Castro,** Northwestern University, CEES
- **Marco Govoni,** Argonne National Laboratory/ University of Chicago, MICCoM
- **Arny Leroy,** MIT, S3TEC
- **Haylie Lobeck,** Notre Dame, MSA
- **Ernesto Martinez Baez,** Washington State University, IDREAM
- **Camille May,** University of Minnesota, ICDC
- **Robert Sacci,** Oak Ridge National Laboratory, FIRST
- **Gen (Jason) Yin,** University of California, Los Angeles, SHINES

DESCRIPTION

Have FUN at The Board Room DC near Dupont Circle (1737 Connecticut Ave NW). BYO food (many options nearby), order drinks on premises, play board games.

Contacts:

Michael Guerette
mguerette@carnegiescience.edu

Stacey Chin
stacey.chin@u.northwestern.edu

BASEBALL GAME

TUESDAY, JULY 25, 2017, 6:15PM – late
Open to All

ECN COMMITTEE MEMBERS

- **Michael Guerette (Co-chair)**, Carnegie Institution of Washington, EFree
- **Haylie Lobeck (Co-chair)**, Notre Dame, MSA
- **Robert Sacci (Co-chair)**, Oak Ridge National Laboratory, FIRST
- **Jacob Artz**, Washington State University, BETCy
- **Fernando Castro**, Northwestern University, CEES
- **Stacey Chin**, Northwestern University, CBES
- **Marco Govoni**, Argonne National Laboratory/ University of Chicago, MICCoM
- **Arny Leroy**, MIT, S3TEC
- **Ernesto Martinez Baez**, Washington State University, IDREAM
- **Camille May**, University of Minnesota, ICDC
- **Gen (Jason) Yin,** University of California, Los Angeles, SHINES

DESCRIPTION

Washington Nationals vs. Milwaukee Brewers at 7:05 pm. We will leave from the Wardman Park and take the Metro (red line connected to green line ~31 minutes) to and from Nationals Stadium. Group tickets at the discounted rate of $11 were purchased in advance by contacting Robert Sacci before June 15.

Contacts:
Robert Sacci
saccirl@ornl.gov

Haylie Lobeck
hlobeck@nd.edu

Michael Guerette
mguerette@carnegiescience.edu

CAREER PATHS FOR YOUNG PROFESSIONALS PANEL

Monday, July 24, 2017, 11:50 – 12:50PM
Lincoln 3/4
Open to All

ECN COMMITTEE MEMBERS

- **Hang Deng (Chair)**. Lawrence Berkeley National Laboratory, NCGC
- **Felipe da Jornada**, Lawrence Berkeley National Laboratory, C2SEPEM
- **Pin Lu**, QuesTek Innovations LLC, WastePD
- **Renato Sampaio**, UNC Chapel Hill, UNC
- **Dan Trainer**, Temple University, CCDM
- **Ian Walton**, Georgia Tech, UNCAGE-ME
- **Shuai Yuan**, Texas A&M University, CGS

PANELISTS

- **Jonathan Ajo-Franklin**, Staff Scientist at Lawrence Berkeley National Lab
- **Omar Farha**, Professor at Northwestern University
- **Gerald Meyer,** Professor at the University of North Carolina
- **Ashley Predith**, Senior Technical Advisor in the DOE Office of Science

DESCRIPTION

The goal is to provide graduate students and postdocs with information on the transition from postdoc to faculty positions, management of research groups, and paths to national laboratory, industry, and other non-traditional careers. There will be a brief opening statement from each panelist about their career trajectory, followed by prepared questions and a Q&A session with the audience.

SPEAKER BIOGRAPHIES

Jonathan Ajo-Franklin is currently the Geophysics Department Head and works as a Staff Scientist in the Energy Geoscience Division at Lawrence Berkeley National Laboratory (LBNL). He received his BA in Computer Science and History at Rice University (1998) followed by an MS (2003) and Ph.D. (2005) in Geophysics at Stanford University. From 2005 to 2007 he was a postdoctoral fellow at the Earth Resources Laboratory at MIT. Since 2007, he has led a group at LBNL, first as a researcher (2007-2013) and since 2013 as a staff scientist. He leads the Environmental and Applied Geophysics Lab (EAGLe) and the Reservoir Processes group in the Center for Nanoscale Control of Geologic Carbon (NCGC). He will inform the participants about opportunities in national laboratories.

Omar Farha is a research professor in the Department of Chemistry at Northwestern University. He received his Ph.D. in chemistry at University of California, Los Angeles in 2006, and was a postdoctoral fellow working on porous materials at Northwestern University from 2007 to 2008. His current research focuses on the rational design of metal–organic frameworks (MOFs) and porous-organic polymers for sensing, catalysis, storage, separations and light harvesting. He is also a distinguished adjunct professor at King Abdulaziz University and the president of NuMat Technologies. Professor Farha's work and research leadership have been recognized widely. He received the Satinder Ahuja Award for Young Investigators in Separation Science from American Chemical Society in 2016. His experiences in academia and industry will provide insight into career development in both sectors.

Gerald J. Meyer is a professor of chemistry at University of North Carolina at Chapel Hill and the Deputy Director of UNC's Energy Frontier Research Center on Solar Fuels. Professor Meyer's research concerns experimental investigations of the excited states of transition metal compounds that can drive subsequent electron or energy transfer reactions in fluid solution and at semiconductor interfaces. Professor Meyer received his Ph.D. in Chemistry at University Wisconsin – Madison in 1989, and held a post-doctoral position in Chapel Hill until 1991. Before he moved to UNC in 2014, he was the Bernard N. Baker Professor of Chemistry at Johns Hopkins University and served two years as the Chemistry Department Chair. His extensive experiences in different academic institutions will provide insight into academic job search from a perspective of the hiring committee.

Ashley Predith is a Senior Technical Advisor in the DOE Office of Science, where she advances DOE's basic research program in emerging biosciences and their intersection with physical sciences, applied math, and computer science. From 2013-2017, she was first the Assistant Director and then the Executive Director of the President's Council of Advisors of Science and Technology (PCAST) in the White House Office of Science and Technology Policy (OSTP). She managed a wide range of PCAST policy studies in technology development, healthcare, and national security. Before OSTP, Dr. Predith was the Associate Director for Programs in the Nanostructures for Electrical Energy Storage (NEES) EFRC and previously held positions in science policy and science writing and editing. She has a Ph.D. in Materials Science (MIT) and a BS in Materials Science and Engineering (University of Illinois at Urbana-Champaign). She will inform the attendees of opportunities in non-traditional careers and offer her perspective on how to navigate a non-traditional career path.

DIVERSITY IN ENERGY SCIENCE BREAKFAST

Tuesday, July 25, 2017, 7:30 – 8:20 AM
Lincoln 3/4
Open to All

ECN COMMITTEE MEMBERS

- **Stacey Chin (Co-chair),** Northwestern University, CBES
- **Carissa Eisler (Co-chair),** Lawrence Berkeley National Laboratory, LMI
- **Alexander Chemey,** Florida State University, CAST
- **Mathew Huie,** Stony Brook, m2M
- **Gene Nolis,** University of Illinois at Chicago, JCESR

PANELISTS

- **Ethan Crumlin,** Research Scientist at the Advanced Light Source, Lawrence Berkeley National Lab
- **Laura Greene,** Professor at Florida State University and Chief Scientist at the National High Magnetic Field Laboratory
- **Jennifer A. Lewis,** Professor at Harvard University
- **Krista Walton,** Professor at Georgia Institute of Technology

DESCRIPTION

This interactive panel will bring together scientists from academic and national research institutes to address diversity and inclusion within STEM fields. This panel will focus on effective practices for increasing inclusion and how to recruit and maintain underrepresented groups. Questions will be solicited from the audience.

SPEAKER BIOGRAPHIES

Ethan Crumlin is a scientist at the Advanced Light Source (ALS), an X-ray synchrotron user facility at Lawrence Berkeley National Laboratory (LBNL). He is also a principle investigator in JCESR and an affiliate with JCAP. He earned his Ph.D. in mechanical engineering from Massachusetts Institute of Technology in 2012 before joining ALS as a postdoctoral fellow and then becoming a scientist in 2014. His work at ALS revolves around supporting users from all around the world and guiding his research group to perform innovative surface and interface science characterization investigations of the solid/gas, solid/liquid, and solid/solid interface from a wide range of disciplines spanning environmental to energy systems. He will offer perspectives on the opportunities provided by the national laboratories and user facilities.

Laura H. Greene is the Chief Scientist at the National MagLab, the Francis Eppes Professor of Physics at Florida State University, and an Associate Director of the EFRC Center for Emergent Superconductivity. She is also the 2017 President of the American Physical Society with Science Diplomacy and Human Rights as her themes; while continuing her emphasis on increasing diversity in physics through multiple avenues. Greene is also co-chairing the NAS Decadal Survey for Materials Research and is on the AAAS Board of Directors. Her research is in experimental condensed matter physics, investigating strongly correlated electron systems, including high-temperature superconductivity. Greene is a member of the National Academy of Sciences; and a Fellow of the American Academy of Arts and Sciences, the Institute of Physics (U.K.), the American Academy of Arts and Sciences, the AAAS, and the APSS. She has been a Guggenheim

Fellow, received the E.O. Lawrence Award for Materials Research, the Maria Goeppert-Mayer Award, and the Bellcore Award of Excellence. She has co-authored > 200 publications and given > 500 invited talks.

Jennifer A. Lewis joined the faculty of the School of Engineering and Applied Sciences and the Wyss Institute for Biologically Inspired Engineering at Harvard University in 2013. Prior to joining Harvard, she was a professor and served as Director of the Materials Research Laboratory at University of Illinois. Her research focuses on the directed assembly of functional, structural and biological materials. She can provide insight based on her experience as a faculty member, administrator and entrepreneur.

Krista Walton is Professor and Marvin R. McClatchey and Ruth McClatchey Cline Faculty Fellow in the School of Chemical & Biomolecular Engineering at the Georgia Institute of Technology. She earned her Ph.D. in chemical engineering from Vanderbilt University in 2005 and completed her postdoctoral work at Northwestern University in 2006 as an ACS PRF Fellow. Dr. Walton is the Director and Lead PI of Georgia Tech's DOE Energy Frontier Research Center, UNCAGE-ME, and also serves as Associate Editor for the ACS journal Industrial & Engineering Chemistry Research. She will provide perspectives into tenure-track faculty positions at R1 institutions, building collaborative research programs, and conducting research with industry.

R&D BUDGET PROCESS PANEL

Tuesday, July 25, 2017, 12:20 – 1:20pm
Lincoln 3/4
Open to All

ECN COMMITTEE MEMBERS

- **Alexander Chemey (Chair)**, Florida State University, CAST
- **Joseph Christensen**, Northwestern University, ANSER
- **Raymond Clay**, Sandia National Laboratories, CPSFM
- **Felipe da Jornada**, Lawrence Berkeley National Laboratory, C2SEPEM
- **Hang Deng**, Lawrence Berkeley National Laboratory, NCGC
- **Kristeen Joseph**, University of Minnesota, CCEI
- **Sarah Kiemle**, Penn State University, CLSF
- **Haylie Lobeck**, Notre Dame, MSA
- **Pin Lu**, QuesTek Innovations LLC, WastePD
- **Robert Sacci**, Oak Ridge National Laboratory, FIRST
- **Renato Sampaio**, UNC Chapel Hill, UNC
- **Gideon Segev**, Lawrence Berkeley National Laboratory, JCAP
- **Wenhao Sun**, Lawrence Berkeley National Laboratory, CNGMD
- **Dan Trainer**, Temple University, CCDM
- **Lichun Wang**, University of Texas at Austin, CFSES

PANELISTS

- **Julie A. Carruthers,** Senior Science and Technical Advisor in the DOE Office of the Deputy Director for Science Programs
- **Kei Koizumi,** Visiting Scholar in Science Policy at the American Association for the Advancement of Science (AAAS)
- **Leland Cogliani,** Senior Consultant with Lewis-Burke Associates

DESCRIPTION

The multi-year federal R&D budget process involves many stakeholders including elected officials, congressional staff, executive branch employees, scientists, and members of the general public. The panel brings together experts in the federal budget process to discuss how the federal R&D budget is created. Each panelist will give a short presentation about different aspects of the budget process, followed by prepared questions from the committee and open questions from the audience.

SPEAKER BIOGRAPHIES

Julie A. Carruthers is a Senior Science and Technical Advisor in the DOE Office of Science, Office of the Deputy Director for Science Programs. Her responsibilities include advising the Deputy Director on science program management and policy issues, and providing coordination and analysis of budget, scientific, technical, programmatic, and operational issues regarding the Office of Science Program Offices and national laboratories. She also coordinates Office of Science participation in interagency committees on science and technology. She received her Ph.D. in Chemistry from Yale University, and a B.S. in Chemistry from the University of California, Santa Cruz.

Kei Koizumi is a Visiting Scholar in Science Policy at the American Association for the Advancement of Science (AAAS). He joined AAAS in February 2017 after 8 years as Assistant Director for Federal Research and Development and Senior Advisor to the Director for the National Science and Technology Council at the White House Office of Science and Technology Policy (OSTP). He received his M.A. from the Center for International Science, Technology, and Public Policy program at the George Washington University (where he is currently an instructor), and received his B.A. in Political Science and Economics from Boston University.

Leland Cogliani is a Senior Consultant with Lewis-Burke Associates, a government relations firm advocating for the public policy interests of over 35 research universities, associations and federal research centers. Prior to joining Lewis-Burke two years ago, he served on the Senate Energy and Water Appropriations subcommittee and had lead budget responsibilities over the National Nuclear Security Administration (NNSA), the Office of Science, the Advanced Research Projects Agency-Energy (ARPA-E), and other defense programs. He has a Bachelor of Arts in international studies from Boston College, a Master of Arts in international affairs from the George Washington University Elliott School of International Affairs, and a Juris Doctor from Catholic University Columbus School of Law.

2017 EFRC-HUB-CMS PI MEETING – GRAPHIC AGENDA FOR MONDAY, JULY 24, 2017

		A. Biosciences/ C. Catalysis	D. Energy Storage	H. Solar Energy Conversion	J. Materials and Chemistry by Design	B. Carbon Sequest/ G. Separation Science	E. Nuclear Energy & Waste	F. Quantum Materials
Room		***Thurgood North***	***Thurgood East***	***Thurgood South***	***Thurgood West***	***Lincoln 2***	***Lincoln 5***	***Lincoln 6***
Chair		***Robert Stack***	***Craig Henderson***	***Chris Fecko***	***Matthias Graf***	***P. Thiyagrajan***	***Philip Wilk***	***Mick Pechan***
O-1	**1:00 PM**	[**CCEI**] Dionisios Vlachos *U. Delaware* Catalysis Center for Energy Innovation	[**CEES**] Paul Fenter *ANL* Center For Electrochemical Energy Science	[**JCAP**] Harry Atwater *Caltech* Joint Center for Artificial Photosynthesis	[**CCDM**] John Perdew *Temple* Computational Design of Functional Layered Materials	[**NCGC**] Donald DePaolo *LBNL* Center for Nanoscale Controls on Geologic CO_2	[**EDDE**] Yanwen Zhang *ORNL* Energy Dissipation to Defect Evolution	[**S3TEC**] Gang Chen *MIT* Solid-State Solar Thermal Energy Conversion Center
O-2	**1:13 PM**	[**CLSF**] Daniel Cosgrove *Penn State* Center for Lignocellulose Structure and Formation	[**FIRST**] D. J. Wesolowski *ORNL* Fluid Interface Reactions, Structures and Transport	[**UNC**] Thomas Meyer *UNC Chapel Hill* Center for Solar Fuels	[**CNGMD**] W. Tumas *NREL* Center for Next Generation of Materials by Design	[**CFSES**] Larry Lake *UT Austin* Center for Frontiers of Subsurface Energy Security	[**WastePD**] G. Frankel *Ohio State* Performance & Design of Nuclear Waste Forms & Containers	[**CPSFM**] Paul Kent *ORNL* Center for Predictive Simulation of Functional Materials
O-3	**1:26 PM**	[**C3Bio**] M. C. McCann *Purdue* Center for Direct Catalytic Conversion of Biomass to Biofuels	[**JCESR**] George Crabtree *ANL, U. Illinois Chicago* Joint Center for Energy Storage Research	[**ANSER**] M. Wasielewski *Northwestern, ANL* Argonne-Northwestern Solar Energy Research Center	[**MAGICS**] P. Vashishta *U. Southern California* MAterials Genome Innovation for Computational Software	[**GSCO2**] Scott Frailey *UIUC* Center for Geologic Storage of CO_2	[**CHWM**] H. zur Loye *U. South Carolina* Center for Hierarchical Wasteform Materials	[**EFree**] Russell Hemley *Carnegie Institution, George Washington* Energy Frontier Research in Extreme Environments
O-4	**1:39 PM**	[**PARC**] R. Blankenship *Wash U. St. Louis* Photosynthetic Antenna Research Center	[**NECCES**] Whittingham *Binghamton* NorthEast Center for Chemical Energy Storage	[**CASP**] Victor Klimov *LANL* Center for Advanced Solar Photophysics	[**ICDC**] Laura Gagliardi *U. Minnesota* Inorganometallic Catalyst Design Center	**[Invited Talk]** James Glownia *DOE Office of Science* Office of Science Sponsored Undergraduate and Graduate Student Placement Opportunities at DOE Laboratories	[**CDMFTS**] G. Kotliar *Rutgers* Computational Design of Functional Strongly Correlated Materials & Theoretical Spectroscopy	[**CES**] Peter Johnson *BNL* Center for Emergent Superconductivity
O-5	**1:52 PM**	[**CBES**] Samuel Stupp *Northwestern* Center for Bio-Inspired Energy Science	[**m2M**] Esther Takeuchi *Stony Brook* Center for Mesoscale Transport Properties	[**C2SEPEM**] Steven Louie *LBNL, UC Berkeley* Computational Study of Excited-State Phenomena in Energy Materials	[**IMASC**] Cynthia Friend *Harvard* Integrated Mesoscale Architectures for Sustainable Catalysis		[**IDREAM**] Sue Clark *PNNL* Interfacial Dynamics in Radiation Environments and Materials	[**SHINES**] Jing Shi *UC Riverside* Spins and Heat in Nanoscale Electronic Systems
O-6	**2:05 PM**	[**BETCy**] John Peters *Montana State, Washington State* Biological Electron Transfer and Catalysis EFRC	[**NEES**] Gary Rubloff *U. Maryland* Nanostructures for Electrical Energy Storage	[**CE**] Marc Baldo *MIT* Center for Excitonics	[**MICCoM**] Giulia Galli *U. Chicago, ANL* Midwest Integrated Center for Computational Materials	[**UNCAGE-ME**] K.Walton *Georgia Tech* Understanding & Control of Acid Gas-Induced Evolution of Materials for Energy	[**MSA**] Peter Burns *Notre Dame* Materials Science of Actinides	**[Invited Talk]** Roger Falcone *Advanced Light Source, LBNL* DOE Light Sources: Capabilities, Opportunities, and Access
O-7	**2:18 PM**	[**CME**] R. Morris Bullock *PNNL* Center for Molecular Electrocatalysis		[**LMI**] Ralph Nuzzo *UIUC* Light-Material Interactions in Energy Conversion		[**CGS**] Jeffrey Long *UC Berkeley* Center for Gas Separations Relevant to Clean Energy Technologies	[**CAST**] T. Albrecht-Schmitt *Florida State* Center for Actinide Science and Technology	

* Team Science Finalist

2:30 – 3:00 PM Break

		C. Catalysis	**D. Energy Storage**	**H. Solar Energy Conversion**	**J. Materials and Chemistry by Design**	**I. Synthesis Science**	**E. Nuclear Energy & Waste**	**F. Quantum Materials**
Room		***Thurgood North***	***Thurgood East***	***Thurgood South***	***Thurgood West***	***Lincoln 2***	***Lincoln 5***	***Lincoln 6***
Chair		***Viviane Schwartz***	***Greg Fiechtner***	***Mark Spitler***	***Matthias Graf***	***Mike Markowitz***	***Tim Fitzsimmons***	***Jim Davenport***
I-1	**3:00 PM**	[**CCEI**] O. Abdelrahman *U. Minnesota* Biomass-Derived Butadiene by Dehydra-Decyclization of Tetrahydrofuran	[**m2M**] Amy Marschilok, Guihua Yu *Stony Brook, UT Austin* Exploiting "Passive Materials" in Electrochemical Energy Storage Systems: The Significant Impacts of Hard Material – Soft Material …	[**UNC**] Kirk S. Schanze *UT San Antonio* Molecular and Polymer Chromophore-Catalyst Assemblies for Solar Fuels Production	[**JCAP**] J. T. Feaster; D. A. Torelli; Z. W. Ulissi* *Stanford/SLAC; Caltech* Materials Discovery, Theory, & Characterization of Intermetallics for Electrochemical CO_2 Reduction	[**EFree**] Xiang Li *Penn State* Novel Carbon Materials Synthesis in Extreme Environments	[**CAST**] Kenneth Hanson *Florida State* Wavelength selective photochemical transformations using electroactive ligands	[**C2SEPEM**] D. Qiu; F. da Jornada; M. Utama* *LBNL, UC Berkeley* Environmental Screening Effects in 2D Materials: Renormalization of the Bandgap, Electronic Structure, and Optical Spectra
I-2	**3:20 PM**	[**IMASC**] Robert J Madix *Harvard* Moving from Model Studies on Single Crystal Gold to Higher Pressure Conditions: Kinetic and Mechanistic Understanding from TAP Studies on npAu Catalysts	[**NECCES**] Y.-M. Chiang *MIT* Integrated Experimental-Computational Investigation of a Polycrystalline Battery-Electrode Particle	[**PARC**] M. Maiuri *Princeton* Coherent Wavepackets in tho FMO Complex are Robust to Spectral Perturbations by Mutagenesis	[**JCESR**] K. A. Persson *LBNL* Materials Genomics Design and Electrochemical Realization of Improved Electrodes and Electrolytes for Future Multivalent Energy Storage	[**CBES**] G. Whitesides *Harvard* Soft Robotics	[**CDMFTS**] Yongxin Yao *Ames Lab* The recent development of the DFT/GW + Gutzwiller slave-boson method and package	[**CCDM**] Arun Bansil *Northeastern* The SCAN Density Functional: Success Stories for 2D, Layered and 3D Materials
I-3	**3:40 PM**	[**ICDC**] M. A. Ortuño; Z. Li; A. E. Platero-Prats* *U. Minnesota; Northwestern; ANL* Post-functionalized Metal–Organic Frameworks for Catalysis	[**FIRST**] N. Osti; M. W. Thompson; K.Van Aken* *ORNL; Vanderbilt; Drexel* Understanding Room Temperature Ionic Liquids & their Performance in Supercapacitors	[**CE**] G. Schlau-Cohen *MIT* Controlling energy transfer in DNA-based excitonic circuits	[**CES**] Wai-Kwong Kwok *ANL* Critical-Current-by-Design	[**CLSF**] Jochen Zimmer *U. Virginia* In vitro Reconstitution of Plant Cellulose Biosynthesis	[**CHWM**] N. B. Shustova *U. South Carolina* Well-Defined Actinide-Based Frameworks	[**CPSFM**] Olle Heinonen *ANL* Towards experimentally validated, predictive quantum simulations of vanadium and nickel oxides
I-4	**4:00 PM**	[**BETCy**] C. E. Lubner *NREL* Electron Bifurcation – Mechanistic First Principles	[**JCESR**] Brett A. Helms *LBNL* Tailoring Polymers of Intrinsic Microporosity to Meet the Growing Demands for Fast Ion Transport in Electrochemical Energy Storage Devices	[**UNC**] J. M. Papanikolas *UNC Chapel Hill* Ultrafast Injection and Recombination Dynamics at SnO2/TiO2 Core/Shell and NiO Interfaces for Solar Fuels Production	[**ICDC**] Donald G. Truhlar *U. Minnesota* Modeling Structure and Activity for Catalysts Supported on Metal-Organic Frameworks	[**CBES**] Sharon Glotzer *U. Michigan* Clathrate Colloidal Crystals	[**WastePD**] Jie Lian *RPI* Design and Performance of Ceramic Waste Forms for Iodine and Chlorine Sequestration with High Waste Loadings	[**MAGICS**] David Fritz *SLAC/Stanford* Ultrafast experiments and quantum dynamics of layered materials

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2017 EFRC-Hub-CMS PI Meeting – Graphic Agenda for Monday, July 24, 2017

		C. Catalysis	**D. Energy Storage**	**H. Solar Energy Conversion**	**J. Materials and Chemistry by Design**	**I. Synthesis Science**	**E. Nuclear Energy & Waste**	**F. Quantum Materials**
Room		***Thurgood North***	***Thurgood East***	***Thurgood South***	***Thurgood West***	***Lincoln 2***	***Lincoln 5***	***Lincoln 6***
I-5	**4:20 PM**	[**ANSER**] J. T. Hupp *Northwestern* A new family of catalysts for solar fuels: Cofactor-like catalysts on mesoporous MOF supports	[**m2M**] Y.Zhu,K.Takeuchi *BNL, Stony Brook* Contributions to Inter- and Intra-Rod Ion Transport in Tunnel Structured Materials: Implications for Electrochemical Energy Storage	[**JCAP**] Chengxiang Xiang *Caltech* Modeling, Simulation and Prototyping of Solar-Fuel Devices	[**CGS**] Berend Smit *UC Berkeley* Computational Screening of Nanoporous Materials for Gas Separations	[**EFree**] Tianshu Li *George Washington* Silicon Clathrates as New Energy Materials	[**CAST**] Eric Schelter *U. Pennsylvania* Synthesis of actinide hydroxylamine complexes and characterization of their electronic structures	[**CPSFM**] L.Shulenburger *SNL* Advances in many-body simulations of materials
I-6	**4:40 PM**	[**CME**] Simone Raugei *PNNL* Reversible Enzymatic H_2 production/oxidation Uses Different Pathways for the Forward and reverse Reaction	[**FIRST**] Jianzhong Wu *UC Riverside* Electrical Double Layer in Porous Electrodes - Capacitance, Capacitive Mixing, and Electro-Osmosis	[**ANSER**] B. Rudshteyn; K. Materna; N. La Porte* *Yale; Northwestern* The Pyridine Alkoxide Ligand Works for Water Oxidation Catalysts Both in Theory & in Practice	[**ICDC**] Omar Farha *Northwestern* Tuning the Catalytic Activity of Few-atom Clusters Deposited in Metal–Organic Frameworks	[**LMI**] Jennifer A. Lewis *Harvard* Patterning Polarized Photonic Nanocomposites via Direct Ink Writing	[**MSA**] May Nyman *Oregon State* Actinide Polynuclear Speciation and Implications in Nuclear Energy	[**CCDM**] John P. Perdew *Temple* Band Gaps from Hybrid Density Functionals for 1D, 2D, and 3D Solids: The Right Answer for the Right Reason

5:00 – 6:30 PM	**Poster Session, Exhibition Hall C**
7:00 – late	**ECN Event: Board Games with Dinner at The Board Room DC (all welcome)**

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2017 EFRC-Hub-CMS PI Meeting – Graphic Agenda for Tuesday, July 25, 2017

		C. Catalysis	D. Energy Storage	H. Solar Energy Conversion	G. Separation Science	I. Synthesis Science	E. Nuclear Energy & Waste	A. Biosciences
Room		***Thurgood North***	***Thurgood East***	***Thurgood South***	***Thurgood West***	***Lincoln 2***	***Lincoln 5***	***Lincoln 6***
Chair		***Chris Bradley***	***Michael Sennett***	***Refik Kortan***	***P. Thiyagrajan***	***Bonnie Gersten***	***John Vetrano***	***Bob Stack***
II-1	**8:30 AM**	[**IMASC**] M. Stamatakis *University College London* First-Principles Kinetic Monte Carlo Simulations of C1 Chemistries on Pure Metals and Single Atom Alloys	[**NECCES**] Y.-C. Lin; M. V. Hidalgo; S. Sallis* *UCSD; Binghamton* Thermodynamic Stability, Voltage and Diffusion Kinetics of Li$_x$VOPO$_4$ (x=0,1,2) Vanadyl Phosphate …	[**ANSER**] M. Kanatzidis *Northwestern* Lead-free Perovskite Films for Heterojunction Depleted Perovskite Solar Cells	[**UNCAGE-ME**] R. Lively *Georgia Tech* Engineering Nanoporous Materials with Increased Acid Gas Resistance	[**CNGMD**] Gerbrand Ceder, Andriy Zakutayev *LBNL, NREL* Discovery and Synthesis of Novel Nitrides with Targeted Functionality	[**IDREAM**] Kevin Rosso *PNNL* Interfacial Dynamics of Boehmite & Gibbsite in Extreme Environments: Connecting Across Spatial Scales	[**CLSF**] A. Singh; J. N. Burris; X. Xin* *North Carolina State; Penn State* The Nanomachine that Synthesizes Cellulose in Plants
II-2	**8:50 AM**	[**UNCAGE-ME**] Zili Wu *ORNL* Role of Surface Structure and Dopants on the Interaction Between Acid Gases and Metal Oxide Catalysts	[**m2M**] Alan West, Amy Marschilok *Columbia, Stony Brook* Electrochemically Induced Phase evolution of High Capacity Layered Materials: Complementary Insights …	[**CE**] William Tisdale *MIT* Luminescent 2D Metal Halide Perovskite Nanoplatelets	[**CGS**] Walter S. Drisdell *LBNL* Determining Mechanisms of Gas Adsorption in MOFs by Combining X-ray Spectroscopy & Theory	[**MAGICS**] P. Vashishta *U. Southern California* Computational synthesis of layered materials using CVD & exfoliation	[**EDDE**] Eva Zarkadoula *ORNL* Molecular Dynamics Simulations of Cascades: Effects of Ion-Electron Interactions in Irradiated Alloys	[**C3Bio**] N. C. Carpita *Purdue* Redesigning the structure of biomass for carbon- and energy-efficient catalytic & pyrolytic transformations
II-3	**9:10 AM**	[**ICDC**] Bruce Gates *UC Davis* Zr6 Nodes of Metal Organic Frameworks as Platforms for Single-Site Metal Catalysts	[**CEES**] Jeffrey P. Greeley *Purdue* Atomistic Studies of Nucleation and Growth in Conversion Reactions for Lithium-Ion Batteries	[**S3TEC**] J. Shuai,D. Singh *U. Houston, U. Missouri* Novel High Performance P- and N-Type Zintl Thermoelectrics	[**UNCAGE-ME**] Bobby G. Sumpter *ORNL* Linking Morphology and Interfacial Interactions to Acid Gas Uptake	[**EDDE**] Shijun Zhao; Taini Yang; Shi Shi* *ORNL; U. Michigan; U. Wisconsin* Effects of Alloy Complexity on Defect Production & Microstructural Evolution in Concentrated Alloys	[**CHWM**] Hui Wang *U. South Carolina* Multimetallic Nanoparticles: Alloys, Intermetallics, and Heterostructures	[**CLSF**] D. J. Cosgrove *Penn State* Cellulose structure, Organization and Interactions with Matrix Polysaccharides and Proteins
II-4	**9:30 AM**	[**IMASC**] M. Salmeron *LBNL* Structure And Reactivity of Noble Metal & Alloy Catalysts Characterized By In Situ Microscopy and Spectroscopy	[**NECCES**] I. D. Seymour *U. Cambridge* Advances in NMR Methodology of Paramagnetic Li-ion Battery Cathode Materials	[**LMI**] A. Paul Alivisatos *LBNL* Luminescent Concentrators as Light Compressors	[**CGS**] R. L. Siegelman; A. C. Forse* *UC Berkeley* Rational Design of New Materials for Carbon Dioxide Capture	[**CNGMD**] David Ginley, Kristin Persson *NREL, LBNL* Synthesis of Functional Polymorphic Materials	[**WastePD**] Seong Kim *Penn State* Understanding the formation, structure, and stability of the passivating layer formed on nuclear waste glass during aqueous corrosion	[**CBES**] Kyle Bishop *Columbia* Programming the Dynamics of Colloidal Machines
II-5	**9:50 AM**	[**JCAP**] Guiji Liu *LBNL* Integrated Photoelectrodes for CO$_2$RR	[**FIRST**] Nina Balke *ORNL* Heterogeneity of Charge Storage Processes in Electrochemical Capacitors	[**CE**] Mircea Dinca *MIT* Transport in 2D Metal-Organic Frameworks	[**UNCAGE-ME**] R. M. Marti; J. D. Howe* *Wash. U.; Georgia Tech* Understanding Structure and Dynamics of CO$_2$ Adsorbed in Open-Site MOFs	[**CGS**] Brett A. Helms *LBNL* Diamine-Appended Mg$_2$(dobpdc) Nanorods as Fillers in Mixed-Matrix Membranes for Efficient CO$_2$/N$_2$ Separt.	[**IDREAM**] Jay LaVerne *Notre Dame* Radiation Driven Modification of Beohmite and Gibbsite	[**CLSF**] Yaroslava Yingling *North Carolina State* All-Atom Structural Model of Plant Cellulose Synthase and Cellulose Synthase Complex

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2017 EFRC-Hub-CMS PI Meeting – Graphic Agenda for Tuesday, July 25, 2017

10:10 – 10:40 AM Break

		C. Catalysis	D. Energy Storage	H. Solar Energy Conversion	J. Materials and Chemistry by Design	B. Carbon Sequestration	A. Biosciences	F. Quantum Materials
Room		***Thurgood North***	***Thurgood East***	***Thurgood South***	***Thurgood West***	***Lincoln 2***	***Lincoln 5***	***Lincoln 6***
Chair		***Wade Sisk***	***Lane Wilson***	***Tom Settersten***	***Matthias Graf***	***Tom Russell***	***Bob Stack***	***Jim Rhyne***
III-1	**10:40 AM**	[**C3Bio**] M. Abu-Omar *UC Santa Barbara* Catalytic conversion of lignin first to chemical synthons for making materials and fuels	[**CEES**] R. Warburton; B. Nicolau; K. Letchworth-Weaver* *Purdue; UIUC; ANL* Understanding and Controlling the Reactivity of LiMn$_2$O$_4$-Electrolyte Interfaces	[**S3TEC**] Marin Soljacic *MIT* Nanophotonics for tailoring emission and absorption of light	[**CPSFM**] Paul Kent *ORNL* Effectively developing and distributing open source code and data: experiences from QMCPACK	[**NCGC**] Sally Benson *Stanford* Towards Resolution of Conflicting Information about the Influence of CO$_2$ Exposure on Wetting Properties and Residual Gas Trapping	[**BETCy**] Diep Nguyen; Jonathan Yuly* *U. Georgia; Duke* Mechanistic insights into energy conservation by flavin-based electron bifurcation	[**SHINES**] C.-L. Chien *Johns Hopkins* Exploiting spin-chiral topological surface states in Kondo insulator SmB$_6$ thin films
III-2	**11:00 AM**	[**CCEI**] M. J. Gilkey *U. Delaware* Metal-free cleavage of C-O bonds to form adipic acid from biomass derivatives	[**NEES**] K. Gregorczyk *U. Maryland* Vapor Phase Chemistry for Protection Layers and Solid-state 3D Batteries	[**CASP**] J. M. Luther *NREL* Quantum Dot Device Structures for High Efficiency Photoconversion	[**MICCoM**] F. Gygi *UC Davis* Development and Interoperability of the Qbox First-Principles Molecular Dynamics Code	[**GSCO2**] J. Druhan *UIUC* Linking Chemical Transformations to Physical Integrity Through Direct Imaging of Fluid Transport Properties in Mt. Simon Core During CO$_2$ Injection	[**PARC**] Rafael Saer *Wash U. St. Louis* Energy Transfer Fundamentals in Nature's Molecular Wires: Lessons from Native & Genetically-Modified FMO Pigment-Protein Complexes	[**CES**] Mark P M. Dean *BNL* Nature of the charge density waves in cuprate superconductors
III-3	**11:20 AM**	[**C3Bio**] H. I. Kenttämaa *Purdue* Fast hydropyrolysis, catalytic conversion & in situ hydrodeoxygenation produce drop-in hydrocarbon fuels from biomass	[**JCESR**] Kevin R. Zavadil *SNL* Polysulfide Solubility Suppression Through Electrolyte Redesign as a Path Toward Practical Lithium-Sulfur Batteries	[**LMI**] Paul V. Braun *UIUC* 3D Gradient Refractive Index Micro-Optics for Enhanced Control of Light	[**C2SEPEM**] J. DeSlippe *LBNL* Large-Scale GW Calculations on Pre-Exascale HPC Systems	[**CFSES**] Tip Meckel *UT Austin* Advances in Understanding Buoyancy-Dominated Flow in Heterogeneous Geologic Systems	[**BETCy**] Anne K. Jones, Paul W. King *Arizona State; NREL* Oxidative Inactivation of [FeFe]-Hydrogenase as a Model for Redox Tuning of Enzyme Active Site Reactivity	[**SHINES**] C.-N. Lau *UC Riverside/OSU* Long-Distance Spin Transport Through a Graphene Quantum Hall Antiferromagnet
III-4	**11:40 AM**	[**CCEI**] K. E. Joseph *U. Minnesota* Tunable synthesis of Oleo-Furan Surfactants via Acylation of Biomass-Derived Furans	[**CEES**] Kan-Sheng Chen *Northwestern* Interfacial Properties of Graphene/Lithium Manganese Oxide Spinel Cathodes for Lithium-Ion Batteries	[**S3TEC**] David Bierman; Veronika Stelmakh* *MIT* Tailoring Thermal Emission for High Performance Solar Thermophotovoltaic Devices	[**MAGICS**] A. Nakano *U. Southern California* Scalable simulation software and data analytics for Layered materials	[**NCGC**] Ian Bourg *Princeton* Solubility of Gases (CO$_2$, CH$_4$, H$_2$, Noble Gases) in Clay Interlayer Nanopore Water	[**PARC**] Matt Cuneo *ORNL* Probing Photosynthetic Antenna Complexes with Neutrons: from Individual Hydrogen Atoms to Hierarchal Assemblies	[**EFree**] M. Somayazulu *Carnegie Institution* Potential New Superhydride Superconductors

12:00 – 1:30 PM Lunch

* Team Science Finalist

2017 EFRC-Hub-CMS PI Meeting – Graphic Agenda for Tuesday, July 25, 2017

		C. Catalysis	**D. Energy Storage**	**H. Solar Energy Conversion**	**J. Materials and Chemistry by Design**	**B. Carbon Sequestration**	**E. Nuclear Energy & Waste**	**F. Quantum Materials**
Room		***Thurgood North***	***Thurgood East***	***Thurgood South***	***Thurgood West***	***Lincoln 2***	***Lincoln 5***	***Lincoln 6***
Chair		***Chris Fecko***	***Craig Henderson***	***Jane Zhu***	***Jim Davenport***	***Jim Rustad***	***Philip Wilk***	***Mick Pechan***
IV-1	**1:30 PM**	[**CME**] James M. Mayer *Yale* Advancing Molecular Electrocatalysis using Linear Free Energy Relationships	[**JCESR**] Joaquin Rodriguez-Lopez *UIUC* Versatile Macromolecular Design for Emerging Size-Selective Non-Aqueous Redox Flow Batteries	[**UNC**] Taylor H. Moot; Lesheng Li* *UNC Chapel Hill* Identification and Passivation of the Defect States in NiO for Photovoltaic and Solar Fuel Applications	[**MICCoM**] J. de Pablo *U. Chicago, ANL* SSAGES and COPSS - Modern Software for Advanced Materials Modeling	[**GSCO2**] R. Makhnenko *UIUC* Hydro-Mechanical Aspects of Deep CO$_2$ Storage	[**MSA**] Maik Lang *U. Tennessee* Actinide Materials Under Exterme Condition: Local Defect Structure and Disorder	[**SHINES**] G. Yin; X. Ma* *UCLA; UT Austin* Magnetic skyrmions in ferromagnetic/heavy-metal multi-layers
IV-2	**1:50 PM**	[**BETCy**] Lance Seefeldt, Caroline Harwood *Utah State;* *U. Washington* Light Driven N-H and C-H Bond Formation by Nitrogenase	[**FIRST**] Yury Gogotsi *Drexel* High-Rate Electrical Energy Storage Enabled by Metallic Conductivity of MXenes	[**ANSER**] T. J. Marks *Northwestern* Soft Matter and Hybrid Solar Cell Interfacial Science	[**C2SEPEM**] Chao Yang *LBNL* Low-Rank Approximation for Solving the Bethe-Salpeter Equation	[**CFSES**] Pania Newell *SNL* Performance Assessment of Jointed/Faulted Caprock During CO$_2$ Sequestration	[**EDDE**] Karren L. More *ORNL* Defect Generation, Evolution, and Dynamics in Irradiated Concentrated Solid Solution Alloys	[**CES**] James Eckstein *UIUC* Superconductivity in the Topological Insulator Bi$_2$Se$_3$
IV-3	**2:10 PM**	[**UNC**] Gerald J. Meyer *UNC Chapel Hill* A General Approach for Generation of Catalytic High Valent Metal Oxo Species Reveals Photoinduced One Electron, Two Proton Transfer Reactivity	[**NEES**] A. Alec Talin *SNL* Solid State Li-ion Batteries: Advancing Performance Through Fundamental Understanding	[**JCAP**] Jeff B. Neaton *LBNL* Discovery of new solarfuels photoanode materials with a combination of high-throughput theory and experiment	[**MICCoM**] M. Govoni *ANL, U. Chicago* Development of the WEST Code for Large Scale GW Code and of Data Infrastructure	[**GSCO2**] Dalton; M. G. D. Ordonez; S. Fuchs; P. Kabir; Z. Shi; M. Tkach* *NETL; UIUC; UT Austin; U. Southern California* Geochemical Reactions During Geological Carbon Sequestration Can Decrease Fracture …	[**WastePD**] J. R. Scully *U. Virginia* Integrated Computational Materials Design of a Corrosion Resistant High Entropy Alloy for Harsh Environments: The Science Behind it	[**SHINES**] Kang L. Wang *UC Los Angeles* Topological spintronic heterostructures and their properties – examples of the collaborative research in SHINES
IV-4	**2:30 PM**	[**CCDM**] D. R. Strongin *Temple* Theory and Computation Working with Experiment to Understand and Improve Water Splitting Catalysts	[**NECCES**] M. D. Radin *UC Santa Barbara* The Materials Physics of Lithium (De)intercalation in Layered Oxide Cathodes	[**CASP**] Cherie R. Kagan *U. Pennsylvania* Mechanisms for Charge Transport and Photoconductance in Mesoscale Quantum Dot Assemblies	[**CNGMD**] S. Lany, J.Tate *NREL, OSU* Novel Phase Diagram Behavior and Materials Design in Heterostructural Semiconductor Alloys	[**NCGC**] Hang Deng *LBNL* Investigation of Fracture Alteration using a Coupled Modeling and Experimental Approach	[**CHWM**] T. M. Besmann *U. South Carolina* Volume Based Thermodynamics Approach Applied to Salt Inclusion Materials	[**CDMFTS**] C. C Homes *BNL* Optical properties of the narrow-gap semiconductor FeSb$_2$

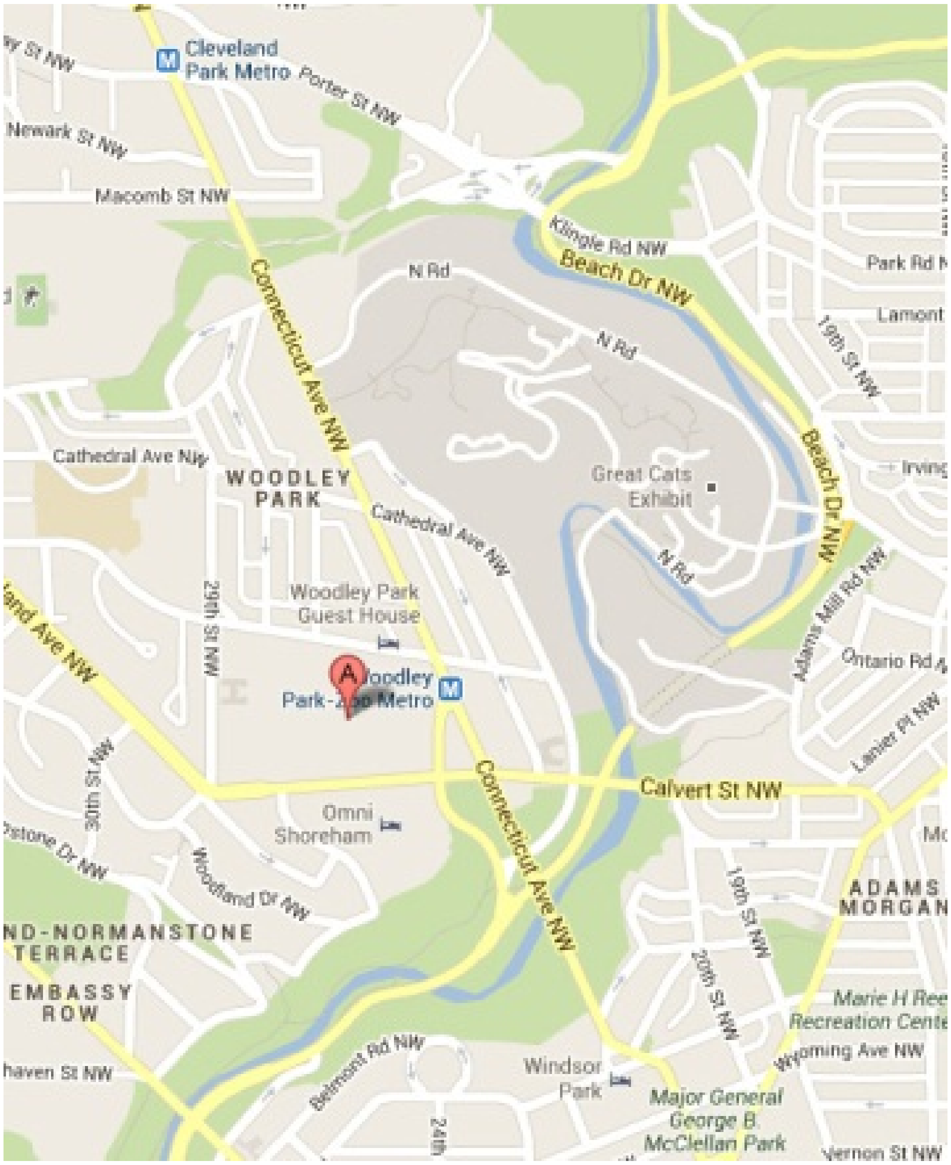
* Team Science Finalist

2017 EFRC-HUB-CMS PI MEETING – GRAPHIC AGENDA FOR TUESDAY, JULY 25, 2017

		C. Catalysis	D. Energy Storage	H. Solar Energy Conversion	J. Materials and Chemistry by Design	B. Carbon Sequestration	E. Nuclear Energy & Waste	F. Quantum Materials
Room		***Thurgood North***	***Thurgood East***	***Thurgood South***	***Thurgood West***	***Lincoln 2***	***Lincoln 5***	***Lincoln 6***
IV-5	**2:50 PM**	[**CME**] Shannon S. Stahl *U. Wisconsin* Development of Molecular Mediators for Improved Electrochemical Energy Conversion	[**CEES**] Maria Chan *ANL* Characterization and modeling of oxygen reactivity and structural evolution during electrochemical charging of Li-rich Li_5FeO_4	[**C2SEPEM**] J. B. Neaton *LBNL, UC Berkeley* Origins of Singlet Fission in Solid Pentacene from an Ab Initio Green's-Function Approach	[**EDDE**] Yuri N. Osetskiy *ORNL* Diffusion and Mass Transport in Concentrated Solid Solution Alloys: Features and Effects to Radiation Damage	[**CFSES**] Matt Balhoff *UT Austin* Rock Mechanical Alteration Due to Flow of CO_2-Charged Brine: Shear Strength of Crystal Geyser Outcrop Samples	[**CAST**] Ryan Baumbach *Florida State/NHMFL* Harnessing the f-electron state in novel high temperature waste forms	[**S3TEC**] Vazrik Chiloyan, Keith Nelson *MIT* Thermal transport on experimentally imposed length scales: Non-diffusive kinetics, phonon mean free paths, and first- …
IV-6	**3:10 PM**	[**JCAP**] Jens K. Nørskov *SLAC* Understanding trends in CO_2 reduction electro-catalysis	[**NEES**] Yue Qi *Michigan State* Quantify the Fundamental Irreversible Structural and Chemical Changes for Nanostructure Designs in Battery Applications	[**CASP**] Matthew Beard *NREL* Carrier Multiplication in Semiconductor Quantum Dots: Current Status and Future Prospects	[**IDREAM**] Aurora Clark *Washington State* Developing a Multiscale Understanding of Aluminum Transformations with Integrated Simulation and Spectroscopy	[**GSCO2**] A. Elbanna *UIUC* Towards a Multiscale Physics Based Framework for Modeling Fluid Infiltrated Fault Zones with an Eye for Induced Seismicity in Energy Applications	[**MSA**] Albert Migliori *LANL* New Insights into the Physics and Aging of Plutonium Metal	[**CDMFTS**] S. Choi *BNL* Transport properties of correlated $FeSb_2$: first principles combined with dynamical mean field theory

3:30 – 5:00 PM Poster Session II, Exhibition Hall C; 4:15 Announce winners of the *Graduate Student and Postdoctoral Team Science Competition*

HOTEL MAPS

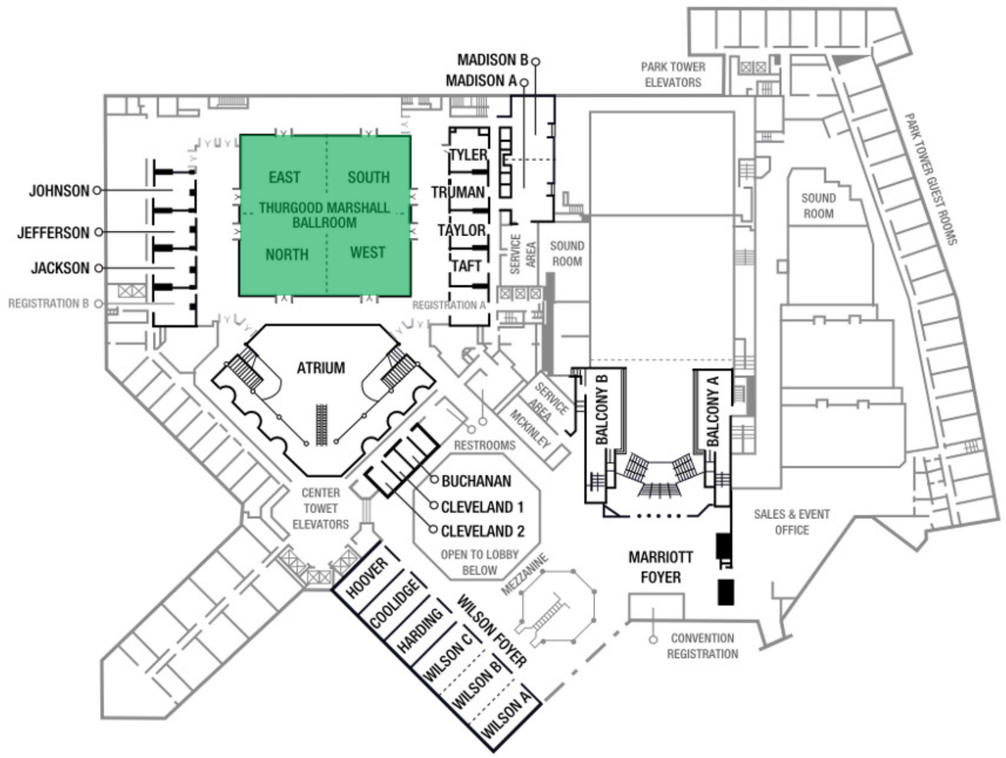


Washington Marriott Wardman Park
2660 Woodley Road NW
Washington, DC 20008

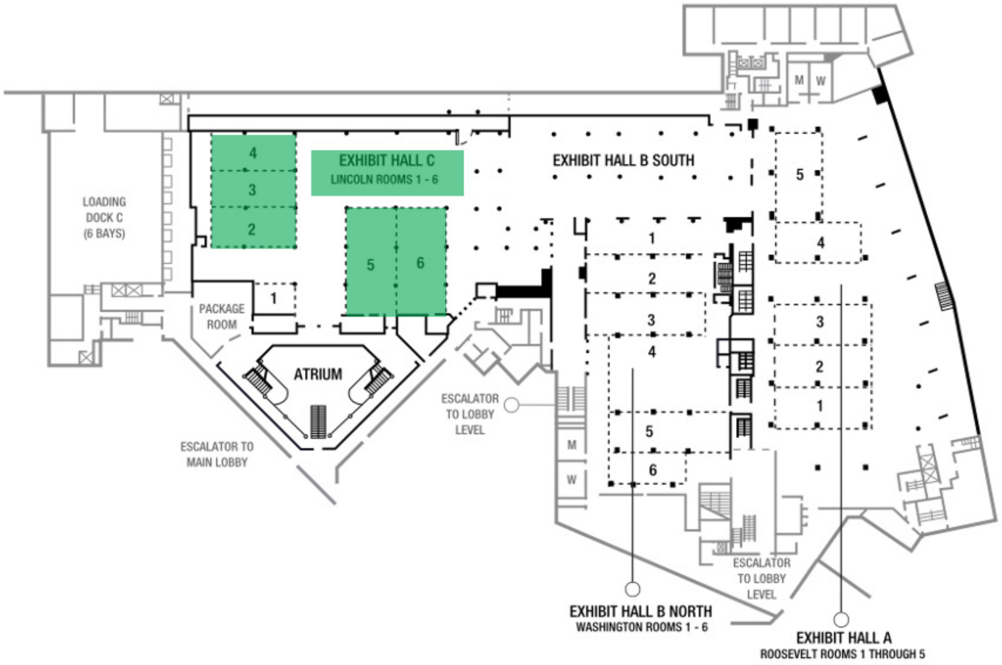
Subway Station: Woodley Park-Zoo/Adams Morgan Metro Red line

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

MEZZANINE LEVEL



EXHIBITION LEVEL



HIGHLIGHT TALK ABSTRACTS

A. BIOSCIENCES / C. CATALYSIS, *THURGOOD MARSHALL NORTH*

1:00 PM

O-A-1: CATALYSIS CENTER FOR ENERGY INNOVATION

Award Period: 2009 – 2014; 2014 – 2018

[EFRC – CCEI] Stavros Caratzoulas[1], Jingguang Chen[2], Paul Dauenhauer[3], Mark Davis[4], Doug Doren[1], Wei Fan[5], Anatoly Frenkel[6], Ray Gorte[7], Marianthi Ierapetritou[8], Friederike Jentoft[5], Chris Jones[9], Raul Lobo[1], Chris Murray[7], Basu Saha[1], Stan Sandler[1], Ilja Siepmann[3], Mark Snyder[10], Klaus Theopold[1], Michael Tsapatsis[3], Dion Vlachos[1], Don Watson[1], Bingjun Xu[1]

[1]University of Delaware (lead institution); [2]Columbia University; [3]University of Minnesota; [4]California Institute of Technology; [5]University of Massachusetts; [6]Brookhaven National Laboratory and Stony Brook University; [7]University of Pennsylvania; [8]Rutgers University; [9]Georgia Institute of Technology; [10]Lehigh University

CCEI is a transformative catalysis center for energy innovation that addresses one of today's most challenging problems: the transformation of lignocellulosic biomass into renewable transportation fuels and chemicals.

1:13 PM

O-A-2: CENTER FOR LIGNOCELLULOSE STRUCTURE AND FORMATION

Award Period: 2009 – 2014; 2014 – 2018

[EFRC – CLSF] Daniel J. Cosgrove[1], Charles T. Anderson[1], Ying Gu[1], Candace Haigler[2], Mei Hong[3], Seong H. Kim[1], James D. Kubicki[4], Manish Kumar[1], Chang-Jun Liu[5], Janna Maranas[1], Karl Mueller[1], B. Tracy Nixon[1], Hugh O'Neill[6], Alison W. Roberts[7], Ming Tien1, Yaroslava G. Yingling[2], Jochen Zimmer[8]

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

CLSF's mission is to develop a nano- to meso-scale understanding of plant cell walls, the main structural material in plants, and the mechanisms of their assembly, forming the foundation for significant advances in sustainable energy and novel biomaterials.

1:26 PM

O-A-3: CENTER FOR DIRECT CATALYTIC CONVERSION OF BIOMASS TO BIOFUELS

Award Period: 2009 – 2014; 2014 – 2018

[EFRC – C3Bio] Maureen C, McCann[1], Mahdi M. Abu-Omar[2], Rakesh Agrawal[1], Gregg T. Beckham[3], Joseph J. Bozell[4], Nicholas C. Carpita[1], Clint C. S. Chapple[1], Michael F. Crowley[3], W. Nicholas Delgass[1], Bryon S. Donohoe[3], Michael E. Himmel[3], Hilkka I. Kenttämaa[1], Lee Makowski[5], Richard Meilan[1], Nathan S. Mosier[1], Fabio H. Ribeiro[1], Melvin P. Tucker[3]

[1]Purdue University (lead institution); [2]University of California Santa Barbara; [3]National Renewable Energy Lab; [4]University of Tennessee; [5]Northeastern University

Mission: To master the ability to reconfigure all partially reduced carbon from plant cell walls into desired molecules.

1:39 PM

O-A-4: PHOTOSYNTHETIC ANTENNA RESEARCH CENTER

Award Period: 2009 – 2014; 2014 – 2018

[EFRC – PARC] Robert Blankenship[1], Dewey Holten[1], David Bocian[2], Donald Bryant[3], Richard Cogdell[4], P. Leslie Dutton[5], Michael Gross[1], Neil Hunter[6], Christine Kirmaier[1], Jonathan Lindsey[7], Paul Loach[8], Zaida Luthey-Schulten[9], Gabriel Montaño[10], Christopher Moser[5], Dean Myles[11], Himadri Pakrasi[1], Pamela Parkes-Loach[8], Greg Scholes[12], Melih Sener[9], Andrew Shreve[13], Jerilyn Timlin[14], Volker Urban[11]

[1]Washington University in St. Louis (lead institution); [2]University of California, Riverside; [3]The Pennsylvania State University; [4]University of Glasgow; [5]University of Pennsylvania; [6]University of Sheffield; [7]North Carolina State University; [8]Northwestern University; [9]University of Illinois at Urbana-Champaign; [10]Los Alamos National Laboratory; [11]Oak Ridge National Laboratory; [12]Princeton University; [13]University of New Mexico; [14]Sandia National Laboratories

The objective of PARC is to understand the basic scientific principles that underpin the efficient functioning of natural photosynthetic antenna systems as a basis for design of biohybrid and bioi nspired architectures for next-generation systems for solar-energy conversion.

1:52 PM

O-A-5: CENTER FOR BIO-INSPIRED ENERGY SCIENCE

Award Period: 2009 – 2014; 2014 – 2018

[EFRC – CBES] Samuel I. Stupp[1], Chad A. Mirkin[1], Monica Olvera de la Cruz[1], Mark A. Ratner[1], George C. Schatz[1], Igal G. Szleifer[1], Emily A. Weiss[1], George M. Whitesides[2], Anna C. Balazs[3], Kyle J.M. Bishop[4], Paul Chaikin[5], Sharon C. Glotzer[6]

Northwestern University[1] (lead Institution), Harvard University[2], University of Pittsburgh[3], Columbia University[4], New York University[5], University of Michigan[6]

The goal of the Center for Bio-inspired Energy Science (CBES) is to develop artificial materials and systems that take inspiration from biology to optimize the way we use energy and interconvert between different energy forms, for example converting chemical energy into mechanical energy the way muscles do in living organisms. Our team has innovated in the areas of self-assembly, the interface of biology and materials science, as well as in theory and simulation of materials.

2:05 PM

O-A-6: BIOLOGICAL ELECTRON TRANSFER AND CATALYSIS EFRC

Award Period: 2014 – 2018

[EFRC – BETCy] John W. Peters[1,2], Michael W.W. Adams[3], David N. Beratan[4], Brian Bothner[1], Eric S. Boyd[1], Ross P. Carlson[1], Caroline S. Harwood[5], Anne K. Jones[6], Paul W. King[7], Pin-Ching Maness[7], Anne-Frances Miller[8], Lance C. Seefeldt[9]

[1]Montana State University (lead institution); [2]Washington State University; [3]University of Georgia; [4]Duke University; [5]University of Washington; [6]Arizona State University; [7]National Renewable Energy Laboratory; [8]University of Kentucky; [9]Utah State University

The mission of the BETCy EFRC is to define the molecular mechanisms controlling electron flow in coupling electrochemical potential energy to chemical bond formation. BETCy EFRC uses advanced physical techniques to delineate the molecular and atomic determinants of factors that support highly efficient electron transfer reactions. The studies provide a framework of design principles to advance the development of next generation catalysts.

2:18 PM

O-A-7: CENTER FOR MOLECULAR ELECTROCATALYSIS

Award Period: 2009 – 2014; 2014 – 2018

[EFRC – CME] R. Morris Bullock[1], Shannon S. Stahl[2], James M. Mayer[3], Sharon Hammes-Schiffer[4], Aaron M. Appel[1], Simone Raugei[1], Michael M. Mock[1], Eric S. Wiedner[1], Molly O'Hagan[1]

[1]Pacific Northwest National Laboratory (lead institution); [2]University of Wisconsin-Madison; [3]Yale University; [4]University of Illinois at Urbana-Champaign

The mission of the CME is to make transformational changes in our ability to design molecular electrocatalysts for the interconversion of electricity and fuels, by understanding, predicting, and controlling proton and electron transfers in processes of critical importance to a secure energy future.

B. CARBON SEQUESTRATION / G. SEPARATION SCIENCE, *LINCOLN 2*

1:00 PM

O-B-1: CENTER FOR NANOSCALE CONTROLS ON GEOLOGIC GO_2

Award Period: 2009 – 2014; 2014 – 2018

[EFRC – NCGC] Donald J. DePaolo[1], Jonathan Ajo-Franklin[1], Lawrence Anovitz[2], Sally M. Benson[3], Ian C. Bourg[4], David R. Cole[5], Benjamin Gilbert[1], Young-Shin Jun[6], Timothy J. Kneafsey[1], Laura Pyark-Nolte[7], Gernot Rother[2], Peter J. Schuck[1], Andrew Stack[2], Carl I. Steefel[1], Hamdi Tchelepi[3], Tetsu K. Tokunaga[1], David Trebotich[1], Jiamin Wan[1]

[1]Lawrence Berkeley National Laboratory (lead institution); [2]Oak Ridge National Laboratory; [3]Stanford University; [4]Princeton University; [5]The Ohio State University; [6]Washington University St. Louis; [7]Purdue University

The NCGC's mission is to enhance the performance and predictability of subsurface storage systems by understanding the molecular and nanoscale origins of CO_2 trapping processes, and developing computational tools to translate to larger-scale systems.

1:13 PM

O-B-2: CENTER FOR FRONTIERS OF SUBSURFACE ENERGY SECURITY

Award Period: 2009 – 2014; 2014 – 2018

[EFRC – CEFRC] Larry Lake[1], Grant Heffelfinger[2], Anastasia Ilgen[2], Hilary C. Olson[1], Matt Balhoff[1], Bayani Cardenas[1], Thomas Dewers[2], David DiCarlo[1], Nicolas Espinoza[1], Nick Hayman[1], Marc Hesse[1], Susan Hovorka[1], Anastasia, Ilgen[2], Keith Johnston[1], Toti Larson[1], Mario Martinez[2], Tip Meckel[1], Pania Newell[2], Mary Wheeler[1], Changbing Yang[1], Hongkyu Yoon[2]

[1]The University of Texas at Austin (lead institution); [2]Sandia National Laboratories

The Center for Frontiers of Subsurface Energy Security (CFSES) is pursuing scientific understanding of multiscale, multiphysics processes to ensure safe and economically feasible storage of carbon dioxide and other byproducts of energy production without harming environments.

1:26 PM

O-B-3: CENTER FOR GEOLOGIC STORAGE OF CO_2

Award Period: 2014 – 2018

[EFRC – GSCO2] Scott M. Frailey[1], Steve Whittaker[1], Robert Bauer[1], Roland Okwen[1], Ed Mehnert[1], Ange-Therese Akono[2], James Best [2], Alexey Bezryadin[2], Jennifer Druhan[2], Ahmed Elbanna[2], Roman Makhnenko[2], John Popovics[2], Al Valocchi[2], Stephen Marshak[2], Charlie Werth[3], Pierre Cerasi[4], Michael Jordan [4], Sergey Stanchits[5], Volker Oye[6], Bettina Goertz-Allman[6], Muhammad Sahimi[7], Kristian Jessen[7], Theodore Tsotsis[7], Ken Christensen[8], Dustin Sweet[9], Calvin Barnes[9], Paul Sylvester[9], Melanie Barnes[9], Dustin Crandall[10], Angela Goodman[10], William Harbert[10], Paul Johnson[11], Pierre-Yves Le Bas[11], Nicolas Espinoza[12]

[1]Illinois State Geologic Survey, [2]University of Illinois at Urbana-Champaign (lead institution), [3]University of Texas-Austin, [4]SINTEF, [5]Schlumberger, [6]NORSAR, [7]University of Southern California, [8]University of Notre Dame, [9]Texas Tech University, [10]National Energy Technology Laboratory, [11]Los Alamos National Laboratory, [12]University of Texas-Austin

Mission: To generate new conceptual, mathematical, and numerical models applicable to geologic storage systems in specific and strategically identified research areas, based on uncertainty and limitations observed in field pilots and CO_2 injection demonstration projects, laboratory experiments, and the experience of researchers.

1:39 PM

SPONSORED UNDERGRADUATE AND GRADUATE STUDENT PLACEMENT OPPORTUNITIES AT DOE LABORATORIES

[Invited Talk] James Glownia

Director, Office of Workforce Development for Teachers and Scientists

DOE Office of Science

The Office of Science sponsors several workforce mission programs that place undergraduate or graduate students in paid appointments at DOE Laboratories. These programs, which enable undergraduate and graduate students to work directly on mission relevant research projects, will be described.

2:05 PM

O-B-6: THE CENTER FOR UNDERSTANDING AND CONTROL OF ACID GAS-INDUCED EVOLUTION OF MATERIALS FOR ENERGY

Award Period: 2014 – 2018

[EFRC – UNCAGE-ME] Jonas Baltrusaitis[3], Sheng Dai[2], David A. Dixon[6], Michael A. Filler[1], Phillip N. First[1], Sophia E. Hayes[5], Christopher W. Jones[1], Ryan P. Lively[1], Sankar Nair[1], Thomas M. Orlando[1], Gernot Rother[2], J.R. Schmidt[7], David S. Sholl[1], Susan B. Sinnott[4], Tjerk P. Straatsma[2], Bobby G. Sumpter[2], Sergey Vasenkov[8], Israel E. Wachs[3], Krista S. Walton[1], Zili Wu[2]

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

UNCAGE-ME seeks to develop a deep knowledge base in the characterization, prediction, and control of acid-gas interactions with a broad class of materials to accelerate materials discovery for large-scale energy applications.

2:18 PM

O-B-7: Center for Gas Separations Relevant to Clean Energy Technologies

Award Period: 2009 – 2014; 2014 – 2018

[EFRC – 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[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 (lead institution); [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

CGS
Center for Gas Separations
Relevant to Clean Energy Technologies

The mission of CGS is to develop the fundamental science necessary for tailor-making new materials and membranes that enable energy-efficient separation of gas mixtures, as required in the clean use of fossil fuels and in reducing emissions from industry. Emphasis is placed on separations that reduce CO_2 emissions from power plants and energy-intensive gas separations in industry and agriculture, as well as development of computational tools and *in situ* characterization methods to guide and support the synthetic efforts.

D. ENERGY STORAGE, *THURGOOD MARSHALL EAST*

1:00 PM

O-D-1: CENTER FOR ELECTROCHEMICAL ENERGY SCIENCE

Award Period: 2009 – 2014; 2014 – 2018

[EFRC – CEES] Paul Fenter[1], Jeff Elam[1], Tim Fister[1], Christopher Johnson[1], Michael Thackeray[1], Scott Barnett[2], Michael Bedzyk[2], Vinayak Dravid[2], Mark Hersam[2], Tobin Marks[2], Chris Wolverton[2], Andrew Gewirth[3], Ralph Nuzzo[3], Nancy Sottos[3], Scott White[3], Jeffrey Greeley[4]

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

The CEES mission is to understand and control the molecular-scale reactivity of electrified oxide interfaces and materials that limit the performance of lithium-ion battery systems.

1:13 PM

O-D-2: FLUID INTERFACE REACTIONS, STRUCTURES AND TRANSPORT

Award Period: 2009 – 2014; 2014 – 2018

[EFRC – FIRST] David J. Wesolowski[1], Nina Balke[1], Peter Cummings[2], Sheng Dai[1], Nancy Dudney[1], Paul Fenter[3], Yury Gogotsi[4], De-en Jiang[5], Paul Kent[1], Alexander Kolesnikov[1], Daniel Lutterman[1], Shannon Mahurin[1], Eugene Mamontov[1], Haoxiang Liu[2], David Mullins[1], Michael Naguib[1], Alexandra Navrostky[6], Matthew Neurock[7], Joel Rosenthal[8], Gernot Rother[1], Robert Sacci[1], Raymond Unocic[1], Adri Van Duin[9], Jianzhong Wu[5], Huiyuan Zhu[1]

[1]Oak Ridge National Laboratory (lead institution); [2]Vanderbilt University; [3]Argonne National Laboratory; [4]Drexel University; [5]University of California at Riverside; [6]University of California at Davis; [7]University of Minnesota; [8]University of Delaware; [9]Penn State University

The FIRST Center mission is to develop fundamental understanding and validated, predictive models of the unique nanoscale environment at fluid-solid interfaces that will enable transformative advances in electrical energy storage and electrocatalysis. Much of our work related to electrical energy storage focuses on capacitive and pseudocapacitive processes and systems that have the potential to deliver high power and long cycle life as well as high energy density.

1:26 PM

O-D-3: Joint Center for Energy Storage Research

Award Period: 2012 – 2017

[Hub – JCESR] George Crabtree[1,2], Venkat Srinivasan[1], Nenad Markovic[1], Robert Darling[3], Brian Ingram[1], Jeff Moore[4], Kevin Zavadil[5], Kristin Persson[6], Karl Mueller[7], Nitash Balsara[6], Fikile Brushett[8], Gerbrand Ceder[6], Linda Nazar[9], Yet-Ming Chiang[8]

[1]*Argonne National Laboratory (lead institution);* [2]*University of Illinois at Chicago;* [3]*United Technologies Research Center;* [4]*University of Illinois at Urbana-Champaign;* [5]*Sandia National Laboratories;* [6]*Lawrence Berkeley National Laboratory;* [7]*Pacific Northwest National Laboratory;* [8]*Massachusetts Institute for Technology;* [9]*University of Waterloo*

JCESR launched in 2012 with a vision to transform transportation and the electricity grid with high performance, low cost electrochemical energy storage. The JCESR mission has been to deliver battery platforms with five times the energy density and one-fifth the cost of 2012 Li-ion commercial batteries within five years.

1:39 PM

O-D-4: NorthEast Center for Chemical Energy Storage

Award Period: 2009 – 2014; 2014 – 2018

[EFRC – NECCES] M. Stanley Whittingham[1], Louis F.J. Piper[1], Guangwen Zhou[1], Natasha A. Chernova[1], Glenn Amatucci[2], Natalie Pereira[2], Frederic Cosandey[2], Philip E. Batson[2], Clare P. Grey[3], Gerbrand Ceder[4], Yet-Ming Chiang[5], Karena W. Chapman[6], Peter J. Chupas[6], Katsuyo Thornton[7], Anton Van der Ven[8], Ying Shirley Meng[9], Shyue Ping Ong[9] , Jordi Cabana[10]

[1]*Binghamton University (lead institution);* [2]*Rutgers The State University of New Jersey;* [3]*University of Cambridge;* [4]*University of California, Berkeley;* [5]*Massachusetts Institute of Technology;* [6]*Argonne National Laboratory;* [7]*University of Michigan;* [8]*University of California, Santa Barbara;* [9]*University of California, San Diego;* [10] *University of Illinois at Chicago*

The mission of the Center is to develop an understanding of how key electrode reactions occur, and how they can be controlled to improve electrochemical performance, from the atomistic level to the macroscopic level through the life-time of the operating battery. Three thrust areas have been established in order to achieve the Center's goals: intercalation materials, transport in mesoscale systems and one cross-cutting on characterization.

1:52 PM

O-D-5: Center for Mesoscale Transport Properties

Award Period: 2014 – 2018

[EFRC – m2M] Esther Takeuchi[1], Nitash Balsara[2], Joseph DeSimone[3], Nancy Dudney[4], Maria Fernandez-Serra[1], Hong Gan[5], Robert Hull[6], Mark Hybertsen[5], Yan Li[7], Ping Liu[5], Amy Marschilok[1], Elsa Reichmanis[8], Eric Stach[5], Kenneth Takeuchi[1], Feng Wang[5], Jun Wang[5], Alan West[9], Stanislaus Wong[1], Guihua Yu[10], Yimei Zhu[5].

[1]Stony Brook University (lead institution), [2]University of California at Berkeley, [3]University of North Carolina at Chapel Hill, [4]Oak Ridge National Laboratory, [5]Brookhaven National Laboratory, [6]Rensselaer Polytechnic Institute, [7]American Physical Society, [8]Georgia Institute of Technology, [9]Columbia University, [10]University of Texas at Austin.

The mission of the Center for Mesoscale Transport Properties is to understand and to ultimately control transport properties in complex battery systems with respect to multiple length scales, from molecular to Mesoscale (m2M); to minimize heat and maximize work of electrical energy storage devices.

2:05 PM

O-D-6: Nanostructures for Electrical Energy Storage

Award Period: 2009 – 2014; 2014 – 2018

[EFRC – NEES] Gary Rubloff[1], Sang Bok Lee[1], Phil Collins[2], John Cumings[1], Bruce Dunn[3], Bryan Eichhorn[1], Farid El Gabaly[4], Sean Hearne[4], Liangbing Hu[1], Katherine Jungjohann[4], Kevin Leung[4], Charles Martin[5], Reginald Penner[2], Yue Qi[6], Mark Reed[7], Janice Reutt-Robey[1], Zuzanna Siwy[2], A. Alec Talin[4], Chunsheng Wang[1], YuHuang Wang[1], Henry White[8]

[1]University of Maryland (lead institution); [2]University of California, Irvine; [3]University of California, Los Angeles; [4]Sandia National Laboratories; [5]University of Florida; [6]Michigan State University; [7]Yale University; [8]University of Utah

Mission: To reveal scientific insights and design principles that enable a next-generation electrical energy storage technology based on dense mesoscale architectures of multifunctional nanostructures.

E. NUCLEAR ENERGY AND WASTE, *LINCOLN 5*

1:00 PM

O-E-1: ENERGY DISSIPATION TO DEFECT EVOLUTION

Award Period: 2014 – 2018

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

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

> EDDE's Mission is to develop a fundamental understanding of energy dissipation and defect evolution mechanisms in tunable concentrated solid solution alloys (CSAs), and ultimately to control defect evolution in a radiation environment. Our goal is to reveal energy dissipation mechanisms through electrons, phonons, and magnons, and utilize this knowledge to understand the process of radiation damage formation and evolution in its early stages. We aim to design materials that can intrinsically recover from the damaged state.

1:13 PM

O-E-2: CENTER FOR PERFORMANCE AND DESIGN OF NUCLEAR WASTE FORMS AND CONTAINERS

Award Period: 2016 – 2020

[EFRC – WastePD] Gerald S. Frankel,[1] Jincheng Du,[2] Stephane Gin,[3] Seong Kim,[4] Jie Lian,[5] Jenifer Locke,[1] Gregory B. Olson,[6] Joseph V. Ryan,[7] John R. Scully,[8] Chris 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) seeks 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, in particular, improved resistance to degradation over long periods of exposure to aqueous environments.

1:26 PM

O-E-3: Center for Hierarchical Wasteform Materials

Award Period: 2016 – 2020

[EFRC – CHWM] Hans-Conrad zur Loye[1], Theodore M. Besmann[1], Natalia Shustova[1], Hui Wang[1], Jake Amoroso[2], Scott Misture[4], Simon R. Phillpot[7], Charles Henager, Jr.[3], Simerjeet Gill[6], Lynne Ecker[6], Agnes Grandjean[8], Kyle Brinkman[5], Shenyang Hu[3], David DiPrete[2], Charles Crawford[2]

[1]University of South Carolina (lead institution); [2]Savannah River National Laboratory; [3]Pacific Northwest National Laboratory; [4]Alfred University; [5]Clemson University; [6]Brookhaven National Laboratory; [7]University of Florida; [8]Commissariat à l'Energie Atomique

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.

1:39 PM

O-E-4: Center for Computational Design of Functional Strongly Correlated Materials and Theoretical Spectroscopy

Award Period: 2015 – 2019

[CMS – CDMFTS] Gabriel Kotliar[1,3], Kristjan Haule[3], Yongxin Yao[2], Sangkook Choi[1], Hubertus van Dam[1], Nick D'imperio[1], Robert Harrison[1], Cristian Batista[5], Gia-Wei Chern[4], Alexei Tsvelik[1], Emil Bozin[1], Simon Billinge[1], Andrey Kutepov[1], Igor Zaliznyak[1], Peter Johnson[1], Mark Dean[1], Robert Konik[1], Christopher Homes[1], Cedomir Petrovic[1], Martha Greenblatt[3]

[1]Brookhaven National Lab (lead Institution); [2]Ames Lab; [3]Rutgers University; [4]University of Virginia; [5]University of Tennessee

The goal of CDMFTS is to develop, disseminate, and validate methodologies (theory, algorithms and codes) to accurately describe the electronic properties in complex strongly correlated materials. These tools will accelerate scientific progress in strongly correlated materials research by enabling theoretical spectroscopy and theoretically guided material design. The validation effort will focus on materials holding a promise of revolutionary functionalities for energy applications, ranging from energy transmission to superior thermoelectric performance.

1:52 PM

O-E-5: Interfacial Dynamics in Radioactive Environments and Materials

Award Period: 2016 – 2020

[EFRC – IDREAM] Sue B. Clark[1], Aurora E. Clark[2], Nigel D. Browning[1], Jaehun Chun[1], James J. De Yoreo[1], Andrew R. Felmy[2], Sebastien Kerisit[1], Gregory A. Kimmel[1], Jay A. La Verne[6], Xiaosong Li[3], Thomas M. Orlando[5], Katharine Page[4], Carolyn I. Pearce[1], Kevin M. Rosso[1], Gregory K. Schenter[1], Andrew G. Stack[4], David J. Wesolowski[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.

2:05 PM

O-E-6: MATERIALS SCIENCE OF ACTINIDES

Award Period: 2009 – 2014; 2014 – 2018

[EFRC – MSA] Peter C. Burns[1], Rodney C. Ewing[2], Alexandra Navrotsky[3], Mark Asta[3], Christopher L. Cahill[4], William H. Casey[3], Jeremy Fein[1], Laura Gagliardi[5], Amy E. Hixon[1], Maik Lang[6], Tianbo Liu[7], Edward J. Maginn[1], Wendy Mao[2], Albert Migliori[8], May Nyman[9]

[1]University of Notre Dame (lead institution); [2]Stanford University; [3]University of California-Davis; [4]George Washington University; [5]University of Minnesota; [6]University of Tennessee; [7]University of Akron; [8]Los Alamos National Laboratory; [9]Oregon State University

The mission of MSA is to conduct collaborative, multidisciplinary, novel and transformative research on actinide materials emphasizing actinide ceramic, metallic, hybrid, and nanoscale materials, effective integration of experimental and computational approaches, and solving research questions that are critical to the energy future of the nation. Workforce development is a fundamental and inherent goal of this university-based center.

2:18 PM

O-E-7: THE CENTER FOR ACTINIDE SCIENCE AND TECHNOLOGY

Award Period: 2016 – 2020

[EFRC – CAST] Thomas Albrecht-Schmitt[1,2], Susan Latturner[1,2], Kenneth Knappenberger[1,2]. Kenneth Hanson[1,2], Eugene DePrince[1,2], Stan Tozer[1,2], David Hobart[1,2], Ines Triay[3], Christopher Dares[3], Konstantinos Kavallieratos[3], David Graf[2], Ryan Baumbach[2], John Gibson[4], Susanne Bart[5], Stosh Kozimor[6], Andrew Gaunt[6], Enrique Batista[6], Ping Yang[6], Eric Schelter[7]

[1]Florida State University (lead institution); [2]National High Magnetic Field Laboratory; [3]Florida International University; [4]Lawerence Berkeley National Laboratory; [5]Purdue University; [6]Los Alamos National Laboratory; [7]University of Pennsylvania;

The CAST mission is to advance understanding of nuclear materials through use-inspired, basic research that leads to improvements in nuclear energy utilization, environmental remediation, and training of the next generation of nuclear scientists. CAST unites materials chemists, condensed-matter physicists, and theoreticians into a cohesive research unit with the common goal of solving long-standing nuclear waste legacy issues.

F. QUANTUM MATERIALS, *LINCOLN 6*

1:00 PM

O-F-1: SOLID-STATE SOLAR THERMAL ENERGY CONVERSION CENTER

Award Period: 2009 – 2014; 2014 – 2018

[EFRC – S^3TEC] David Broido[1], Gang Chen[2], Olivier Delaire[3,4], Mildred Dresselhaus[2], Liang Fu[2], Nicolas Hadjiconstantinou[2], Alexie Kolpak[2], Keith Nelson[2], Zhifeng Ren[5], Caroline Ross[2], Yang Shao-Horn[2], David J. Singh[6], G. Jeffrey Snyder[7], Marin Soljacic[2], Evelyn Wang[2], Yimei Zhu[8]

[1]Boston College; [2]Massachusetts Institute of Technology (lead Institution); [3]Oak Ridge National Laboratory; [4]Duke University; [5]University of Houston; [6]University of Missouri; [7]Northwestern University; [8]Brookhaven National Laboratory

Mission: To advance fundamental science and to develop materials for harnessing heat from the sun and terrestrial sources and converting this heat into electricity via solid-state thermoelectric, thermophotovoltaic, and thermogalvanic technologies.

1:13 PM

O-F-2: CENTER FOR PREDICTIVE SIMULATION OF FUNCTIONAL MATERIALS

Award Period: 2016 – 2020

[CMS – CPSFM] Anouar Benali[1], Anand Bhattacharya[1], Panchapakesan Ganesh[2], Olle Heinonen[1], Paul Kent[2], Jaron Krogel[2], Ho-Nyung. Lee[2], Lubos Mitas[3], Miguel Morales[4], Eric Neuscamman[5], Luke Shulenburger[6]

[1]Argonne National Laboratory; [2]Oak Ridge National Laboratory (lead institution); [3]North Carolina State University; [4]Lawrence Livermore National Laboratory; [5]University of California Berkeley; [6]Sandia National Laboratories

The mission of the Center for Predictive Simulation of Functional Materials is the development, application, validation, and dissemination of parameter-free methods and open source codes to predict and explain the properties of functional materials for energy applications.

1:26 PM

O-F-3: ENERGY FRONTIER RESEARCH IN EXTREME ENVIRONMENTS

Award Period: 2009 – 2014; 2014 – 2018

[EFRC – EFree] Russell Hemley[1], Timothy Strobel[2], Stephen Gramsch[2], Nasim Alem[3], Neil Ashcroft[4], John Badding[3], Vincent Crespi[3], Brent Fultz[5], Roald Hoffmann[4], Lakshmi Krishna[6], Kai Landskron[7], Tianshu Li[1], P. Craig Taylor[6], Maria Baldini[2], Reinhard Boehler[2,8], Konstantin Lokshin[9], Maddury Somayazulu[2]

[1]George Washington University, [2]Carnegie Institution of Washington (lead institution), [3]Pennsylvania State University, [4]Cornell University, [5]California Institute of Technology, [6]Colorado School of Mines, [7]Lehigh University, [8]Spallation Neutron Source, Oak Ridge National Laboratory, [9]University of Tennessee

The mission of EFree is to accelerate the discovery and synthesis of new energy materials using extreme conditions. We study materials under extreme conditions to deepen the understanding of material behavior, enabling new materials to be discovered, and ultimately produced by design, for use at ambient conditions.

1:39 PM

O-F-4: CENTER FOR EMMERGENT SUPERCONDUCTIVITY

Award Period: 2009 – 2014; 2014 – 2018

[EFRC – CES] Peter D. Johnson[1], J.C. Seamus Davis[1], John Tranquada[1], James Eckstein[2], Wai-Kwong Wok[3], Mike Norman[3], Laura H. Greene[4].

[1]*Brookhaven National Laboratory (lead institution),* [2]*University of Illinois, Urbana Champaign,* [3]*Argonne National Laboratory,* [4]*National High Magnetic Field Laboratory*

The central mission of the CES is the development of an understanding of High Tc Superconductivity that will enable the prediction and perfection of new High Tc materials for use in a range of energy technologies including applications in generation, storage and transmission.

1:52 PM

O-F-5: SPINS AND HEAT IN NANOSCALE ELECTRONIC SYSTEMS

Award Period: 2014 – 2018

[EFRC – SHINES] Alexander Balandin[1], Chia-Ling Chien[2], Tingyong Chen[3], Nathaniel Gabor (seed)[1], Javier Garay[4], Alexander Khitun[1], Ilya Krivorotov[5], Roger Lake[1], Chun-Ning (Jeanie) Lau[1], Xiaoqin (Elaine) Li[6], Jianlin Liu (seed)[1], Allan MacDonald[6], Jing Shi[1], Kang L. Wang[7], Mingzhong Wu[8], Ruqian Wu[5]

[1]*University of California, Riverside (lead institution);* [2]*Johns Hopkins University;* [3]*Arizona State University;* [4]*University of California, San Diego;* [5]*University of California, Irvine;* [6]*University of Texas at Austin;* [7]*University of California, Los Angeles;* [8]*Colorado State University.*

The SHINES EFRC explores the interplay of spins, charge, and heat to control the transport of spins and energy to achieve significantly higher energy efficiencies in nanoscale electronic devices.

2:05 PM

DOE LIGHT SOURCES: CAPABILITIES, OPPORTUNITIES, AND ACCESS

[Invited Talk] Roger Falcone
Director, Advanced Light Source
Lawrence Berkeley National Lab

Basic Energy Sciences in the Department of Energy supports five world-leading x-ray light source facilities in the US. These facilities are open to all scientists through a proposal and review system, as well for proprietary work in a mode typically utilized by industry. These x-ray facilities offer unique instrumentation, a highly skilled and collaborative workforce of scientists and engineers, and data analysis for complex research problems, beyond the capabilities found outside of the national laboratories. The spectrum of light available stretches from the infrared, to the vacuum ultraviolet, to soft x-rays, and to hard x-rays. Techniques include spectroscopy, imaging, scattering, and dynamics, and the science typically involves determining the electronic, chemical, and physical structure of materials, as well as matter in gas and liquid phases. An example of research is the determination of the electronic band structure of quantum materials through photoemission and inelastic x-ray scattering, at the nanoscale.

H. SOLAR ENERGY CONVERSION, *THURGOOD MARSHALL SOUTH*

1:00 PM
O-H-1: JOINT CENTER FOR ARTIFICIAL PHOTOSYNTHESIS

Award Period: 2010 – 2015; 2015 – 2020

[Hub – JCAP] Theodor Agapie[1], Joel. W. Ager[2], Harry A. Atwater[1], Alexis T. Bell[2], Marco Bernardi[1], Bruce Brunschwig[1], Walter Drisdell[2], William A. Goddard[1], John M. Gregoire[1], Robert. H. Grubbs[1], Joel A. Haber[1], Martin P. Head-Gordon[2], John C. Hemminger[4], Frances A. Houle[2], Thomas Jaramillo[3], Clifford P. Kubiak[5], Hans J. Lewerenz[1], Nathan S. Lewis[1], Daniel J. Miller[2], Thomas F. Miller[1], Jeffrey B. Neaton[2], Jens K. Norskov[3], Kristin A. Persson[2], Jonas C. Peters[1], Ian D. Sharp[2], Manuel P. Soriaga[1], Francesca M. Toma[2], Dean Toste[2], Lin-Wang Wang[2], Adam Z. Weber[2], Chengxiang Xiang[1], Junko Yano[2]

[1]California Institute of Technology (lead institution); [2]Lawrence Berkeley National Laboratory; [3]SLAC National Accelerator Laboratory; [4]University of California Irvine; [5]University of California San Diego

JCAP's mission is to create the scientific foundation for a scalable technology that converts carbon dioxide, water, and sunlight into renewable transportation fuels.

1:13 PM
O-H-2: CENTER FOR SOLAR FUELS

Award Period: 2009 – 2014; 2014 – 2018

[EFRC – UNC] Thomas J. Meyer[1], John M. Papanikolas[1], Gerald J. Meyer[1], Joanna M. Atkin[1], Maurice S. Brookhart[1], James F. Cahoon[1], Jillian L. Dempsey[1], Yosuke Kanai[1], Rene Lopez[1], Alexander J.M. Miller[1], Andrew M. Moran[1], James T. Muckerman[2], John R. Reynolds[3], Kirk S. Schanze[4], Cynthia K. Schauer[1], Joseph L. Templeton[1], M. Kyle Brennaman[1]

[1]University of North Carolina at Chapel Hill (lead institution); [2]Brookhaven National Laboratory; [3]Georgia Institute of Technology; [4]University of Texas at San Antonio

The mission of the UNC EFRC: Center for Solar Fuels is to conduct research on dye sensitized photoelectrosynthesis cells (DSPECs) for water splitting, and tandem cells for the reduction of carbon dioxide to carbon-based solar fuels.

1:26 PM

O-H-3: Argonne-Northwestern Solar Energy research Center

Award Period: 2009 – 2014; 2014 – 2018

[EFRC – ANSER] Michael R. Wasielewski[1], Joseph T. Hupp[1], David M. Tiede[2], Victor S. Batista[3], Gary W. Brudvig[3], Robert H. Crabtree[3], Mercouri G. Kanatzidis[1], Alex B. F. Martinson[2], James M. Mayer[3], Samuel I. Stupp[1], Sharon Hammes-Schiffer[5], Tobin J. Marks[1], Lin X. Chen[1,2], Michael Bedzyk[1], Robert P. H. Chang[1], Mark C. Hersam[1], Michael J. Pellin[2], Mark A. Ratner[1], George C. Schatz[1], Emily A. Weiss[1], Luping Yu[4]

[1]Northwestern University (lead institution); [2]Argonne National Laboratory; [3]Yale University; [4]University of Chicago; [5]University of Illinois Urbana-Champaign

ANSER Center research seeks to revolutionize our understanding of the molecules, materials, and physical phenomena necessary to create dramatically more efficient technologies for solar fuels and electricity production. At the same time, the ANSER Center works to create and mentor a technically excellent workforce engaged in team science that is capable of solving energy-related problems far into the future.

1:39 PM

O-H-4: Center for Advanced Solar Photophysics

Award Period: 2009 – 2014; 2014 – 2018

[EFRC – CASP] Victor I. Klimov[1], Jeffrey M. Pietryga[1], Istvan Robel[1], Kirill A. Velizhanin[1], Matthew C. Beard[2], Justin C. Johnson[2], Joseph M. Luther[2], Arthur J. Nozik[2], Matt Law[3], Uwe R. Kortshagen[4], Alexander L. Efros[5], Andrew Shabaev[5], Cherie R. Kagan[6], Giulia Galli[7]

[1]Los Alamos National Laboratory (lead institution); [2]National Renewable Energy Laboratory; [3]University of California, Irvine; [4]University of Minnesota; [5]George Mason University; [6]University of Pennsylvania; [7]University of Chicago

Mission: To exploit fundamental interactions between nanomaterials and light with the goal of producing disruptive advances in the efficiency of solar energy conversion.

1:52 PM

O-H-5: Center for Computational Study of Excited-State Phenomena in Energy Materials

Award Period: 2016 – 2020

[CMS – C2SEPEM] Steven G. Louie[1, 2], James R. Chelikowsky[4], Jack Deslippe[1, 2], Jeffrey B. Neaton[1,2], Daniel Neuhauser[3], Eran Rabani[1, 2], Feng Wang[1, 2], Lin-Wang Wang[1], Chao Yang[1]

[1]Lawrence Berkeley National Laboratory (lead institution); [2]University of California, Berkeley; [3]University of California, Los Angeles; [4]University of Texas at Austin

The mission of the Center for Computational Study of Excited-State Phenomena in Energy Materials (C2SEPEM) is to develop and implement new theories, methods, algorithms, and computer codes to explain and predict excited-state phenomena in energy materials.

2:05 PM

O-H-6: CENTER FOR EXCITONICS

Award Period: 2009 – 2014; 2014 – 2018

[EFRC – CE] Alan Aspru-Guzik[2], Marc Baldo[4], Mark Bathe[4], Moungi Bawendi[4], Charles Black[1], Vladmir Bulovic[4], Eric Dauler[4], Mircea Dinca[4], Dirk Englund[4], Pablo Jarillo-Herrero[4], Jing Kong[4], Leonid Levitov[4], Ju Li[4], Keith Nelson[4], Gabriela Schlau-Cohen[4], Eric Stach[1], William Tisdale[4], T. Van Voorhis[4], A. Willard[4].

[1]Brookhaven National Laboratory; [2]Harvard University; [3]Lincoln Laboratory; [4]Massachusetts Institute of Technology (lead institution)

Excitons are the crucial intermediate for energy transduction in materials that are more suitable for large scale production – low cost, disordered semiconductors. Thus, we seek to supersede traditional electronics with lower cost devices that use excitons to mediate the flow of energy.

2:18 PM

O-H-7: LIGHT-MATERIAL INTERACTIONS IN ENERGY CONVERSION

Award Period: 2009 – 2014; 2014 – 2018

[EFRC – LMI] Ralph G. Nuzzo[1,2], A. Paul Alivisatos[3], Harry A. Atwater[1], Paul V. Braun[2], Mark L. Brongersma[4], Jennifer A. Dionne[4], Shanhui Fan[4], Andrei Faraon[1], Jennifer A. Lewis[5], Nathan S. Lewis[1], Austin J. Minnich[1], John A. Rogers[2], Eli Yablonovitch[3], Xiang Zhang[3]

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

The scientific mission of the Light-Material Interactions in Energy Conversion EFRC (LMI-EFRC) is to tailor the morphology, complex dielectric structure, and electronic properties of matter so as to sculpt the flow of sunlight and heat, enabling light conversion to electrical energy with unprecedented efficiency.

J. Materials and Chemistry by Design, *Thurgood Marshall West*

1:00 PM

O-J-1: Center for the Computational Design of Functional Layered Materials

Award Period: 2014 – 2018

[EFRC – CCDM] J.P. Perdew[1], A. Bansil[2], E. Borguet[1], L. Cao[3], M. Haataja[4], M. Iavarone[1], G. Karapetrov[5], M.L. Klein[1], A. Ruzsinsky[1], G.E. Scuseria[6], D. Srolovitz[7], D.R. Strongin[1], J. Sun[8], X. Wu[1], X. Xi[1], Q. Yan[1], W. Yang[9], M.J. Zdilla[1] and Y. Zhu[11]

[1]*Temple University (lead institution),* [2]*Northeastern University,* [3]*North Carolina State University,* [4]*Princeton University,* [5]*Drexel University,* [6]*Rice University,* [7]*UPenn,* [8]*University of Texas-El Paso,* [9]*Duke University,* [10]*Brookhaven National Laboratory*

The Center develops, applies, and validates theoretical methods to calculate the electronic structure of materials. While these methods can be useful for the design of many new materials, we focus on the layered and two-dimensional materials that have potential for clean-energy technologies. We aim to predict how the properties of these materials are affected by composition, structure, interfacial support, defects, and strain, and to assist the design of such materials for practical applications including catalysis of water-splitting.

1:13 PM

O-J-2: Center for Next Generation of Materials by Design

Award Period: 2014 – 2018

[EFRC – CNGMD] William Tumas[1], Gerbrand Ceder[2], David Ginley[1], John Perkins[1], Stephan Lany[1], Andriy Zakutayev[1], Kristin Persson[2], Alexie Kolpak[3], Tonio Buonassisi[3], Roy Gordon[4], Daniel Nocera[4], Brian Gorman[5], Vladan Stevanovic[5], Janet Tate[6], Michael Toney[7]

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

The mission of the Center for Next Generation of Materials by Design (CNGMD) is to dramatically transform the discovery of functional energy materials using high-throughput multiple-property search, incorporation of metastable materials into predictive design, and the development of theory to guide materials synthesis.

1:26 PM

O-J-3: MATERIALS GENOME INNOVATION FOR COMPUTATIONAL SOFTWARE

Award Period: 2015 – 2019

[CMS – MAGICS] Priya Vashishta[1], Malancha Gupta[1], Rajiv K. Kalia[1], Aiichiro Nakano[1], Oleg Prezhdo[1], Pulickel M. Ajayan[2], Uwe Bergmann[3], David Fritz[3], William A. Goddard, III[4], Kristin A. Persson[5], David J. Singh[6]

[1]*University of Southern California (lead institution)*; [2]*Rice University*; [3]*SLAC National Accelerator Laboratory, Stanford University*; [4]*California Institute of Technology*; [5]*Lawrence Berkeley National Laboratory, University of California Berkeley*; [6] *University of Missouri*

MAGICS center develops first-principles based computational synthesis software for layered materials genome (LMG). MAGICS software aids the synthesis of stacked LMs by chemical vapor deposition, liquid phase exfoliation and intercalation. The software also provides function-property-structure relationships in functionalized LMs. The software runs on all platforms from desktops to petascale and evolving exascale architectures.

1:39 PM

O-J-4: INORGANIC CATALYSIS DESIGN CENTER

Award Period: 2014 – 2018

[EFRC – ICDC] Laura Gagliardi[1], Joseph T. Hupp[2], Aditya Bhan[1], E.M. Calverley[3], Donald M. Camaioni[4], Karena W. Chapman[5], Christopher J. Cramer[1], Omar K. Farha[2], Bruce C. Gates[6], Rachel B. Getman[7], Johannes A. Lercher[4], Connie C. Lu[1], Alex B. F. Martinson[5], William Morris[8], Justin M. Notestein[2], R. Lee Penn[1], Randall Q. Snurr[2], Andreas Stein[1], Ian Tonks[1], Donald G. Truhlar[1]

[1]University of Minnesota (lead institution); [2]Northwestern University; [3]The Dow Chemical Company; [4]Pacific Northwest National Laboratory; [5]Argonne National Laboratory; [6]University of California Davis, Davis; [7]Clemson University; [8]NuMat Technologies

The mission of the Inorganometallic Catalyst Design Center (ICDC) is to guide the discovery of superior catalysts by integrating computational modeling with experiments in well-defined systems that are amenable to high-throughput search and discovery methods.

1:52 PM

O-J-5: INTEGRATED MESOSCALE ARCHITECTURES FOR SUSTAINABLE CATALYSIS

Award Period: 2014 – 2018

[EFRC – IMASC] Cynthia M Friend,[1] Efthimios Kaxiras,[1] Robert J Madix,[1] Maria Flytzani-Stephanopoulos,[2] Miquel Salmeron,[3] E. Charlie H Sykes,[2] Juergen Biener,[4] Monika Biener,[4] David Bell,[1] Eric Stach,[5] Joanna Aizenberg,[1] Michael Aizenberg,[1] Michail Stamatakis,[6] Philippe Sautet,[7] Evgeniy Redekop,[8] Michelle L. Personick[9]

[1]Harvard University (lead institution); [2]Tufts University; [3]Lawrence Berkeley National Laboratory; [4]Lawrence Livermore National Laboratory; [5]Brookhaven National Laboratory; [6]University College London; [7]UC Los Angeles; [8]University of Oslo; [9]Wesleyan University

The mission of IMASC is to drive and conduct transformative research in mesoscale science for sustainable catalysis, with full integration of multi-scale experimental, theoretical and computational approaches.

2:05 PM

O-J-6: MIDWEST INTEGRATED CENTER FOR COMPUTATIONAL MATERIALS

Award Period: 2015 – 2019

[CMS – MICCoM] Giulia Galli[1,2], Juan de Pablo[1,2], Francois Gygi[3], Marco Govoni[1], Jonathan Whitmer[4], John Mitchell[1], Paul Fenter[1], Mercouri Kanatzidis[1,5], Monica Olvera de la Cruz[5], Sharon Glotzer[6], Olle Heinonen[1], Dmitri Talapin[2], Paul Nealey[2], Nicola Ferrier[1]

[1]Argonne National Laboratory; [2]University of Chicago; [3]University of California Davis; [4]University of Notre Dame; [5]Northwestern University; [6]University of Michigan

MICCoM (http://miccom-center.org/) develops predictive computational tools to design synthetic materials from specific building blocks while incorporating consideration of efficient assembly routes into the design process. The Center's mission is to develop and disseminate interoperable open source software, data and validation procedures, enabling the community to simulate and predict properties of functional materials for energy conversion processes. Emphasis is on interfaces, the transport across them, and the manipulation of matter under conditions far from equilibrium.

TECHNICAL TALK ABSTRACTS

A. BIOSCIENCE

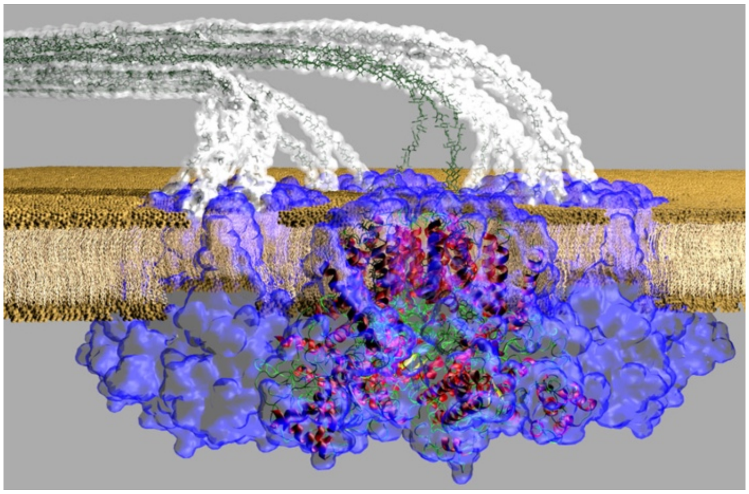
SESSION II: TUESDAY, JULY 25, 2017; 8:30 – 10:10 AM; LINCOLN 6

8:30 AM – Team Science Finalist

A-II-1: THE NANOMACHINE THAT SYNTHESIZES CELLULOSE IN PLANTS

[EFRC – CLSF] Abhishek Singh[1], Yaraslova Yingling[1], Jason N. Burris[1], Jonathan K. Davis[1], Alison W. Roberts[2], Candace H. Haigler[1], Xiaoran Xin[3], Ying Gu[3], Hui Yang[3], James D. Kubicki[4], Jochen Zimmer[5]
[1]North Carolina State University, [2]University of Rhode Island, [3]Pennsylvania State University, [4]University of Texas at El Paso, [5]University of Virginia

Using sugar derived from photosynthesis, plants annually produce gigatons of cellulose, a global sink for atmospheric carbon and stored solar energy. Despite its importance as a structural material and a source of renewable energy, many aspects of cellulose synthesis are unresolved. Eighteen β1,4-glucan chains are polymerized in parallel by a remarkable multimeric nanomachine, the cellulose synthase complex (CSC), which is embedded in the cell's plasma membrane, harvests UDP-glucose from the cytoplasm and spins oriented microfibrils outside the cell to construct a complex cell wall. The CSC contains an estimated 18 cellulose synthase proteins (CESAs) in a rosette-like configuration and other protein partners help to regulate CSC activity. Here we report on complementary computational and experimental studies of CSC structure and regulation. Biochemical methods demonstrate the membrane topology of CESA and guide atomistic modeling of CESA with seven transmembrane helices and a predicted substrate-binding motif in the cytoplasm. QM/MM modeling of the catalytic domain gives insights into transition states and activation free energy for glucan polymerization. Using laser scanning confocal microscopy we demonstrate the association of cellulose synthase interactive 1 protein (CSI1) with the CSC. We constructed an atomistic model of CSI1 structure and developed an interaction model in which CSI1 links CESA with cytoskeletal microtubules, providing a means of orienting the direction of cellulose microfibril deposition to the cell wall. These results form the basis for many ongoing experiments in our center, with the goal of manipulating plant cellulose synthesis in beneficial ways.



Right: Molecular model of the CSC embedded in the plasma membrane (brown) and extruding glucan chains (white) to the outside surface of the cell, forming an ordered microfibril.

Contributions: Experiments were designed, implemented, or interpreted as follows: atomistic modeling: A.S., C.H.H, and Y.Y.; biochemistry: J.N.B., J.K.D., A.W.R. and C.H.H.; microscopy: X.X. and Y.G.; and quantum modeling: H.Y., J.D.K. and J.Z.

8:50 AM

A-II-2: REDESIGNING THE STRUCTURE OF BIOMASS FOR CARBON- AND ENERGY-EFFICIENT CATALYTIC AND PYROLYTIC TRANSFORMATIONS

[EFRC – C3Bio] NICHOLAS C. CARPITA[1], Matheus Benatti[1], Rucha Karve[1], Chien-Yuan Lin[2], Hao Luo[3], Anna T. Olek[1], Phillip Rushton[1], Hui Wei[2], Haibing Yang[1], Ximing Zhang[1], Mahdi M. Abu-Omar[3], Clint C. S. Chapple[1], Peter Ciesielski[2], Mike F. Crowley[2], Bryon S. Donohoe[2], Michael E. Himmel[2], Lee Makowski[4], Maureen C. McCann[1], Richard, Meilan[1], Nathan S. Mosier[1], and Melvin P. Tucker[2]

[1]Purdue University; [2]National Renewable Energy Lab, [3]University of California Santa Barbara; [4]Northeastern University

Our goal is to gain genetic control of molecular to mesoscale cell-wall architecture in plants optimized for specific catalytic transformations. For example, we have generated transgenic poplar lines expressing iron-binding peptides/proteins targeted to cell-wall components to deliver iron catalysts directly to cellulose substrates for enhanced deconstruction. However, the complexity of wall architecture demands new fundamental understandings of cellulose and lignin structure and biosynthesis to inform our genetic strategies. Cellulose microfibrils bundle into largely anhydrous domains, constituting a more significant barrier to catalytic disassembly than previously recognized. Cellulose is dissolved by trifluoroacetic acid (TFA) into amorphous forms with enhanced rates of catalytic conversion into biofuel intermediates. In fundamental studies to build new cellulose microfibrils with intrinsic catalytic susceptibilities, we expressed two recombinant plant-unique domains of cellulose synthase to determine their roles in recruitment of the catalytic units into multimeric cellulose synthase complexes and in regulation of catalysis. As lignin composition greatly impacts cellulose swelling and dissolution in TFA, we explored the potential of enhanced catalytic susceptibility through generation of tailored lignins with wide S- and G-monolignol variation, novel monolignols, and altered aldehyde composition. We have also generated and characterized poplar mutants using CRISPR/Cas9 gene editing technology for knockout of genes of monolignol synthesis and xylan substitution, and expression of pectolytic enzymes. We have used these various transgenic lines to identify the molecular determinants of cell-cell adhesion in poplar, providing a knowledge base for tailoring biomass with reduced energy inputs for deconstruction.

9:10 AM

A-II-3: CELLULOSE STRUCTURE, ORGANIZATION AND INTERACTIONS WITH MATRIX POLYSACCHARIDES AND PROTEINS

[EFRC – CLSF] Mei Hong[1], Yun Zhen Zheng[2], Tian Zhang[2], Tuo Wang[1], Pyae Phyo[1], Liza Wilson[2], Yong Bum Park[2], Hui Yang[2], James D. Kubicki[3] and Daniel J. Cosgrove[1]

[1]Massachusetts Institute of Technology; [2]The Pennsylvania State University; [3]University of Texas at El Paso

We are developing new insights into plant cell wall structure, mechanics and other properties using solid-state NMR, atomic force microscopy (AFM), scanning electron microscopy (SEM), nano-gold affinity tags, selective enzymatic treatments, genetic mutants, and computational approaches. In ^{13}C-enriched primary cell walls, high resolution SSNMR spectra reveal cellulose polymorphism in unprecedented detail, identifying cellulose forms with ^{13}C chemical shifts significantly different from those of Iα and Iβ allomorphs. AFM experiments show that cellulose microfibril movements differ for cell wall extension caused by applied force versus extension induced by enzymatic loosening. Moreover, nanomechanical mapping shows that both cellulose microfibrils and matrix polymers bear tensile stresses. AFM and FESEM studies show that cellulose microfibril organization is remarkably altered in the xyloglucan-deficient mutant *xxt1/xxt2*. High-resolution FESEM is combined with selective enzyme digestions to identify the form and locations of matrix polymers in the cell wall at the nanoscale. Complementary studies are being carried out with nano-gold affinity tags, including proteins that selectively bind cellulose, xyloglucan and pectin. These experiments reveal the distribution of cellulose surfaces that are bound with matrix components. Studies of cell wall mechanics along the growing Arabidopsis inflorescence stem were carried out in parallel with SSNMR characterization of polysaccharide properties. The results show that changes in matrix properties, not cellulose organization, are associated with cell wall stiffening and reduced wall hydration. Our research is revealing the plant cell wall as a complex material with many properties beyond current understanding of cell wall structure and mechanisms of its assembly.

9:30 AM

A-II-4: PROGRAMMING THE DYNAMICS OF COLLOIDAL MACHINES

[EFRC – CBES] Kyle J.M. Bishop[1], Sabrina Syeda[1], Allan M. Brooks[1], Yong Dou[1], Mykola Tasinkevych[2], Aysuman Sen[3], Thomas E. Mallouk[3], Monica Olvera de la Cruz[2]
Columbia University[1], Northwestern University[2], Pennsylvania State University[3]

The creation of colloidal machines – that is, dynamic assemblies of colloidal components that perform useful functions – requires advances in our ability to rationally engineer the dynamics of active colloids operating outside of thermodynamic equilibrium. Owing to their small size (nanometers to microns), such machines must assemble spontaneously and operate autonomously in response to simple energy inputs due to chemical fuels or external fields. Achieving non-trivial dynamical behaviors and ultimately function demands the use of complex components, into which the desired behaviors can be effectively encoded. The challenge is conceptually similar to that of programmable self-assembly, whereby assembly information encoded in the building blocks directs their organization into a specific structure. Extending this approach to design colloidal machines will require control over particle organization in time as well as space – that is, over dynamics as well as structure. Here, we describe how top down fabrication processes can be used to program the desired dynamics of active colloidal particles powered by a variety of simple (high symmetry) energy inputs. We show how particle shape and symmetry can be used to direct particle motions powered by electric fields, acoustic waves, and chemical fuels. Additionally, we demonstrate that useful collective motions such as traveling wave excitations can be rationally engineered using patterned arrays of many colloidal actuators.

9:50 AM

A-II-5: ALL-ATOM STRUCTURAL MODEL OF PLANT CELLULOSE SYNTHASE AND CELLULOSE SYNTHASE COMPLEX

[EFRC – CLSF] Abhishek Singh[1], Arielle M. Chaves[5], Hugh O'Neill[3], B. Tracy Nixon[2], Seth DeBolt[6], Alison W. Roberts[5], Candace H. Haigler[1], Yaroslava G. Yingling[1]
[1]North Carolina State University; [2]The Pennsylvania State University; [3]Oak Ridge National Laboratory; [5]University of Rhode Island; [6]University of Kentucky

Cellulose synthase (CESA) is an enzyme that polymerizes glucose into cellulose which is a principal component of plant cell walls and lignocellulosic biomass. Despite the importance of plant cellulose to nature and industry, we have little understanding of the 3D structure of proteins required for plant cellulose biosynthesis and the mechanism of how CESA produces cellulose is not completely understood. In this talk, we will show how computational models can facilitate better understanding of the CESA function and the assembly of CESAs into cellulose synthesis complex (CSC). We used a combination of de-novo, ab-initio, partial homology modeling and molecular dynamics simulations to predict an all-atom 3D structural model of cotton CESAs protein structure. Using our 3D model we were able to design new experiments and shed light on the specific roles of various conserved regions of plant CESA, such as regions unique to plant CESA and Zn-finger. Moreover, we predicted how CESAs can assemble into CSC complex and show possible formation of oligomeric assemblies from dimers to hexamers. Our 3D model and available biochemical/structural data of cellulose synthase complex suggests that each rosette lobe preferably contains a trimer of CESA producing 18 cellulose chains per CSC and allows for exploration and testing of the structure-to-function relations of CESAs.

Session III: Tuesday, July 25, 2017; 10:40 AM – 12:00PM; Lincoln 5

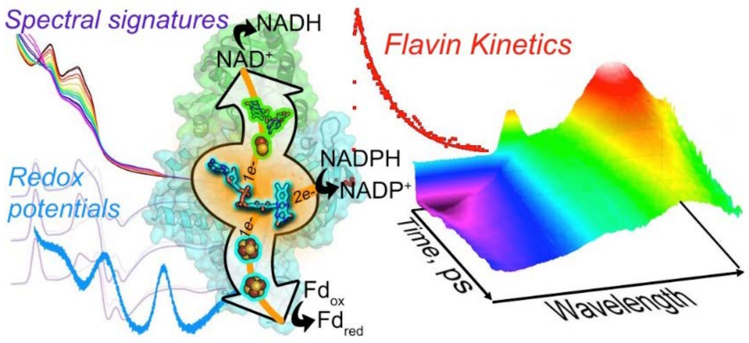
10:40 AM – Team Science Finalist

A-III-1: MECHANISTIC INSIGHTS INTO ENERGY CONSERVATION BY FLAVIN-BASED ELECTRON BIFURCATION

[EFRC – BETCy] D. Nguyen[1], J. Yuly[2], C. Lubner[3], D. Jennings[4], D. Mulder[3], G. Schut[1], O. Zadvornyy[5], J. Hoben[6], P. Zhang[1], M. Tokmina-Lukaszewska[7], L. Berry[7], G. Lipscomb[1], B. Bothner[7], A. Jones[4,] A. Miller[6], P. King[3], D. Beratan[2], M. Adams[1], J. Peters[5,7]

[1]Univ. of Georgia, [2]Duke, [3]NREL, [4]Arizona State, [5]Washington State, [6]Univ. of Kentucky, [7]Montana State

The recently realized biochemical phenomenon of energy conservation through electron bifurcation provides biology with an elegant means to maximize energy efficiency. Flavin based electron bifurcation couples endergonic and exergonic oxidation-reduction reactions into an overall thermodynamically favorable reaction with minimal energy loss. The catalysts that affect these reactions are enzyme complexes that possess numerous redox cofactors to coordinate electron flow between three diffusible electron carriers. At the inception of the Biological Electron Transfer and Catalysis (BETCy) Energy Frontier Research Center (EFRC) little was known about the mechanism of these unique enzymes. The BETCy EFRC team has used a multidisciplinary approach resulting in profound advances in our mechanistic understanding of flavin-based bifurcation, revealing novel features of redox cofactors. Structure determination using x-ray diffraction, coupled with chemical cross-linking, mass spectrometry, and computational modeling reveals the unique architecture and the arrangement of redox cofactors providing a framework for mechanistic studies. Optical and electron paramagnetic spectroscopy coupled with protein film electrochemistry have revealed unique features of redox cofactors, including highly energetic intermediates and large ranges of cofactor oxidation-reduction potentials invoking low potential electron carriers that have yet to be observed outside of light energy-dependent photosynthesis. Pairs of electrons are bifurcated over more than 1 volt of electrochemical potential by generating a low-potential, highly energetic, unstable flavin semiquinone and directing electron flow to an iron–sulfur cluster with a highly negative potential to overcome the barrier of the endergonic half reaction. Theoretical work supports that gating of electron flow committing the coordination of exergonic and endergonic paths can occur electronically through Marcus inversion. The nature of our results has had transformative effects on understanding this fascinating electron transfer phenomena.



Reference: C.E. Lubner, D.P. Jenning, D.W. Mulder, G.J. Schut, O.A. Zadvornyy, J. Hoben, M. Tokmina-Lukaszewska, L. Berry, D. Nguyen, G.L. Lipscomb, B. Bothner, A.K. Jones, A-F. Miller, P.W. King, M.W.W. Adams, J.W. Peters. "Mechanistic Insights into Energy Conservation by Flavin-Based Electron Bifurcation" *Nature Chem. Bio.* 2017 Apr 10. doi: 10.1038/nchembio.2348

Contributions: Diep Nguyen determined the biochemical properties of the bifurcating enzyme, used genetic tools to generate mutants, provided the bifurcating enzyme to collaborators for spectroscopic, electrochemical and structural analyses, and composed the presentation. Jonathon Yuly contributed to the development of the kinetic models for electron bifurcation, analyzed the electron bifurcation results analysis in collaboration with the experimental team, and composed the presentation.

11:00 AM

A-III-2: ENERGY TRANSFER FUNDAMENTALS IN NATURE'S MOLECULAR WIRES: LESSONS FROM NATIVE AND GENETICALLY-MODIFIED FENNA-MATTHEWS-OLSON PIGMENT-PROTEIN COMPLEXES

[EFRC – PARC] Rafael G. Saer[1], Margherita Maiuri[2], Evgeny Ostroumov[2], Gregory Scholes[2], and Robert E. Blankenship[1]
[1]Washington University in St. Louis; [2]Princeton University

Photosynthetic organisms capture and mobilize light energy with specialized pigment-protein antennas. To accomplish this goal, nature has designed these antenna complexes such that they are capable of moving excitation energy over long distances in ultrafast timescales. As the ability to move excitation energy over long distances with high efficiency is useful for designing artificial light-harvesting systems, understanding the mechanisms of energy transfer in their natural systems will provide researchers with a toolkit of design principles for bio-inspired devices. One such natural model system is the Fenna-Matthews-Olson (FMO) complex, present in green sulfur bacteria and acidobacteria. This complex is a stable, water-soluble, pigment-protein complex that mobilizes excitation energy in a directional fashion over tens of Angstroms in under a picosecond. The dynamics of energy transfer in FMO complexes are thought to be assisted by quantum coherent effects, however the source of these coherences are a debated issue. In our work, we have probed the origin of these effects by using a combination of site-directed mutagenesis and ultrafast pump-probe spectroscopic techniques at room temperature and cryogenic temperatures (77 K). Despite the presence of the mutations, however, the coherent oscillation frequencies were the same. Such oscillation frequencies were also independent of the excitation wavelength used when narrow-band excitation of the samples was employed. The results suggest that the nature of coherent oscillations in FMO complexes arises from the delocalization of ground states in the embedded pigment molecules.

11:20 AM

A-III-3: OXIDATIVE INACTIVATION OF [FEFE]-HYDROGENASE AS A MODEL FOR REDOX TUNING OF ENZYME ACTIVE SITE REACTIVITY

[EFRC – BETCy] Anne K. Jones[1], Paul W. King[2], S. Garrett Wiliams[1], Jacob Artz[3,4], David W. Mulder[2], Michael W. Ratzloff[2], Michael W.W. Adams[5] and John W. Peters[3,4]
[1]Arizona State University; [2]National Renewable Energy Laboratory; [3]Montana State University; [4]Washington State University; [5]University of Georgia

[FeFe]-hydrogenases are enzymes that catalyze H–H bond activation at a unique organometallic cofactor known as the H-cluster. The structural organization and catalytic behavior of this family of enzymes is diverse and includes electron bifurcation. Thus [FeFe]-hydrogenases are an ideal model system to establish fundamental mechanistic principles of how enzymes use the coordination environment of cofactors to exquisitely tune function in electron transfer and catalysis. *Clostridium pasteurianum* produces an [FeFe]-hydrogenase, CpII, with catalytic properties that are unlike any other [FeFe]-hydrogenase. CpII has an intrinsic bias towards the H_2 oxidation reaction over proton reduction. As we show in this talk, it also inactivates under mildly oxidizing conditions in which other characterized [FeFe]-hydrogenases are active. We have begun to explain this unprecedented reactivity in CpII using electrochemical and biophysical approaches. We are using these experiments to define the roles played by secondary and outer coordination sphere interactions with the H-cluster in modulating its reduction potentials and tuning catalytic bias of the enzyme. This talk will summarize our latest results.

11:40 AM

A-III-4: PROBING PHOTOSYNTHETIC ANTENNA COMPLEXES WITH NEUTRONS: FROM INDIVIDUAL HYDROGEN ATOMS TO HIERARCHAL ASSEMBLIES

[EFRC – PARC] Brinda Selvaraj[1], Xun Lu[1], Gregory Orf[2], Robert Blankenship[2], Matthew Cuneo[1], Dean Myles[1]
[1]*Oak Ridge National Laboratory*; [2]*Washington University in St. Louis*

An understanding of the molecular details that underlie solar energy capture in photosynthetic organisms will lead to a better understanding of energy transfer in natural photosynthetic systems, and aid in the development of biohybrid photosynthetic systems. Current x-ray crystal structures of the photosynthetic machinery reveal details of the pigment-protein architecture and interactions that regulate and control energy transfer, but do not resolve hydrogen atoms. This is significant, because the individual site energies of protein bound chlorophyll molecules are thought to be modulated and tuned through local hydrogen bonding and electrostatic interactions with the surrounding protein scaffold. Neutron scattering and diffraction are exquisitely sensitive to the location of hydrogen atoms in biological systems, and allow for atomic-resolution analysis of individual hydrogen atoms in proteins, and for multi-scale analysis of hierarchical structures and assemblies. Here we will describe recent neutron-based structural studies on several photosynthetic antennae complexes, with a particular focus on the first high resolution neutron analysis of the Fenna-Matthews-Olsen (FMO) antenna complex, which provides a more complete atomic resolution description and detail of the protein-pigment interactions that are involved.

B. CARBON SEQUESTRATION

SESSION III: TUESDAY, JULY 25, 2017; 10:40 AM – 12:00PM; LINCOLN 2

10:40 AM

B-III-1: TOWARDS RESOLUTION OF CONFLICTING INFORMATION ABOUT THE INFLUENCE OF CO_2 EXPOSURE ON WETTING PROPERTIES AND RESIDUAL GAS TRAPPING

[EFRC – NCGC] Sally M. Benson[1], Charlotte Garing[1], Tetsu K. Tokunaga[2], Jiamin Wan[2]
[1]Stanford University; [2]Lawrence Berkeley National Laboratory

The influence of exposure to supercritical CO_2 on the wetting and capillary trapping properties of rocks remains the subject of uncertainty. Experiments on micromodels and unconsolidated sand-packs by a number of research groups show that the wettability can decrease when exposed to supercritical CO_2 and capillary trapping can increase. At the same time, experiments on consolidated rocks exposed to CO_2 show that the rocks remain strongly water wet and that residual gas trapping is similar to that with other fluid pairs such as nitrogen and water. Here we present data documenting the evidence for both arguments and new information to help resolve this issue. In particular, we show new data demonstrating that the presence of dissolved organic compounds can explain some of the changes in wettability. We also show new data for consolidated rocks, demonstrating that pre-treatment from firing the samples does not alter the wettability of the rocks. Steps to resolution of this conflicting information are presented and discussed.

11:00 AM

B-III-2: LINKING CHEMICAL TRANSFORMATIONS TO PHYSICAL INTEGRITY THROUGH DIRECT IMAGING OF FLUID TRANSPORT PROPERTIES IN MT. SIMON CORE DURING CO_2 INJECTION

[EFRC – GSCO2] Jennifer L. Druhan[1], Gabriela Davila[1], Christopher Zahasky[2], Sally Benson[2], Dustin M. Crandall[3], Ange T. Akono[1], Theo Tsotsis[4], Kristian Jessen[4], Charles L. Werth[5]
[1]University of Illinois at Urbana-Champaign, [2]Stanford University, [3]National Energy Technology Laboratory, [4]University of Southern California, [5]University of Texas at Austin

During CO_2 injection into sedimentary basins, characteristic geochemical reactions alter the pore structure of the formation, and thus ultimately influence the mechanical integrity of the reservoir. We suggest that these processes may be coupled through the influence of reactivity on fluid transport properties such as the permeability of the medium. At the laboratory scale, it has been demonstrated that local heterogeneities result in low permeability zones, presenting a higher resistance to fluid phase pressure gradients. We are currently developing a novel experimental procedure in order to facilitate (*1*) acquisition of a 3D permeability map in real time, (*2*) evaluation of the retardation effect as the disparity between inert tracer and CO_2 injection, and (*3*) quantification of mineral dissolution/precipitation processes altering permeability during injection of a CO_2-rich brine through Mt. Simon core rock.

A key novelty of this work is the use of a non-invasive, real-time radiotracer imaging technique, Positron Emission Tomography (PET). The PET imaging study consists of injection pulses using inert flouuride-18 labeled radiotracer during a CO_2-saturated brine flow-through experimental. Geochemical alteration is induced between PET images using a continuous flow-through experiment under CO_2 supercritical conditions (P_{Total} = 100 bar and T = 53°C) with the synthetic CO_2-rich brine circulated at constant flow rate of 0.17mL min^{-1} through a core sample (2.3cm in

diameter and 8.6cm in length). The pH of the injected solution was acidic (~3.5) promoting the dissolution of feldspar, chloride, illite, kaolinite, calcite/dolomite and pyrite and precipitation of secondary minerals, resulting in a net porosity increase.

11:20 AM

B-III-3: ADVANCES IN UNDERSTANDING BUOYANCY-DOMINATED FLOW IN HETEROGENEOUS GEOLOGIC SYSTEMS

[EFRC – CFSES] Tip Meckel[1], Mario Martinez[2], Hongkyu Yoon[2], David DiCarlo[1], Luca Trevasan[1], Prasanna Krishnamurthy[1], Alec Kucala[1], Sid Senthilnathan[1]
[1]The University of Texas at Austin; [2]Sandia National Laboratories

Geologic CO_2 storage (GCS) is a key technology for mitigating greenhouse gas emissions, but to be meaningful GCS must overcome three key technical challenges: sustaining large storage rates for decades, using pore space with unprecedented efficiency, and controlling undesired or unexpected behavior in the geostorage system. Because viscous forces decline rapidly with distance from injection wells, even at the large material rates anticipated, buoyancy dominates the majority of the storage complex during and after injection. *A primary research theme within CFSES is to improve the scientific understanding of buoyancy-dominated multiphase displacements in heterogeneous geomaterials.* While informed by field-scale observations of natural analogs and active GCS projects, the primary focus is on the meso-scale, where the interaction with geologic heterogeneity yields behavior that is extremely difficult to predict for natural materials. This research investigates a specific range of length scales (cm to m) and time scales (years to decades) within which significant patterns and behaviors emerge, but for which both data and models are traditionally lacking. The research establishes a new scientific foundation for defining the physical constraints on key challenges for GCS, and for identifying novel materials and strategies to overcome these constraints. This foundation is the first to account for the crucial but currently intractable aspect of intermediate scale heterogeneity, which is relevant to several other large-scale subsurface applications. This presentation will highlight research for prediction and control of CO_2 flow from integrated results from model development of realistic geologic heterogeneity, lab-scale experimentation, and numerical simulation techniques.

11:40 AM

B-III-4: SOLUBILITY OF GASES (CO_2, CH_4, H_2, NOBLE GASES) IN CLAY INTERLAYER NANOPORE WATER

[EFRC – NCGC] Greeshma Gadikota[1], Baptiste Dazas[1], Gernot Rother[2], Michael C. Cheshire[2], Ian C. Bourg[1,]
[1]Princeton University; [2]Oak Ridge National Laboratory

The migration of dissolved gases in sedimentary rocks is a recurrent topic in subsurface hydrology, from the widespread use of noble gases as tracers of fluid migration in sedimentary rocks to specific energy technologies including carbon capture and storage (CO_2), radioactive waste storage (H_2), and shale gas extraction (CH_4). In all these applications, hydrologic studies almost invariably assume that dissolved gases behave as inert tracers, even in clay-rich nanoporous rocks (shale, mudstone). Over the last few years, however, experimental studies have shown that CO_2 is about five times more soluble in water-saturated clay interlayer nanopores than in bulk liquid water. The fundamental basis of this selectivity and its relevance to other gases remain unknown. Here, we use molecular dynamics (MD) simulations and gravimetric adsorption experiments to determine the solubility of CO_2, CH_4, H_2, and noble gases in clay interlayer water. Our results demonstrate that clay minerals, despite their well-known hygroscopic nature, have a significant hydrophobic character at the atomistic scale. The affinity of different dissolved gases for the clay surface shows significant variations related to the size and shape of the adsorbing molecules and the structuring of interfacial water by the clay surface. For example, intermediate-size noble gases (Ne, Ar) partition into the clay interlayer nanopores more strongly than their smaller (He) or larger (Kr) counterparts. Our results have implications for the fundamental science of hydrophobic adsorption and for specific applications related to gas migration in sedimentary rocks.

SESSION IV: TUESDAY, JULY 25, 2017; 1:30 – 3:30PM; LINCOLN 2

1:30 PM

B-IV-1: HYDRO-MECHANICAL ASPECTS OF DEEP CO_2 STORAGE

[EFRC – GSCO2] Roman Makhnenko[1], Ali Tarokh[1], Victor Vilarrasa[2]
[1]University of Illinois at Urbana-Champaign, [2]Spanish National Research Council

Field-scale geological CO_2 storage projects indicated a number of factors that can compromise the integrity of the involved geomaterials. CO_2 leakage to the near-surface and induced seismicity are the major concerns. Accurate evaluation of rock response is needed to investigate possible problems and predict long-term storage strategies. Novel experimental techniques have been developed to characterize fluid-saturated rock behavior at elevated temperatures and pressures. Tested materials included sandstones and limestones as high-permeable host rock representatives, and shale and granite as low-permeable caprock and crystalline basement formations, respectively. Poromechanical and inelastic parameters, microseismic activity, brine and CO_2 permeability of rock are measured. Obtained material properties are used to simulate fault stability and caprock deformation for industrial-scale CO_2 storage, where cooling is likely to occur around injection wells and clay-rich faults may induce microseismic events.

1:50 PM

B-IV-2: PERFORMANCE ASSESSMENT OF JOINTED/FAULTED CAPROCK DURING CO_2 SEQUESTRATION

[EFRC – CFSES] Pania Newell[1&2], Mario J. Martinez[2], Peer Eichhubl[3], Thomas Dewers[2], Richard Reguerio[4]
[1]The University of Utah; [2]Sandia National Laboratories; [3]The University of Texas at Austin; [4]The University of Colorado-Boulder

Deep geological formations have shown potential as permanent storage units for large amounts of carbon dioxide over long periods of time (103-104 years). Success of the overall performance of geological carbon storage (GCS) units depends on various trapping mechanisms such as structural, capillary, solubility, and mineral mechanisms within geological systems. Structural trapping within deep geological formations is highly influenced by rock formation, newly-formed and pre-existing fractures and faults across many scales. The growth and reactivation of these fracture networks are fluid- driven which may or may not be assisted by chemical-mechanical alterations. The magnitude of the pore pressure due to injection not only depends on hydrological and geomechanical properties of rock formation, but also on the wellbore orientation, the injection rate and the injection schedule. In this presentation: (i) geomechnical testing at core scale for the calibration of material models will be reviewed, (ii) chemo-mechanical coupling impact on fracture propagation at the laboratory scale will be addressed, (iii) the impact of formation thickness, wellbore orientation, injection rate, presence of fault and pre-existing fractures within the caprock is computationally investigated at the reservoir scale. These studies will highlight the importance of the spatial and temporal scales and coupled processes within geological formations and their influences on the overall performance for GCS.

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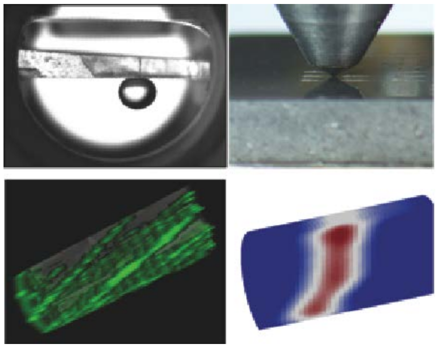
2:10 PM – Team Science Finalist

B-IV-3: GEOCHEMICAL REACTIONS DURING GEOLOGICAL CARBON SEQUESTRATION CAN DECREASE FRACTURE TOUGHNESS OF RESERVOIR ROCK AND CONTRIBUTE TO MICROSEISMIC EVENTS

[EFRC – GSCO2] L Dalton[1], MG Davila Ordonez[2], S Fuchs[3], P Kabir[2], Z Shi[4], MK Tkach[1], A Akono[2], DM Crandall[1], J Druhan[2], AL Goodman[1], K Jessen[4], T Tsotsis[4], CJ Werth[3]

[1]National Energy Technology Laboratory, [2]University of Illinois at Urbana-Champaign, [3]University of Texas at Austin, [4]University of Southern California



Many reservoirs proposed for geological storage of carbon dioxide contain reactive minerals that can dissolve under acidic conditions created during CO_2 injection. In some cases, the most reactive minerals act as cementing agents that bind less reactive minerals together. For example, illite clays bind together quartz and feldspar grains in the Mount Simon formation, a siliciclastic storage reservoir being used in a DOE pilot study to geologically sequester carbon dioxide. Bench-scale core studies indicate dissolution and displacement of clays can occur during CO_2 injection, suggesting that this cementing agent can be removed during long-term storage operations. The objectives of our team effort are to quantify the geochemical reactions that occur in reservoir materials during exposure to carbon dioxide, and the subsequent effects on fluid flow paths, the location of geochemical reactions, and reservoir geomechanical properties. Our team is aging common reservoir materials from the Mount Simon formation in supercritical CO_2 and brine at representative pressures and temperatures, under both static and flowing conditions. Pre- and post-aging, we are probing the materials for geochemical and pore-space changes using a suite of gas adsorption, optical, spectroscopic and tomographic methods, including permporometry and CT scanning. During aging, we are mapping preferential flow paths using positron emission tomography (PET scan). We are probing changes in geomechanical properties using a scratch test to measure fracture toughness, as well as triaxial tests that subject rock cores to representative pore fluid and confining pressures. These various experiments span a range of scales, and are being performed by different team members. The results are collectively contributing to our project objectives, and to our collaborative goal of identifying implications of geomechanical weakening on induced microseismicity in the Mount Simon Formation.

Contributions: L. Dalton and M. Tkach are contributing to CT scans of the Mount Simon Material, optical, spectroscopic, and triaxial tests. M. Davila is contributing to PET scan measurements of flow, and geochemical reaction modeling. S. Fuchs is contributing to sample aging and geochemical reaction characterization. P. Kabir is contributing to scratch testing. Z. Shi is contributing to permporometry and strain measurements.

2:30 PM

B-IV-4: INVESTIGATION OF FRACTURE ALTERATION USING A COUPLED MODELING AND EXPERIMENTAL APPROACH

[EFRC – NCGC] Hang Deng[1], Sergi Molins[1], Carl Steefel[1], Donald DePaolo[1], Marco Voltolini[1], Jonathan Ajo-Franklin[1], Li Yang[1], Michael Cheshire[2], Andrew Stack[2], Lawrence Anovitz[2]
[1]Lawrence Berkeley National Laboratory; [2]Oak Ridge National Laboratory

Fractures are preferential flow pathways that largely control the migration of injected CO_2 in geological formations, and are subject to alteration due to water-CO_2-rock interactions. In order to accurately assess long-term storage security of Geological CO_2 Storage (GCS), it is critical to understand the dynamic evolution of fractures. Reactive transport models that are developed and tested based on experimental work serve as an important investigative and predictive tool.
In this presentation, we first present a novel reactive transport model that was developed based on an in situ synchrotron X-ray microtomography experiment flowing CO_2-saturated water through a single-fractured Niobrara shale mini-core. The model successfully captures the development and erosion of a porous altered layer on the fracture surfaces, and the evolution of geochemical reactions and morphology observed in the experiment.

We also use this model to investigate the evolution of fracture morphology and hydraulic properties under conditions beyond the experimental studies. Simulations are conducted using mineral compositions with a range of carbonate contents in random fracture fields with similar statistics as previous experimental work. Comparisons of the simulations demonstrate how mineral heterogeneity affects the alteration of the rock matrix bordering the fracture, and the subsequent reactions in the fracture and the extent and spatial pattern of fracture opening.
The reactive transport model has also been used to examine the potential of mineral precipitation in sealing fractures in carbonate rich rocks. Fracture sealing was observed in a fractured Eagle Ford core after flowing CO_2-rich brine through it for 1.5 months.

2:50 PM

B-IV-5: ROCK MECHANICAL ALTERATION DUE TO FLOW OF CO_2-CHARGED BRINE: SHEAR STRENGTH OF CRYSTAL GEYSER OUTCROP SAMPLES

[EFRC – CFSES] Nicolas D. Espinoza[1], Jung Hojung[1], Matthew J Ramos[1], Jonathan Major[1], Peter Eichhbul[1], Zhuang Sun[1], Matthew T. Balhoff[1], Charles R Choens[2], Thomas A. Dewers[2]
[1]The University of Texas at Austin; [2]Sandia National Laboratories

CO_2 geological storage in saline aquifers results in acidification of resident brine. Chemical reactions between acidified brine and rock minerals lead to dissolution and precipitation of minerals at various time scales. Mineral dissolution and precipitation are often neglected in assessing mechanical integrity of target storage formations, yet, changes in rock strength and deformational behavior can impact trapping mechanisms. This study shows impact of flow of CO_2-charged brine on shear strength of various outcrop rocks evaluated through triaxial testing. Rocks were exposed to CO_2-charged brine over geological time at a naturally occurring near-surface seepage in Little Grand Wash Fault, Crystal Geyser site near the town of Green River, Utah. Results show mechanical alteration in various aspects: (1) CO_2-charged brine alteration at near-surface conditions results in mineral dissolution and reduction of shear strength and brittleness of hematite/carbonate-cemented Entrada sandstone and Summerville siltstone samples, (2) carbonate precipitation in fractured Mancos shale leads to matrix stiffening and fracture mineralization resulting in overall stiffer and likely tighter shale. Additional discrete element simulations coupled with bonded-particle-model confirm the role of bond size alteration as one of the main controls for rock chemo-mechanical alteration. A chemo-mechanical alteration path that mimics cement dissolution (under stressed conditions) results in vertical compaction and lateral stress relaxation. Overall, results show that exposure of rocks to CO_2-charged brine can result in either negative or positive implications regarding trapping mechanisms. While mineral dissolution in storage rock may result in undesired reservoir strains and stresses, mineral precipitation downstream can help seal potentially induced fractures.

3:10 PM

B-IV-6: TOWARDS A MULTISCALE PHYSICS BASED FRAMEWORK FOR MODELING FLUID INFILTRATED FAULT ZONES WITH AN EYE FOR INDUCED SEISMICITY IN ENERGY APPLICATIONS

[EFRC – GSCO2] Ahmed Elbanna[1], Setare Hajaroalasvadi[1], Xiao Ma[1], Sahar Bakhshian[2], Muhammad Sahimi[2], Al Valocchi[1], Yu Chen[1]
[1]*University of Illinois at Urbana-Champaign,* [2]*University of Southern California*

In the past decade, there has been a surge in the rate of induced earthquakes of magnitude 3–4 range. With induced seismicity events further approaching M6 (Oklahoma, 2016) the hazard they impose is not negligible. While the basic mechanism for induced seismicity is well understood as a result of fault lubrication due to an increased pore pressure, development of predictive models for their magnitudes, frequency, spatial distribution, and correlation to well operating conditions is still challenging. Part of the challenge is the nature of the problem that requires Multiphysics coupling (hydro-chemo-mechanical coupling) and multiscale techniques to couple small-scale lab measurements to field-scale observations.

In this presentation, I will give an overview of our recent progress in addressing these challenges. In particular, I will present a non-equilibrium statistical physics model for visco-plasticity in pressure sensitive porous media (such as rocks and granular materials). I will show that the model predicts correctly the complex evolution of shear bands and I will further discuss interactions of these instabilities with heterogeneous microstructure and pore fluid pressure and the complex feedback loops between them. Next, I will describe a novel computational scheme integrating the finite difference method with spectral boundary integral algorithms enabling efficient coupling of small-scale nonlinear rheology and damage with large-scale elastodynamics. This integration is scale bridging and will ultimately enable incorporation of high-resolution microstructure and fracture models with field-scale elastic deformation and pore pressure measurements providing a critical link for understanding earthquakes and induced seismicity.

C. CATALYSIS

SESSION I: MONDAY, JULY 24, 2017; 3:00 – 5:00 PM; THURGOOD MARSHALL NORTH

3:00 PM

C-I-1: BIOMASS-DERIVED BUTADIENE BY DEHYDRA-DECYCLIZATION OF TETRAHYDROFURAN

[EFRC – CCEI] Omar A. Abdelrahman[1], Dae Sung Park[1], Katherine P. Vinter[1], Charles S. Spanjers[1], Limin Ren[1], Hong Je Cho[2], Dionisios G. Vlachos[3], Wei Fan[2], Michael Tsapatsis[1], Paul J. Dauenhauer[1]
[1]University of Minnesota; [2]University of Massachusetts Amherst; [3]University of Delaware

Butadiene is an industrially important precursor in the production of polymers, where it is typically reacted with itself or other monomers to produce synthetic rubber. Polymerizing butadiene with styrene and acrylonitrile produces hard ABS plastic for tubing and packaging, while polymers of butadiene and styrene are used in the production of automobile tires. We present a renewable pathway to produce butadiene from biomass-derived tetrahydrofuran (THF), proceeding via dehydrative ring opening of THF (Dehydra-Decyclization). A screening of various solid acid catalysts reveals that all-silica phosphorous-containing zeolites (Phosphorous-self pillared pentasil, P-SPP) result in the highest selectivity for butadiene, *ca*. 95%. The first step in the conversion of THF is proposed to be a ring opening reaction, forming an unsaturated alcohol, which can then proceed via various acid-catalyzed reaction pathways. The most significant undesired reaction is retro-Prins condensation, which converts the unsaturated alcohol to propene and formaldehyde. Increased methyl substitution in the 2 and 5 carbon positions of THF leads to a significant increase in the rate, but not substitution in the 3 carbon position, suggesting that a carbenium ion formation in the 2 and 5 carbon positions is a kinetically relevant step. A combination of in-situ titrations of pyridine and of a bulky base, 2,6-ditertbutyl pyridine, suggest that the surface chemistry is predominantly Brønsted acid catalyzed. A comparison of solid acid catalysts of various acid strengths suggests that a weaker acid site is desirable to achieve higher selectivity for butadiene.

3:20 PM

C-I-2: MOVING FROM MODEL STUDIES ON SINGLE CRYSTAL GOLD TO HIGHER PRESSURE CONDITIONS: KINETIC AND MECHANISTIC UNDERSTANDING FROM TAP STUDIES ON NPAU CATALYSTS

[EFRC – IMASC] Christian Reece,[1] Evgeniy Redekop,[2] Cynthia Friend,[1] and Robert J. Madix[1]
[1]Harvard University; [2]University of Oslo

The reactions involved in the activation of nanoporous gold with ozone and the subsequent reduction by methanol/dioxygen reactant mixtures has been examined using transient pulses of reducing gases. After activation at atmospheric pressure with a flowing stream of dioxygen dilute in ozone, exposure to methanol pulses shows first the removal of surface oxide to form combustion products. As this oxide is depleted a more selective form of adsorbed oxygen emerges that reacts with methanol to form methyl formate and formaldeyde. Progressive removal of the remaining oxygen shifts the product distribution toward formaldehyde. In addition to these overall observations mechanistic information obtained from the transient responses observed for each product will be discussed.

3:40 PM – Team Science Finalist

C-I-3: POST-FUNCTIONALIZED METAL–ORGANIC FRAMEWORKS FOR CATALYSIS

[EFRC – ICDC] Manuel A. Ortuño,[1] Zhanyong Li,[2] Ana E. Platero-Prats,[3] Karena W. Chapman,[3] Joseph T. Hupp,[2] Omar. K. Farha,[2] Christopher J. Cramer,[1] Laura Gagliardi[1]
[1]University of Minnesota; [2]Northwestern University; [3]Argonne National Laboratory

Metal–organic frameworks are a versatile family of mesoporous materials used in gas storage, separation, and catalysis. They are comprised by inorganic nodes connected by organic linkers. The vast number of linker–node combinations provides a high degree of tuning to design and predict unique structure topologies. Within this extensive catalog, the Zr-based MOF NU-1000 stands out as an excellent support material to deposit transition metal catalysts via atomic layer deposition (AIM) or solvothermal deposition (SIM) protocols.

The fine-tuning of MOF nodes with transition metals allows us to prepare different catalysts for different transformations, such as ethylene hydrogenation and dimerization (Ni), epoxidation (Mo), methane oxidation (Cu), and propane oxidative dehydrogenation (Co),[1] among others (Figure 1).

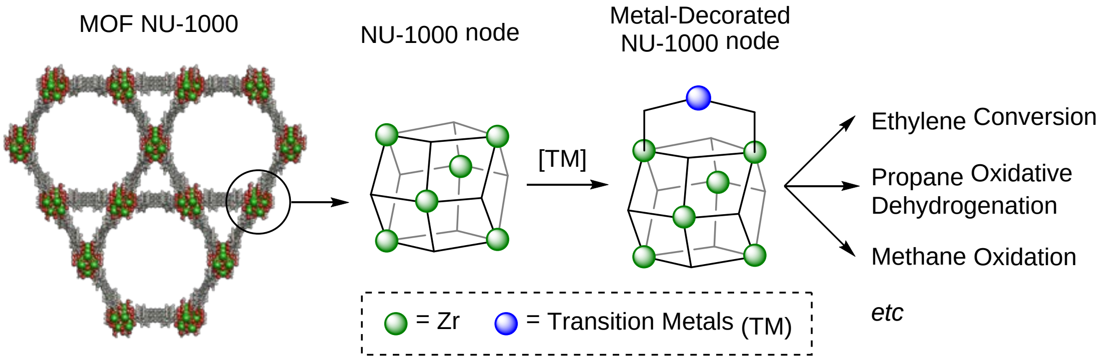


Figure 1. Metal–organic framework (MOF) NU-1000 and further post-functionalization for catalysis.

The synergistic combination of experimental and theoretical techniques becomes crucial to (i) determine the local structure of the post-functionalized materials and (ii) analyze the catalytic reaction mechanisms at the atomic level of precision. These joined efforts would path the way to unravel chemical descriptors and build structure–reactivity relationships leading to rational design of new materials.

Contributions: M. A. O. theoretically modeled structures and reaction mechanisms. Z. L. and A. E. P.-P. carried out the synthesis, characterization, and catalytic testings.

1. Li, Z.; Peters, A. W.; Bernales, V.; Ortuño, M. A.; Schweitzer, N. M.; DeStefano, M. R.; Gallington, L. C.; Platero-Prats, A. E.; Chapman, K. W.; Cramer, C. J.; Gagliardi, L.; Hupp, J. T.; Farha, O. K. *ACS Cent. Sci.* **2017**, *3*, 31.

4:00 PM

C-I-4: ELECTRON BIFURCATION – MECHANISTIC FIRST PRINCIPLES

[EFRC – BETCy] Carolyn E. Lubner[1], David P. Jennings[2], David W. Mulder[1], Gerrit J. Schut[3], Oleg A. Zadvornyy[4,5], John Hoben[6], Monika Tokmina-Lukaszewska[4], Luke M. Berry[4], Diep Nguyen[3], Gina L. Lipscomb[3], Brian Bothner[4], Anne K. Jones[2], Anne-Frances Miller[6], Paul W. King[1], Michael W.W. Adams[3], John W. Peters[4,5]

[1]National Renewable Energy Laboratory; [2]Arizona State University; [3]University of Georgia; [4]Montana State University; [5]Washington State University; [6]University of Kentucky

The recently realized biochemical phenomenon of energy conservation through electron bifurcation provides biology with an elegant means to maximize utilization of metabolic energy. The mechanism of coordinated coupling of exergonic and endergonic oxidation-reduction reactions by a single enzyme complex has been elucidated through optical and paramagnetic spectroscopic studies revealing unprecedented features. Pairs of electrons are bifurcated over more than one volt of electrochemical potential by generating a low potential, highly energetic, unstable flavin semiquinone and directing electron flow to a highly negative potential iron-sulfur cluster to overcome the barrier of the endergonic half reaction. The unprecedented range of thermodynamic driving force that is generated by flavin-based electron bifurcation accounts for unique chemical reactions that are catalyzed by these enzymes.

4:20 PM

C-I-5: A NEW FAMILY OF CATALYSTS FOR SOLAR FUELS: COFACTOR-LIKE CATALYSTS ON MESOPOROUS MOF SUPPORTS

[EFRC – ANSER] Aaron W. Peters[1], Omar K. Farha[1], Alex B. F. Martinson[2], Chung-Wei Kung[1], In Soo Kim[2], Karena Chapman[2], Joseph T. Hupp[1]

[1]Northwestern University; [2]Argonne National Laboratory

This presentation will focus on the synthesis, characterization, and sustainable-energy-relevant application of representative examples of a new class of chemical catalysts. The targeted reactions are carbon dioxide reduction – especially to liquid products, water oxidation, and water reduction. The catalysts are cluster based and, like many enzyme cofactors, contain transition-metal cations and chalcogen anions (sulfur or oxygen ions). The clusters are synthesized from volatile organometallic precursor molecules and are sited on appropriately designed nodes of water-stable, mesoporous metal-organic frameworks. The clusters are obtained with single-atom or close-to-single-atom precision and thus consist of uniform, high-spatial-density arrays when configured on the periodic nodes of the MOFs. Catalyst structures, and structural stability, have been extensively been examined by synchrotron based X-ray methods (APS) and other methods (NU). The mesoporosity of the assemblies ensures that candidate catalysts are accessible to reactants. Finally, the organic linkers of the MOF can be recruited as light-harvesting antennae and energy conduits for accomplishing catalytic reduction chemistry using visible light as the energy input.

4:40 PM

C-I-6: REVERSIBLE ENZYMATIC H_2 PRODUCTION/OXIDATION USES DIFFERENT PATHWAYS FOR THE FORWARD AND REVERSE REACTION

[EFRC – CME] Simone Raugei[1], Neeraj Kumar[1], Bojana Ginovska[1], Wendy J. Shaw[1], Eric S. Weidner[1], Aaron M. Appel[1], R. Morris Bullock[1]
Pacific Northwest National Laboratory

The reversibility of many enzymatic catalytic processes makes them a compelling source of inspiration for design principles for improved catalysts for energy applications. It is generally assumed, because of the microscopy reversibility of elementary reaction steps, that catalytic reversibility is achieved through the same reaction pathway in the forward and reverse directions. Computations carried out at the CME on [FeFe]-hydrogenase have shown that enzymes can achieve reversibility employing multiple pathways, depending on the thermodynamic driving force (*i.e.*, overpotential). [FeFe]-hydrogenase catalyzes the interconversion between protons, electrons and molecular hydrogen at fast rates and low overpotentials. Over the years, several catalytic intermediates have been experimentally identified by various research groups, but little attention has been devoted to characterizing the energetics of all possible elementary steps and connecting them into the full catalytic cycle. We used several complementary computational tools, including quantum chemistry, molecular dynamics and microkinetic modeling, to elucidate the possible thermochemical and electrochemical transformations for the H_2 oxidation and production by the [FeFe]-hydrogenase, taking into account possible protonation states of all the redox forms of the catalytic cofactor. Our results reproduce the most recent experimental evidence and show that while H_2 production involves a super-reduced cofactor, oxidation of H_2 involves only the reduced cofactor. An analysis of the factors influencing the branching points along the catalytic pathways will be discussed, along with implications for the design of molecular electrocatalysts.

SESSION II: TUESDAY, JULY 25, 2017; 8:30 – 10:10 AM; THURGOOD MARSHALL NORTH

8:30 AM

C-II-1: First-Principles Kinetic Monte Carlo Simulations of C1 Chemistries on Pure Metals and Single Atom Alloys

[EFRC – IMASC] Michail Stamatakis[1], Matthew T. Darby[1], Angelos Michaelides[1], E. Charles H. Sykes[2], Maria Flytzani-Stefanopoulos,[2] Ioanna Fampiou[3], Robert J. Madix[3], Cynthia M. Friend[3], Efthimios Kaxiras[3]
[1]University College London; [2]Tufts University; [3]Harvard University

Methane activation is a long-standing challenge in catalysis, and has recently become even timelier, due to the abundant shale gas reserves in the USA and beyond. C-H bond activation of methane towards CH_x fragments and subsequent C-C coupling can yield higher hydrocarbons to be used as fuels, providing a valorization route for such reserves. Using C1 fragments as building blocks towards higher molecular weight compounds can also be achieved via oxidative coupling, for instance, methanol can thus be converted to methylformate, an important precursor in the synthesis of several compounds of commercial interest.

Recent experimental work has demonstrated that it is possible to activate methane without risk of coking on Pt/Cu single atom alloys, and that the oxidative coupling of methanol can proceed on O-precovered Au surfaces. To better understand these two chemistries, we have employed a first-principles based kinetic Monte Carlo (KMC) approach, which enables us to build dynamic

models of the underlying catalytic processes at the molecular level. These models are parameterized using density functional theory (DFT) calculations, and incorporate both the inhomogeneous nature of the alloy surfaces, as well as the adsorbate-adsorbate lateral interactions that result in coverage-dependent reaction rates. Our simulations reproduce the experimental trends, and provide explanations for the coking resistance of Pt/Cu during methane activation, and the dominant pathways and products of methanol coupling on Au. These results showcase the value of combining DFT and KMC to bridge the gap between molecular properties computed at 0 K and experimental observables at realistic conditions.

8:50 AM

C-II-2: ROLE OF SURFACE STRUCTURE AND DOPANTS ON THE INTERACTION BETWEEN ACID GASES AND METAL OXIDE CATALYSTS

[EFRC – UNCAGE-ME] Uma Tumuluri[1], Meijun Li[2], Minghui Zhu[3], Jun-Kun Lai[3], Joshua Howe[4], David Sholl[4], Bobby Sumpter[5], Sheng Dai[1,2], Israel E. Wachs[3], Zili Wu[1,5]
[1]Oak Ridge National Laboratory; [2]University of Tennessee, Knoxville; [3]Lehigh University; [4]Georgia Institute of Technology; [5]Center for Nanophase Materials Sciences, Oak Ridge National Laboratory

The nature of the interaction of acid gases including CO_2, SO_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 and TiO_2 with different morphologies to understand the effect of surface crystallographic termination on the interaction with the acid gases. In addition to the critical role of surface structure, the oxygen vacancies in the metal oxides are also found to play important role in interaction with the acid gases. When doped with various transition metals, the amount and strength of adsorbed acid gas species changes in a trend which is parallel to the change in the density of defect sites, further suggesting the significant role of defects. For supported VO_x/TiO_2 catalysts, the doping of WO_x was shown to increase the total activity of the selective reduction of NOx with NH_3, which is attributed to the cooperativity between the redox sites of VO_x and acid sites associated with WO_x. The underlying mechanisms of the role of surface structure and dopants of oxides on the interaction with acid gases will be presented and discussed.

9:10 AM

C-II-3: ZR$_6$ NODES OF METAL ORGANIC FRAMEWORKS AS PLATFORMS FOR SINGLE-SITE METAL CATALYSTS

[EFRC – ICDC] Dong Yang[1], Varinia Bernales[2], Manuel Ortuño[2], Christopher J. Cramer[2], Laura Gagliardi[2], Bruce C. Gates[1]
[1]University of California Davis; [2]University of Minnesota

Metal−organic frameworks (MOFs) with Zr_6O_8 nodes offer new opportunities as supports for catalysts with well-defined, essentially molecular structures. To understand the bonding of catalytic species to the nodes, we characterized the structure and reactivity of the node surfaces using methanol and ethanol as probe molecules and characterizing the surface species with IR, NMR and DFT calculations. The data demonstrate various ligands bonded to the node vacancies, depending on the synthesis conditions and the modulators. Node surface groups include hydroxo, alkoxy, and carboxylate, and controlling these allows some dialing in of the catalytic properties of the nodes and of metal species anchored to them. These node sites are an ideal platform for anchoring essentially molecular catalysts, and with guidance by theory, design of catalysts in this class is becoming a reality. These points are illustrated for catalysts made from the precursor $Rh(C_2H_4)_2(acac)$ (acac is acetylacetonate) used to anchor Rh(I) complexes to the nodes of UiO-67.

The catalyst performance data characterizing ethylene conversions at room temperature are complemented with structural information determined by IR, EXAFS and by DFT calculations. The agreement between the experimental and calculated structural metrics is good, and the calculations have led to predictions of reaction mechanisms and associated energetics. The data demonstrate a correlation between the catalytic performance of the supported rhodium complexes and the electron-donor tendency of the support (as measured by ν_{CO} of carbonyls bonded to the Rh(I) centers). MOFs are emerging as a potentially broad new class of catalyst supports with tailorable catalytic properties.

9:30 AM

C-II-4: STRUCTURE AND REACTIVITY OF NOBLE METAL AND ALLOY CATALYSTS CHARACTERIZED BY IN SITU MICROSCOPY AND SPECTROSCOPY

[EFRC – IMASC] Miquel Salmeron[1,2], Christian Heine[1], Branko Zugic[3], Baran Eren[1], Barbara Lechner[1], Cheng Hao Wu[1], Cynthia Friend[3]

[1]Lawrence Berkeley National Laboratory; [2]University of California Berkeley; [3]*Harvard University*

Of paramount importance is to understand the structure and evolution of catalysts in the presence of reactants near ambient pressure and temperature conditions. Our studies in Berkeley involve the development and application of instrumentation for molecular level characterization catalysts: model single crystals, nanoparticles, and porous materials. The techniques include ambient pressure Scanning Tunneling and Atomic Force Microscopy (AP-STM, AFM), X-ray phoelectron spectroscopy (AP-XPS), Near edge x-ray absorption fine structure (NEXAFS), and IR, designed for *in situ* operation. We have used them to study the evolution of Cu, Ni and Ag single crystals in the presence of O_2, H_2, CO, CO_2, and CH_3OH. The x-ray spectroscopies made possible to determine the chemical state of the surface reaction products and of metal components in Au-Ag alloys in the presence of alcohols. Also, using AP-STM, AP-XPS and NEXAFS techniques on single crystal Cu and Ag catalysts in the presence of methanol we could observe the formation of products and determine their chemical nature. They fragments such as C, CH_x, and O, in the form of hydrocarbon moieties, carbides and oxides, as well as intermediates closer to the final products such as formaldehyde, methoxy, and methylformate and their orientation on the surface.

9:50 AM

C-II-5: INTEGRATED PHOTOELECTRODES FOR CO_2RR

[Hub – JCAP] Guiji Liu,[1] E. Ashley Gaulding,[1] Francesca M. Toma[1]

[1]Lawrence Berkeley National Laboratory

CO_2 reduction using solar energy could not only help reduce CO_2 emission, but also holds promise to meet the increasing demand for global energy. Over the past three decades, researchers have evaluated lots of materials for CO_2 reduction in aqueous solutions. Among those, Cu based materials have been the focus of most CO_2 reduction studies due to its capability of producing hydrocarbon products. Herein, we aim to construct a copper oxide based photoelectrodes, as they possess abundant active sites to substantially promoting CO_2 reduction

SESSION III: TUESDAY, JULY 25, 2017; 10:40 AM – 12:00PM; THURGOOD MARSHALL NORTH

10:40 AM

C-III-1: CATALYTIC CONVERSION OF LIGNIN FIRST TO CHEMICAL SYNTHONS FOR MAKING MATERIALS AND FUELS

[EFRC – C3Bio]
Mahdi M. Abu-Omar[1], Rebecca Key[2], Will Hartwig[2], Derek Vardon[3], Ximing Zhang[4], Hanyu Zhu[4], Ernesto Zuleta[2], Gregg T. Beckham[3], Joseph J. Bozell[2], Clint C. S. Chapple[4], Hilkka I. Kenttämaa[4], Richard Meilan[4], Nathan S. Mosier[4]
[1]*University of California Santa Barbara;* [2]*University of Tennessee;* [3]*National Renewable Energy Lab;* [4]*Purdue University*

While current biorefinery processes use lignin for its heat value, the conversion of lignin to chemical synthons is an area of emerging interest. We developed transition metal catalysts that are suitable for upgrading lignin directly from lignocellulosic biomass to phenolic molecules. Spectroscopic data coupled with mechanistic investigations revealed the roles of solvent and catalyst in this unique extractive-reaction, which provides high value from lignin. Comparison of wood versus grass species enabled access to synthons with different functionality. Optimal conditions gave over 68% yield of select aromatic products from lignin. After catalytic depolymerization of lignin and upgrading (CDL), the carbohydrates were recovered as a solid residue, accessible for further chemical or biochemical catalytic processing. Overall, 55% of biomass is converted into chemical synthons and closing the mass balance to 98%. We used dynamic nuclear polarization (DNP)-enhanced solid-state (SS)NMR, a technique enabling the measurement of 2D homonuclear ^{13}C-^{13}C correlation SSNMR spectra under natural abundance, to yield, for the first time, an atomic-level picture of the structure of raw and catalytically treated biomass samples. We also explored upgrading lignin by direct catalytic oxidation using metal Schiff base complexes and found catalytic performance is correlated with the level of organization at the metal center. We are synthesizing catalysts that both improve delivery of the substrate to the catalyst as well as delivering the catalyst to the substrate. The implication of CDL on the future biorefinery and use of lignin-derived synthons in making materials will be discussed.

11:00 AM

C-III-2: METAL-FREE CLEAVAGE OF C-O BONDS TO FORM ADIPIC ACID FROM BIOMASS DERIVATIVES

[EFRC – CCEI] Matthew J. Gilkey,[1] Alexander V. Mironenko,[1] Dionisios G. Vlachos,[1] Bingjun Xu[1]
[1]*University of Delaware*

A central challenge in biomass valorization is the selective removal of oxygen-containing functional groups from platform chemicals, e.g., 5-hydroxymethylfurfural, to valuable chemicals without overhydrogenating the substrate to undesired products. Supported metal or metal oxide catalysts have shown promise in removing C-O bonds; however, many catalytically active metals/metal oxides are economically costly and can lead to major selectivity challenges, such as overhydrogenation or C-C cracking. Recently, we have developed a system for the selective removal of C-O single bonds in tetrahydrofuran-2,5-dicarboxylic acid (THFDCA), through employment of hydriodic acid (HI) with molecular H_2 in organic acid solvents, to form adipic acid (AA), a key polymer precursor. In this system, cleavage of C-OH and ether bonds occurs readily without reducing higher order oxygenated functional groups such as carboxylic acids, achieving an AA yield of 89% in the absence of any metal catalyst. In this work, we demonstrate key mechanistic insights in THFDCA hydrogenolysis to AA via computational input, kinetic measurements, and reactivity data, where we shed light onto the interplay between HI, molecular

H_2, and the organic acid solvent. Based on our mechanistic understanding, we propose directions for rational catalyst design to enhance AA yield from THFDCA.

11:20 AM

C-III-3: FAST HYDROPYROLYSIS, CATALYTIC CONVERSION AND IN SITU HYDRODEOXYGENATION PRODUCE DROP-IN HYDROCARBON FUELS FROM BIOMASS

[EFRC – C3Bio] Hilkka I. Kenttämaa, Richard Caulkins, Taufik Ridha, Mckay Easton, Priya Murria, Abhijit Talpade, Zaikuan Yu, Rakesh Agrawal, Fabio H. Ribeiro, W. Nicholas Delgass

Purdue University

Fast-pyrolysis is a potentially viable approach to produce fuels and fuel precursors by thermal fragmentation of biomass. The combined expertise in process systems analysis, reactor design, chemical kinetics, organic synthesis, advanced analytical methods, and high-level quantum chemical calculations has allowed C3Bio to create a detailed understanding of how fast-hydropyrolysis and *in situ* hydrodeoxygenation (HDO) of biomass in the presence of appropriate catalyst(s) can lead to drop-in hydrocarbon fuels. The mechanisms of the reactions occurring during fast pyrolysis have been delineated using isotopically labeled model compounds and theoretical calculations. These studies have demonstrated unambiguously that fast pyrolysis of cellulose, xylan, and lignin are not radical processes, as commonly assumed in literature. The fast pyrolysis products have been quantified using a combination of novel lab-scale reactors, chromatography techniques, and mass spectrometry. These studies revealed that the theoretically proposed mechanisms remain valid for scaled-up reactors. Further, the finding that levoglucosan and glycolaldehyde are the most abundant fast pyrolysis products of cellulose has inspired targeted theoretical and experimental research into upgrading of these molecules. Our results suggest that the opportunity for taking advantage of tailored biomass structures and chemically-driven variations in pyrolysis product distributions is by routes other than direct HDO. For example, we have shown that vapor phase aldol condensation of pyrolysis oxygenates before the HDO step increases the carbon chain length of reaction products. We are in the process of developing a multi-phase kinetic model for fast-pyrolysis processes to enable better reactor design for optimized selectivity to desired products.

11:40 AM

C-III-4: TUNABLE SYNTHESIS OF OLEO-FURAN SURFACTANTS VIA ACYLATION OF BIOMASS-DERIVED FURANS

[EFRC – CCEI] Kristeen E. Joseph[1], Dae Sung Park[1], Christoph Krumm[2], Michael Tsapatsis[1], Raul F. Lobo[3], Dionisios G. Vlachos[3,] Paul J. Dauenhauer[1]

[1]University of Minnesota; [2]Sironix Renewables; [3]University of Delaware, Newark

In this talk, we will present a new, renewable pathway to produce surfactants from biomass-derived feedstocks such as furans from sugars and lauric acid obtained from the hydrolysis of triglycerides found in natural oils. The key enabling chemistry entails acylation of furan with lauric acid or anhydride in the presence of heterogenous catalysts such as zeolites, or homogenous catalysts such as trifluoroacetic anhydride. Our studies show that the zeolite pore size, structure and acidity have a profound effect on the acylation of furan with lauric anhydride. The acylated furan can subsequently be upgraded via several independent and sequential chemistries such as etherification, hydrogenation and aldol condensation and finally be subjected to sulfonation to form a new class of surfactants, oleo-furan sulfonate (OFS), in high yield. Evaluation of surfactant performance of the OFS revealed hundredfold better detergency and stability in hard water conditions in comparison with petroleum-derived counterparts. The synthesis of OFS molecules is highly tunable and selective where the number of carbon atoms in the linear or branched chain can be easily varied to achieve the desired surfactant properties, without compromising reaction yields.

SESSION IV: TUESDAY, JULY 25, 2017; 1:30 – 3:30PM; THURGOOD MARSHALL NORTH

1:30 PM

C-IV-1: ADVANCING MOLECULAR ELECTROCATALYSIS USING LINEAR FREE ENERGY RELATIONSHIPS

[EFRC – CME] James M. Mayer[1], Michael Pegis[1], Catherine F. Wise[1], Daniel J. Martin[1], Neeraj Kumar[2], Simone Raugei[2], Larry Wang[3], Colin W. Anson[3], James B. Gerken[3], Shannon S. Stahl[3], Zach Goldsmith[4], Sharon Hammes-Schiffer[4], Eric S. Weidner[2], Aaron M. Appel[2], R. Morris Bullock[2]
[1]Yale University; [2]Pacific Northwest National Laboratory; [3]University of Wisconsin-Madison; [4]University of Illinois Urbana-Champaign

Studies of molecular catalysts of electrochemical reactions provide fundamental understanding through structure-activity relationships and the basis for development of catalysts that operate at high turnover frequencies (TOFs), low overpotentials (η), and high selectivity. The CME has developed tools to compare different catalysts under different conditions, enabling unprecedented understanding of the molecular electrocatalysis. Studies of the oxygen reduction reaction (ORR) and the hydrogen evolution reaction (HER) have frequently found correlations between the TOF and the effective overpotential (η_{eff}) for sets of related homogeneous catalysts. Examples include iron porphyrin complexes and cobalt macrocycles for the ORR, and nickel amino-phosphines for the HER. These scaling relationships can have quite different slopes (decades of TOF per Volt of η_{eff}). Experimental, computational and theoretical examinations show that these slopes provide fundamental insights into catalytic mechanisms and design principles. The computational studies provide insight into catalysis at the level of individual electron transfer, proton transfer, and other critical reaction steps. The analysis predicts how catalytic systems can be improved using the different slopes of the scaling relationships. This approach is applicable to all multistep proton-coupled electron transfer molecular electrocatalytic processes, such as CO_2 and N_2 reductions, under different conditions. It is being extended to catalytic selectivity, both for different paths from the same reactant and to competition between different reactants (e.g., reduction of N_2 vs. H^+).

1:50 PM

C-IV-2: LIGHT DRIVEN N-H AND C-H BOND FORMATION BY NITROGENASE

[EFRC – BETCy] Lance C. Seefeldt[1], Caroline S. Harwood[2], Yanning Zheng[2], Derek F. Harris[1], Saroj Poudel[3], Rhesa N. Ledbetter[1], Kathryn R. Fixen[2], Zhi-Yong Yang[1], John W. Peters[3,4], Paul W. King[5], and Eric S. Boyd[3]
[1]Utah State University; [2]University of Washington; [3]Montana State University; [4]Washington State University; [5]National Renewable Energy Laboratory

One of the goals in BETCy is to understand how chemical bond energy is used to drive very difficult reduction reactions, with nitrogenase reduction of N_2 to N-H and CO_2 to C-H containing compounds as the paradigm. These reactions normally require ATP and electrons derived from metabolism and the oxidation of sugars. We have discovered ways to provide the energy to drive these reactions using light, both using photosynthetic microbes and biohybrids between nitrogenase and light harvesting CdS nanorods. These studies are providing foundational knowledge about how to utilize energy, including light, to drive these difficult reduction reactions.

2:10 PM

C-IV-3: A GENERAL APPROACH FOR GENERATION OF CATALYTIC HIGH VALENT METAL OXO SPECIES REVEALS PHOTOINDUCED ONE ELECTRON, TWO PROTON TRANSFER REACTIVITY

[EFRC – UNC] Ke Hu, Renato N. Sampaio, Seth L. Marquard, M. Kyle Brennaman, Yusuke Tamaki,
Thomas J. Meyer and Gerald J. Meyer
University of North Carolina at Chapel Hill

A new strategy is reported that enables one to efficiently generate the high valent metal oxo species critical to biological and artificial oxidation catalysis. The strategy is photochemical and utilizes a chromophore or 'sensitizer' and a catalyst anchored to a semiconducting metal oxide surface that is equilibrated with a redox buffer that poises the catalyst's initial protonation and oxidation state. The photo-excited sensitizer injects an electron into the metal oxide and then oxidizes the catalyst whose subsequent reactivity occurs in kinetic competition with back electron transfer. With low sensitizer and catalyst surface coverages a novel trapping process will be reported that inhibits back electron transfer and enables quantification of catalytic reactivity on the nanosecond to hours timescales. Such slow recombination in the absence of the redox buffer allows for the first application of this approach and the realization of a light-driven $1e^-$, $2H^+$ reaction to yield a $Ru^{IV}=O$ species with $k = 0.036\ s^{-1}$, $k_H/k_D = 0.63$, and $\Delta G^o = -70$ meV. The kinetic data also reveal an order of magnitude decrease in charge recombination rate constants that result from having a SnO_2 core with a TiO_2 shell, relative to TiO_2 alone. An almost two order of magnitude increase in the recombination rate constant is observed when all of the catalysts are pre-oxidized by one electron and hence act as electron acceptors. This observation suggests that site isolation of catalysts with high turnover frequencies will be most efficient for light-driven water oxidation.

2:30 PM

C-IV-4: THEORY AND COMPUTATION WORKING WITH EXPERIMENT TO UNDERSTAND AND IMPROVE WATER SPLITTING CATALYSTS

[EFRC – CCDM] D.R. Strongin[1], E. Borguet[1], L. Cao[2], Q. Kang[1], M.L. Klein[1], H. Peng[1], J.P. Perdew[1], R.C. Remsing[1], J. Sun[3], A.C. Thenuwara[1], Q. Yan[1] and M.J. Zdilla[1]
[1]*Temple University,* [2]*North Carolina State University,* [3]*University of Texas-El Paso*

Optimizing catalysts for the oxygen evolution reaction (OER) and hydrogen evolution reaction (HER) plays a central role in water splitting chemistry. The theoretical and computational expertise in the Center for Computational Design of Functional Layered Materials (CCDM) has guided the design of active catalysts for the OER and HER. Importantly, the feedback between theory/computation and experiment validates many of the theoretical and computational developments in the CCDM. To illustrate this synergy, this presentation will highlight how the integration of theory, computation [1], and experiment has led to a new paradigm in the design of water splitting catalysts. In particular, it is shown how this integrated research effort has led to the realization that the confinement of metal ions (active for OER) in the interlayer region of 2D layered metal oxide materials can promote complex dipolar interactions between the metal cations, water, and 2D material and this can lead to improved OER catalysis [2]. Also presented will be how this synergy between theory, computation, and experiment has led to new insights into catalysis on MoS_2 for the HER.

[1] Kang, Q.; Vernisse, L.; Remsing, R. C.; Thenuwara, A.C.; Shumlas, S. L.; McKendry, I.G.; Klein, M.L.; Borguet, E.; Zdilla, M.J.; and Strongin, D.R.: *JACS* 139 (5), 1863 (2017).

[2] Thenuwara, A.C.; Cerkez, E.B.; Shumlas, S.L.; Attanayake, N.H.; McKendry, I.G.; Frazer, L.; Borguet, E.; Kang, Q.; Remsing, R.C.; Klein, M.L.; Zdilla, M.J.; and Strongin, D.R.: *Angewandte Chemie* 55 (35), 10381 (2016).

2:50 PM

C-IV-5: DEVELOPMENT OF MOLECULAR MEDIATORS FOR IMPROVED ELECTROCHEMICAL ENERGY CONVERSION

[EFRC – CME] Shannon S. Stahl[1], James B. Gerken[1], Colin W. Anson[1], Sharon Hammes-Schiffer[2], Soumya Ghosh[2], Mioy T. Huynh[2], Catherine F. Wise[3], James M. Mayer[3]
[1]University of Wisconsin-Madison; [2]University of Illinois at Urbana-Champaign; [3]Yale University

Molecular catalysts have been widely investigated for electrochemical energy conversion, and strategies for practical implementation of these catalysts typically focus on catalyst immobilization or tethering to the electrode surface. The use of soluble redox mediators offers an alternative strategy for efficient interconversion of electrical and chemical energy, particularly for complex transformations involving multiple electron and proton transfer steps, such as those with O_2, N_2 and CO_2. Recent efforts in the CME have begun to provide fundamental insights into the use of electron- and electron-proton-transfer mediators to achieve efficiency in the electrochemical reduction of O_2. Highlights from this work include identification of a metal-free nitroxyl/NO_x mediator/catalyst system that achieves the oxygen reduction reaction (ORR) with a lower overpotential than heterogeneous Pt catalysts. The effectiveness of this system arises from cooperativity between the mediator and catalyst that overcomes kinetic inefficiencies associated with its individual components. Quinones are a particularly appealing class of mediators because they are capable of coupling proton and electron transfer, thereby providing the basis for more efficient redox transformations. A mediator/catalyst system consisting of benzoquinone in combination with Co(salophen) demonstrates this concept and highlights opportunities to improve electrocatalytic performance through tuning of the quinone mediator, rather than the O_2 reduction catalyst. Fundamental and practical advances in the use of quinone-mediated electrochemical transformations will be described.

3:10 PM

C-IV-6: UNDERSTANDING TRENDS IN CO_2 REDUCTION ELECTRO-CATALYSIS

[Hub – JCAP] Karen Chan[1] and Jens K. Nørskov[1]
[1]SLAC National Accelerator Laboratory

A framework is presented for understanding trends in electrocatalytic activity for CO_2 reduction over different metal catalysts. The model rationalizes a number of experimental observations including the selectivity with respect to the competing hydrogen evolution reaction. It also provides design criteria for new catalysts. The understanding is based on density functional theory calculations of potential dependent activation energies and energies of key intermediates combined with an electrochemical kinetic model of the process.

D. ENERGY STORAGE

SESSION I: MONDAY, JULY 24, 2017; 3:00 – 5:00PM; THURGOOD MARSHALL EAST

3:00 PM

D-I-1: EXPLOITING "PASSIVE MATERIALS" IN ELECTROCHEMICAL ENERGY STORAGE SYSTEMS: THE SIGNIFICANT IMPACTS OF HARD MATERIAL – SOFT MATERIAL INTERACTIONS AND MESOSCALE ELECTRODE STRUCTURE ON FUNCTIONAL ELECTROCHEMISTRY

[EFRC – m2M] Lei Wang[1], Ye Shi[2], Xingyi Zhou[2], Jun Zhang[2], Andrew Bond[2], Yo Han Kwon[3], Krysten Minnici[3], Dalsu Choi[3], Mincheol Chang[3], Crystal Lewis[1], Matthew Huie[1], Yiman Zhang[1], Yue Ru Li[1], Andrea Bruck[1], Shihui Zou[1], Megan Scofield[1], Shiyu Yue[1], Coray McBean[1], Jing Li[1], Elsa Reichmanis[3], Stanislaus Wong[1], Eric Stach[4], Kenneth Takeuchi[1], Esther Takeuchi[1], Amy Marschilok[1], Guihua Yu[2].

[1]Stony Brook University, [2]University of Texas at Austin, [3]Georgia Institute of Technology, [4]Brookhaven National Laboratory.

Battery electrodes are most typically prepared by physically mixing "soft" passive materials (carbon conductive additives and non-conductive polymeric binders) with "hard" electroactive materials (inorganic oxides or polyanion framework materials) in a slurry or paste which is tape cast onto a metallic foil current collector to form a composite electrode. While the passive components do not contribute directly to theoretical energy density, their inherent physical and chemical properties, and the way they interact with the active material in the composite electrode can play a critical deterministic role regarding the functional electrochemistry of the energy storage system. Since percolation occurs when a three-dimensional interconnected conducting network is formed throughout a composite, intuition dictates that use of the minimum quantity of conductive additive necessary to develop a percolation network is the goal. However, the hard material-soft material interactions can manifest over multiple length scales, presenting a practical challenge in understanding the locations of localized resistance and addressing these through deliberate electrode design. We will illustrate the importance of considering electrical conductivity, electron transfer, and ion transport in the design of environments incorporating active materials. Specific advances achieved through control of hard material-soft material attachment modalities, control of mesoscale electrode structure and processing, and design of novel electrode architectures will be highlighted.

3:20 PM

D-I-2: INTEGRATED EXPERIMENTAL-COMPUTATIONAL INVESTIGATION OF TRANSPORT KINETICS IN POLYCRYSTALLINE BATTERY-ELECTRODE PARTICLES

[EFRC – NECCES] Ping-Chung Tsai[1], Min-Ju Choe[2], Bohua Wen[1], Hui-Chia Yu[2], Nicholas Faenza[3], Nathalie Pereira[3], Mark Wolf[4], Jordi Cabana[4], Glenn Amatucci[3], Katsuyo Thornton[2]& Yet-Ming Chiang[1].
[1]Massachusetts Institute of Technology; [2]University of Michigan; [3]Rutgers, The State University of New Jersey; [4]University of Illinois at Chicago

Kinetic parameters such as interfacial reaction constants and bulk diffusivity have a critical influence on capacity utilization and rate-performance in lithium ion batteries. In typical cells, electrodes have a complex architecture composed of active materials, binders, and conductive agents, posing a great challenge in extracting the intrinsic kinetic parameters of the electrode-active materials. In this work, we are executing an integrated experimental-computational investigation of the electrochemical behavior of single secondary particles, with the goal of directly measuring particle-level kinetics and elucidating factors that determine electrochemical performance and degradation. $Li_{1-x}Ni_{0.8}Co_{0.15}Al_{0.05}O_2$ (NCA) and $Li_{1-x}Ni_{0.33}Co_{0.33}Mn_{0.33}O_2$ (NCM333) are studied as model cathode materials, common across our EFRC. Single-particle kinetic parameters, including bulk diffusivity and exchange current density, are systematically investigated as a function of state-of-charge and particle size, using electrochemical impedance spectroscopy and potentiostatic intermittent titration technique. Transmission X-ray microscopy is simultaneously used to image physical changes in the particles. In coordination with the experiments, single-particle electrochemical simulations under corresponding conditions are performed, taking the particle geometry, interfacial transport, and surface reactions into account. The synergic integration of experiments and simulations enables examination and interpretation of the bulk and interfacial kinetics of NCA single particles. Furthermore, the simulations show how particle morphology and surface area affect the diffusional impedance behavior. It is demonstrated that the impedance response at varying frequencies yields morphological information about the single particle.

3:40 PM – Team Science Finalist

D-I-3: UNDERSTANDING ROOM TEMPERATURE IONIC LIQUIDS AND THEIR PERFORMANCE IN SUPERCAPACITORS

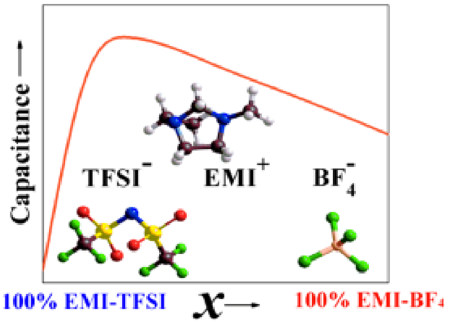
[EFRC – FIRST] Justin Neal[1], Kun Liu[1], Naresh Osti[2], Matthew W. Thompson[3], Katherine Van Aken[4], Yu Zhang[3]

[1]University of California, Riverside, [2]Spallation Neutron Source, Oak Ridge National Laboratory, [3]Vanderbilt University, [4]Drexel University

These graduate students and postdoctoral associates from four of the FIRST Center partner institutions have self-organized into a highly effective team to develop fundamental and predictive understanding of the physicochemical properties of a selection of room temperature ionic liquids and their behavior and performance in nanoporous carbon supercapacitor electrode materials. Through physical meetings at Drexel, ORNL, and U.C. Riverside, as well as numerous teleconferences, they have, with minimal supervision, mapped out and executed a comprehensive research plan that is ongoing, and have published a number of recent joint papers[1-7] briefly summarized below. The team also includes several students and postdoctoral fellows who have now moved on (*e.g.* Cheng Lian and Boris Dyatkin).

Room temperature ionic liquids (RTILs) are a class of molten salts that are liquid at room temperature. Their low vapor pressure and electrochemical stability over a wide voltage window make them viable electrolytes for capacitive energy store. Here, we combine multiscale modeling, electrochemistry, and neutron scattering experiments to probe the fundamental properties of RTILs and how deviations from ideality at the nanoscale affect macroscale properties and capacitive performance.

Classical Density Functional Theory (cDFT) models (figure) predicted that a 20:80 ratio of BF_4^- and Tf_2N^- anions with a common $EMIM^+$ cation exhibited a maximum capacitance over a range of compositions. This result was later confirmed with electrochemistry experiments. cDFT models predict that small concentrations of impurities can boost capacitance energy storage by altering ion affinities and counter-ion adsorption. Molecular dynamics (MD) simulations and cDFT models together predict ion partitioning effects in which larger and smaller ions preferential adsorb into larger and smaller pores, respectively, which help explain capacitance increases observed in electrochemistry experiments.



Quasi-elastic neutron scattering (QENS) measurements revealed the nano-phase separation of an ionic liquid into ionic liquid-rich and solvent-rich phases with a greater diffusivity of ion by the solvent of a higher dipole moment. When confined in functionalized porous carbon, the diffusivity of cation increases significantly. QENS and MD simulations of ions under applied potential in nanoporous carbon demonstrated a totally reversible mechanism of ions immobilized in larger pores (6.7 nm) compared to smaller pores (1.5 nm). These and other emergent nanoconfined RTIL properties are discussed.

References: [1]B. Dyatkin, Y. Zhang, et al., *J. Phys. Chem. C* (2016) *120*:8730-8741. [2]C. Lian, K. Liu, K. Van Aken, et al., *ACS Energy Letters* (2016) *1(1)*:21-26. [3]K. Liu, J. Wu, *J. Phys. Chem. C* (2016) *120*:24041-24047. [4]K. Liu, C. Lian, et al., *Molecular Physics* (2017) *115*:454-464. [5]J. Neal, et al., *J. Chem. Phys.* (2017), *in press.* [6]N. Osti, K. Van Aken, M.W. Thompson, et al., *J. Phys. Chem. Lett.* (2017) *8*:167-171. [7]S.M. Mahurin, M.W. Thompson, et al., *Appl. Phys. Lett.* (2016) *109*:143111.

Contributions: J.N. and K.L. performed classical density functional theory simulations; N.O. conducted and analyzed neutron scattering experiments; M.W.T. and Y.Z. conducted classical molecular dynamics simulations; K.V.A. conducted electrochemical experiments.

4:00 PM

D-I-4: TAILORING POLYMERS OF INTRINSIC MICROPOROSITY TO MEET THE GROWING DEMANDS FOR FAST ION TRANSPORT IN ELECTROCHEMICAL ENERGY STORAGE DEVICES

[Hub – JCESR] Ashleigh L. Ward[1], Sean E. Doris[1], Longjun Li[1], Xiaohui Qu[1], Kristin A. Persson[1], Lin Ma[1], Miranda Baran[1], Jarrod Milshtein[2], Fikile R. Brushett[2], Jeffrey S. Moore[3], Koen Hendrick[4], Melanie S. Sanford[4], Liang Su[2], Yet-Ming Chiang[2], Brett A. Helms[1]

[1]Lawrence Berkeley National Laboratory; [2]Massachusetts Institute of Technology; [3]University of Illinois at Urbana-Champaign; [4]University of Michigan

Selective ion transport across membranes is critical to the performance of many electrochemical energy storage devices. While design strategies enabling ion-selective transport are well-established, enhancements in membrane selectivity are made at the expense of ionic conductivity. To design membranes with both high selectivity and high ionic conductivity, there are cues to follow from biological systems, where regulated transport of ions across membranes is achieved by transmembrane proteins. The transport functions of these proteins are sensitive to their environment: physical or chemical perturbations to that environment are met with an adaptive response. Here we advance an analogous strategy for achieving adaptive ion transport in microporous polymer membranes. Along the polymer backbone are placed redox-active switches that are activated *in situ*, at a prescribed electrochemical potential, by the device's active materials when they enter the membrane's pore. This transformation has little influence on the membrane's ionic conductivity; however, the active-material blocking ability of the membrane is enhanced. We show that when used in lithium–sulfur batteries, these membranes offer markedly improved capacity, efficiency, and cycle-life by sequestering polysulfides in the cathode. The origins and implications of this behavior are explored in detail and point to new opportunities for responsive membranes in battery technology development. In turn, I will describe how these discoveries have led to second generation platforms for a variety of other storage devices.

4:20 PM

D-I-5: CONTRIBUTIONS TO INTER- AND INTRA-ROD ION TRANSPORT IN TUNNEL STRUCTURED MATERIALS: IMPLICATIONS FOR ELECTROCHEMICAL ENERGY STORAGE

[EFRC – m2M] Jianping Huang[1], Altug Poyraz[2], Paul Smith[1], Bingjie Zhang[1], Lijun Wu[2], Xiaobing Hu[2], Seung-Yong Lee[2], Shaobo Cheng[2], Feng Xu[2], Qingping Meng[2], Jessica Durham[1], Merzuk Kaltak[1], Christopher Pelliccione[2], Mark Hybertsen[2], Maria Fernandez-Serra[1], Esther Takeuchi[1], Amy Marschilok[1], Yimei Zhu[2], Kenneth J. Takeuchi[1].

[1]Stony Brook University, [2]Brookhaven National Laboratory.

Tunnel structured manganese dioxide (α-MnO_2, $M_xMn_8O_{16}$) nanorods are interesting cathode materials as they can host various cations (i.e. M = Ag^+, K^+) and molecules (i.e. H_2O) within their 2 x 2 (0.46 x 0.46 nm) tunnels. Conceptually, such structures are appealing for study of one dimensional diffusion processes. However, elucidating the multiple ion transport pathways and local phase changes associated with electrochemical redox requires understanding the limitations for electron and ion transport, including delineation of inter- and intra-rod transport effects. Progress gained through directed synthesis and advanced local characterization will be discussed in this presentation.

4:40 PM

D-I-6: ELECTRICAL DOUBLE LAYER IN POROUS ELECTRODES – CAPACITANCE, CAPACITIVE MIXING, AND ELECTRO-OSMOSIS

[EFRC – FIRST] Cheng Lian[1], Justin N. Neal[1], Kun Liu[1], David J. Wesolowski[2], Douglas Henderson[3], Jianzhong Wu[1]
[1]University of California at Riverside; [2]Oak Ridge National Laboratory; [3]Brigham Young University

This talk presents an overview of our recent theoretical efforts directed at understanding the thermodynamic and transport properties of ionic species in charged micropores based on the classical density functional theory in combination with coarse-grained molecular models and continuous equations to describe fluid mechanics and reaction kinetics. Illustrative examples will be discussed on electrochemical capacitor performance in terms of the electrode pore size, shape and electrolyte composition, optimal operation parameters for capacitive energy extraction with porous electrodes, and the flow effects on ion transport and surface reactions in microchannels.

SESSION II: TUESDAY, JULY 25, 2017; 8:30 – 10:10 AM; THURGOOD MARSHALL EAST

8:30 AM – Team Science Finalist

D-II-1: THERMODYNAMIC STABILITY, VOLTAGE AND DIFFUSION KINETICS OF Li_xVOPO_4 (X=0,1,2) VANADYL PHOSPHATE POLYMORPHS: JOINT FIRST-PRINCIPLES AND EXPERIMENTAL STUDY

[EFRC – NECCES] Yuh-Chieh Lin,[1] Iek-Heng Chu,[1] Marc V. Hidalgo,[2] Carrie Siu,[2] Fredrick Omenya,[2] Natasha A. Chernova,[2] Linda W. Wangoh,[2] Shawn Sallis,[2] Louis F. J. Piper,[2] M. Stanley Whittingham,[1] Shyue Ping Ong[1]

[1]*University of California San Diego,* [2]*Binghamton University*

One of the goals of our center is to attain reversible multi-electron transfer in a cathode material using lithium. We focus on vanadyl phosphates because we can utilize both the $V^{3+/4+}$ and $V^{4+/5+}$ redox couples for a theoretical capacity of 318 mAh/g at about 2.5 and 4 V, respectively. The challenge of this system is its great structural diversity; there are seven known polymorphs of $VOPO_4$ and three for $LiVOPO_4$. No Li_2VOPO_4 has been synthesized directly up to now. In order to identify the most stable Li_xVOPO_4 (x=0,1,2) polymorphs, determine their Li intercalation potentials, diffusion pathways and kinetics, we have combined first-principle calculations with experimental studies involving synthesis, structural and electrochemical characterization of three $LiVOPO_4$ polymorphs. We have demonstrated excellent agreement between the calculated and experimental structures, Li intercalation voltages, and also correlated the calculated diffusion barriers with the electrochemical performance (Figure 1). Our studies reveal that β-$LiVOPO_4$, which was previously thought inferior to ε-$LiVOPO_4$, has comparable electrochemical performance. The significant difference between the two is intermediate low-voltage phases $Li_{1.5}VOPO_4$ and $Li_{1.75}VOPO_4$, which form in ε-, but not in β-$LiVOPO_4$. Using a combination of soft and hard absorption / photoelectron spectroscopy we have demonstrated that a prerequisite for the formation of these intermediates is a uniform distribution of Li, which is achieved when $LiVOPO_4$ is used as a starting material, and in this case full reversible cycling of the second Li can be realized.

Contributions: Y.-C.L. performed the first principles calculations, M.V.H. synthesized the samples and performed structural and electrochemical characterization, S.S. acquired and analyzed spectroscopy data. All nominees discussed the results.

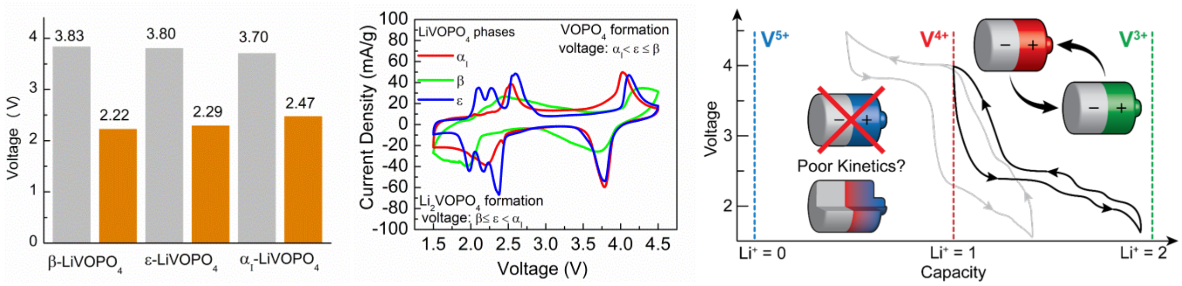


Figure 1 (left) Calculated and (middle) experimental voltages of $LiVOPO_4$ phases. Right: highlight of our ex-situ and operando depth-profile studies confirming full and homogenous second Li^+ insertion and extraction between ε-$LiVOPO_4$ and ε-Li_2VOPO_4 in the low voltage regime.

8:50 AM

D-II-2: ELECTROCHEMICALLY INDUCED PHASE EVOLUTION OF HIGH CAPACITY LAYERED MATERIALS: COMPLEMENTARY INSIGHTS GAINED VIA EXPERIMENT, DENSITY FUNCTIONAL THEORY, AND CONTINUUM MODELING

[EFRC – m2M] Alan West[1], Amy Marschilok[2], Qing Zhang[2], Nicholas Brady[1], Kevin Knehr[1], Alexander Brady[2], Christopher Pelliccione[3], David C. Bock[3], Andrea M. Bruck[2], Jing Li[2], Varun Sarbada[4], Robert Hull[4], Eric Stach[3], Kenneth Takeuchi[2], Ping Liu[3], Esther Takeuchi[3].
[1]Columbia University, [2]Stony Brook University, [3]Brookhaven National Laboratory, [4]Rensselaer Polytechnic Institute

$Li_{1.1}V_3O_8$ is a high capacity (362 mAhg-1) cathode material for Li-ion batteries. The structural evolution during electrochemical discharge and charge processes was investigated using a combination of theoretical calculations and experimental data. Density functional theory was used to predict the intermediate structures at various lithiation states as well as the stability of major phases. In-situ x-ray diffraction (XRD) data was collected as well as operando energy dispersive x-ray (EDXRD) data, allowing for the phase transformations to be monitored under load providing both phase and spatial evolution information. Rietveld refinement was performed to fit the diffraction data with the DFT-derived structures and to analyze the fractions of major phases as a function of dis(charge). Further, the electrochemical behavior of LiV_3O_8 during lithiation, delithiation, and voltage recovery experiments was simulated using a crystal-scale model that accounted for solid-state diffusion, charge-transfer kinetics, and phase transformations. The kinetic expression for phase change was modeled using an approach inspired by the Avrami formulation for nucleation and growth. Agreement between the simulated and experimental results is excellent. Thus, by integrating DFT calculations and continuum modeling with experimental work, a thorough understanding of $Li_{1.1}V_3O_8$ during electrochemical dis(charge) was obtained.

9:10 AM

D-II-3: ATOMISTIC STUDIES OF NUCLEATION AND GROWTH IN CONVERSION REACTIONS FOR LITHIUM-ION BATTERIES

[EFRC – CEES] Robert Warburton[1], Handan Yildirim[1], Maria Chan2, Jae Jin Kim[2], Tim Fister[2], Xiao Chen[2], Paul Fenter[2], Guennadi Evmenenko[3], Bruce Buchholz[3], Michael Bedzyk[3], Zhenpeng Yao[3], Christopher Wolverton[3], Qianqian Li[3], Fernando Castro[3], Xinqi Chen[3], Jinsong Wu[3], Vinayak Dravid[3], Jeffrey P. Greeley[1]
[1]Purdue University, [2]Argonne National Laboratory, [3]Northwestern University

Lithium-ion batteries represent an efficient and versatile energy storage medium, and within this broad class of materials, oxide conversion reactions yield battery electrodes with exceptionally high capacities in comparison to intercalation materials, with Li2O-encompassed transition metal nanoparticles as the ideal charge product. The NiO conversion reaction, in particular, has a high theoretical capacity (718 mAh g-1), but there is significant hysteresis between the experimental and theoretical voltage (0.6 V and 1.9 V, respectively), and the molecular origins of this hysteresis are poorly understood. In this work, we present an integrated computational modeling approach, using classical molecular dynamics, first principles density functional theory calculations, and classical nucleation theory, to directly probe the role of metal/oxide and oxide/oxide interfaces during NiO conversion. Different nucleation schemes are evaluated, considering potential-dependent bulk and interfacial free energies to determine critical nucleation radii and energy barriers, and the results are compared to additional calculations of homogeneous phase transformations that pass through metastable intermediate products. A careful energetic analysis

suggests that both conversion mechanisms may be active, a conclusion that is strongly supported by detailed in-situ x-ray reflectivity and atomic-scale TEM measurements.

9:30 AM

D-II-4: ADVANCES IN NMR METHODOLOGY OF PARAMAGNETIC LI-ION BATTERY CATHODE MATERIALS

[EFRC – NECCES] Ieuan D. Seymour[1], Nicole M. Trease[1], Sylvia Britto[1], Philip J. Reeves[1], Oliver Pecher[1], Paul M. Bayley[1], Maxwell D. Radin[2], Yuh-Chieh Lin[3], Iek-Heng Chu[3], Carrie Siu[4], Yong Shi[4], Haodong Liu[3], Hao Liu[5], Shyue Ping Ong[3], Natasha Chernova[4], Karena W. Chapman[5], Ying S. Meng[3], M. Stanley Whittingham[4], Anton Van der Ven[2] & Clare P. Grey[1]

[1]University of Cambridge; [2]University of California, Santa Barbara; [3]University of California San Diego; [4]Binghamton University; [5]Argonne National Laboratory

Solid-state nuclear magnetic resonance (NMR) is a powerful tool to understand the local structural, electronic and magnetic properties of Li-ion cathode materials. However, the presence of paramagnetic transition metal ions in the majority of conventional cathode systems can lead to significant broadening and highly shifted resonances in the resulting experimental NMR spectra, rendering their interpretation challenging. In recent years, it has been shown that the assignment of paramagnetic NMR spectra can be greatly aided by the use of first principles calculations, allowing a wealth of local structural information to be gained. We will demonstrate how the use of solid-state ^{27}Al and ^{7}Li NMR in combination with density functional theory (DFT) calculations can be used to understand the local distribution of metal ions and delithiation mechanism in $LiNi_{0.8}Co_{0.15}Al_{0.05}O_2$ (NCA). It will further be shown how the combination of ^{7}Li and ^{31}P NMR with first principles calculations can be used to determine the role of lithium disorder during delithiation in the structure of multi-electron cathode material, ε-$LiVOPO_4$. The application of this combined methodology to study the local oxygen environment in layered cathode materials through the use of ^{17}O NMR, a conventionally challenging NMR nucleus, will also be discussed. Finally, we will highlight recent developments in the use of in-situ NMR for the study of local changes on electrochemical cycling of paramagnetic Li-ion battery materials.

9:50 AM

D-II-5: HETEROGENEITY OF CHARGE STORAGE PROCESSES IN ELECTROCHEMICAL CAPACITORS

[EFRC – FIRST] Qiang Gao[1], Wan-Yu Tsai[1], Michael Naguib[1], Nina Balke[1], Paul Fenter[2], Matthew Thompson[3], Peter Cummings[3]

[1]Oak Ridge National Laboratory; [2]Argonne National Laboratory; [3]Vanderbilt University

Electrochemical capacitors (ECs) form an important component of energy storage solutions besides batteries. Charge storage processes in ECs are determined by two main processes: 1) the intercalation of ions into the electrode and 2) the formation of the electric double layer (EDL). Little is known about the nanoscale heterogeneity of these processes and how they link to the overall chare storage properties and kinetics. The first process depends strongly on the microstructure of the electrode and is considered being responsible for performance limitations. The ion intercalation and its heterogeneities can be imaged through the changes in mechanical electrode properties using scanning probe microscopy (SPM) revealing strong variations in active sample volume. This process can be strongly influenced by synergistic effects of co-ion intercalation. The formation of the EDL was believed to be a straightforward process with no effect on the kinetics of ECs. However, recent X-ray scattering for ionic liquid electrolytes results show slow relaxation components and the presence of domains during the re-arrangement of ions in the EDL as response to a change in applied potential. SPM was used to prove the presence of those structural domains in three dimensions and explore their behavior under bias. Complementary molecular dynamics (MD) simulations are used to explore the origin of the structural domains in the EDL. The study of nanoscale heterogeneities of energy storage processes in ECs using SPM provides a pathway to fundamental understanding of how capacitors work and how to modify their performance.

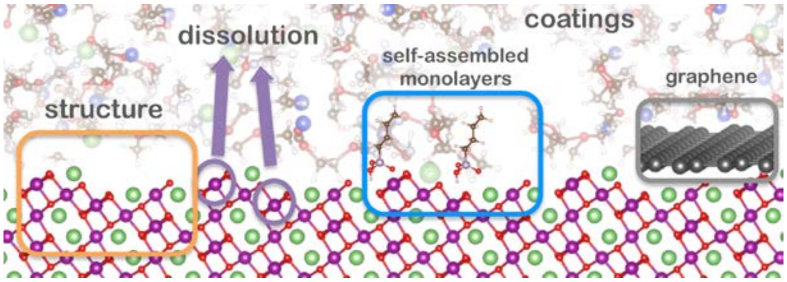
SESSION III: TUESDAY, JULY 25, 2017; 10:40 AM – 12:00PM; THURGOOD MARSHALL EAST

10:40 AM – Team Science Finalist

D-III-1: UNDERSTANDING AND CONTROLLING THE REACTIVITY OF $LiMn_2O_4$-ELECTROLYTE INTERFACES

[EFRC – CEES] Robert Warburton[1], Bruno Nicolau[2], Kendra Letchworth-Weaver[4], Kan-Sheng Chen[3], Aaron Petronico[2], Laila Jaber-Ansari[3], Xiao Chen[4], Yasaman Ghadar,[4] Maria Chan[4], Ralph Nuzzo[2], Andrew Gewirth[2], Jeffrey P. Greeley[1], Mark Hersam[3], Paul Fenter[4]

[1]Purdue University, [2]University of Illinois, [3]Northwestern University, [4]Argonne National Laboratory



The spinel $Li_xMn_2O_4$ ("LMO") is a commercial lithium ion battery cathode material whose use is limited by instabilities at the cathode-electrolyte interface. Specifically, LMO undergoes a disproportionation reaction, 2 Mn(III) → Mn(II) + Mn(IV) for $x \geq 1$ where the presence of Mn(II) at the interface is believed to lead to cathode dissolution. These cathode-electrolyte interface reactions are poorly understood and conceptual advances that enable robust mitigation strategies are needed.

In this context, CEES has been working to develop a suite of experimental and conceptual strategies for understanding and controlling this reactivity through coordinated studies of well-defined model systems. The foundation for these studies is a robust understanding of the structure and stability of the different LMO facets. This is obtained by density functional theory (DFT), revealing that the LMO(111) surface facet is the most stable. X-ray reflectivity measurements of model LMO(111) thin film electrodes confirms their use as model electrodes, including the observation of Mn loss upon lithiation for $x>1$ revealing that this chemical instability is observed even in these ideal systems. Phosphonic acid self-assembled monolayers ("SAMs") were used to create artificial cathode electrolyte interface ("CEI") layers at LMO-electrolyte interfaces, in which the length and functionality of the SAM molecule was used to tune the competing needs of maximizing Li ion conductivity but minimizing secondary reactivity. The observed trends in contact angles and cyclic voltammetry were understood using DFT coupled with a continuum electrolyte description that captures the formation of a stable CEI and the interaction of these layers with the electrolyte. This conceptual advance associated with separating charge and ion transfer functionalities was used to create a composite nanostructured graphene/LMO cathode morphology whose improved properties in a working lithium ion battery cell were demonstrated in both half- and full-cell geometries.

Contributions: Warburton and Greeley performed DFT calculations of the structure and relative stability of LMO interfaces. Chen and Fenter probed the structure and reactivity of model LMO thin-film materials under electrochemical control. Nicolau and Gewirth performed experimental studies of the design of model CEI compounds that control the reactivity of LMO. Letchworth-Weaver, Ghadar, and Chan performed computational studies to understand the suppression of LMO dissolution through the choice of model CEI. Chen and Hersam demonstrated that graphene-coatings in composite electrode are effective at suppressing these chemical instabilities.

11:00 AM

D-III-2: VAPOR PHASE CHEMISTRY FOR PROTECTION LAYERS AND SOLID-STATE 3D BATTERIES

[EFRC – NEES] Keith E. Gregorczyk[1], Alexander Pearse[1], Elliot Fuller[2], Chuan-Fu Lin[1], Dave Steward[1], Malachi Noked[3], Alec Talin[2], Gary Rubloff[1]
[1]University of Maryland; [2]Sandia National Laboratories; [3]Bar-llan University

Vapor phase deposition methods have several unique advantages exploited in a broad range of application spaces. Methods such as atomic layer deposition (ALD), molecular layer deposition (MLD), and chemical vapor deposition (CVD) are uniquely conformal, i.e. able to coat all sides of complex 3D architectures, often have low reaction temperatures, and a broad range of reaction chemistries. The properties of these methods have led to a significant amount of research aimed at exploring energy storage applications. This talk will discuss two of these applications.

Protection layers have garnered substantial interest in Li-ion liquid electrolyte and next generation systems (Li-S, Na, etc.). Ultra-thin layers of Al_2O_3, TiN, TaN, and LiPON have been deposited on a large variety of electrodes including composites, and various nanostructures, and have shown improvements in cell cycling life as well as a variety of other metrics. Here we will review the large amount of protection layer work that has been done in NEES.

3D solid-state batteries (3DSSB) have been discussed since at least 2004. It has been shown that increasing the surface area per unit foot print area can dramatically increase the energy density of thin-film systems without loss to power density. Fabricating such devices, however, has proven to be very difficult and has only recently been accomplished. Any method used must be inherently conformal making vapor phase process attractive. In this second section of the talk we will discuss the first 3DSSB fabricated with entirely conformal processes. including materials development and interface engineering.

11:20 AM

D-III-3: POLYSULFIDE SOLUBILITY SUPPRESSION THROUGH ELECTROLYTE REDESIGN AS A PATH TOWARD PRACTICAL LITHIUM - SULFUR BATTERIES

[Hub – JCESR] Changwook Lee[1], Seungbum Ha[1], Lei Cheng[1], Sang Don Han[1], Mahalingam Balasubramanian[1], Kevin G. Gallagher[1], Quanquang Pang[2], Linda F. Nazar[2], Heng-Liang Wu[3], Minjeong Shin[3], Kim A. See[3], Andrew A. Gewirth[3], Tylan Watkins[4], Kevin R. Zavadil[4]
[1]Argonne National Laboratory; [2]University of Waterloo; [3]University of Illinois at Urbana-Champaign; [4]Sandia National Laboratories

Creating cost competitive, high energy content, and long cycle life lithium – sulfur batteries requires designing for and stabilizing performance at reduced electrolyte content, increased sulfur utilization, and reduced excess lithium metal.[1] Reducing the electrolyte volume fraction poses problems for the standard mixed ether electrolyte as the solution mediated reaction pathway requires sufficient quantity of polysulfide intermediates to mediate the sulfur - sulfide interconversion. Premature saturation and cathode passivation result when the electrolyte volume fraction is reduced to a competitive level, which highlights the importance of successful precipitation/dissolution management.[2] Designing electrolytes that are sparingly solvating of polysulfides offers a unique opportunity to manage product formation by redirecting the redox reaction pathway.[3] The Joint Center for Energy Storage Research has recently demonstrated that the sulfur discharge reaction is redirected as a semi-solid state reaction in a solvate electrolyte.[4] A sufficient reduction in polysulfide solubility is shown to be the primary driver for pathway change. The nature of polysulfide solubility is probed through joint experimental and computational characterization for several solvate electrolytes and correlated with electrochemical performance.[5] The extracted design principles for sparingly solvating electrolytes and the ability to manage precipitation/dissolution processes in the Li-S sulfur system will be discussed in this presentation.

[1] D. Eroglu, et al. *J Electrochem Soc* **2015**, 162, A982
[2] J. Chen, et al. *Nano Lett* **2017**, 17, 3061
[3] L. Cheng, et al. *ACS Energy Lett* **2016**, 1, 503
[4] C.-W. Lee, et al. *ACS Central Sci* **2017**, accepted
[5] K.A. See, et al. ACS Appl Mater **2016**, 8, 34360

11:40 AM

D-III-4: INTERFACIAL PROPERTIES OF GRAPHENE/LITHIUM MANGANESE OXIDE SPINEL CATHODES FOR LITHIUM-ION BATTERIES

[EFRC – CEES] Kan-Sheng Chen[1], Laila Jaber-Ansari[1], Rui Xu[2], Soo Kim[1], Norman S. Luu[1], Ethan B. Secor[1], Koichi Hamamoto[1], Qianqian Li[1], Jinsong Wu[1], Xiankai Yu[1], Hakim Iddir[2], Larry A. Curtiss[2], Vinayak P. Dravid[1], Scott A. Barnett[1], Chris Wolverton[1], Jun Lu[2], Khalil Amine[2], and Mark C. Hersam[1]
[1]Northwestern University, [2]Argonne National Laboratory

Spinel-structured lithium manganese oxide (LMO) is a desirable cathode material for Li-ion batteries due to its low cost, earth abundance, and high power capability. However, its cycling stability is limited by manganese dissolution at the LMO/electrolyte interface. Here, single-layer graphene (Gr) coatings are shown to effectively suppress manganese dissolution, thereby substantially improving the long-term cycling stability of LMO thin-film cathodes. X-ray photoelectron spectroscopy depth profiling and cross-section transmission electron microscopy were utilized to probe chemical and structural changes at the Gr/LMO interface, confirming the suppressed dissolution of manganese in addition to a thin and well-defined solid-electrolyte interphase (SEI) layer. Density functional theory calculations corroborate these experimental results by revealing that graphene serves as an ion-selective diffusion barrier in addition to influencing the oxidation state of manganese at the LMO surface. The Gr/LMO scheme was also extended to Gr/nano-LMO composite cathodes, where few-layered graphene flakes comformally wrap LMO nanoparticles. Similar to the thin film results, Gr/nano-LMO composite cathodes also exhibit superior cycling stability relative to conventional carbon black/LMO control samples. While inductively coupled plasma mass spectrometry indicates suppressed Mn dissolution from the Gr/nano-LMO composite cathode, galvanostatic voltage profile and impedance spectroscopy analysis also suggest that the improved cycling stability of the composite cathode can be attributed to the comparatively low and invariant charge transfer resistance at the Gr/nano-LMO interface. Finally, this talk will show that the Gr/nano-LMO interface provides morphological advantages that enhance electrochemical kinetics, resulting in superlative rate capability and low-temperature performance.

SESSION IV: TUESDAY, JULY 25, 2017; 1:30 – 3:30PM; THURGOOD MARSHALL EAST

1:30 PM

D-IV-1: VERSATILE MACROMOLECULAR DESIGN FOR EMERGING SIZE-SELECTIVE NON-AQUEOUS REDOX FLOW BATTERIES

[Hub – JCESR] Jeffrey S. Moore[1], Kyle C. Smith[1], Randy H. Ewoldt[1], Melanie Sanford[2], Jennifer A. Lewis[3], Rajeev S. Assary[4], Kevin G. Gallagher[4], Robert M. Darling[5], Fikile Brushett[6], Joaquin Rodriguez-Lopez[1]
[1]University of Illinois at Urbana-Champaign; [2]University of Michigan; [3]Harvard University; [4]Argonne National Laboratory; [5]United Technologies Research Center; [6]Massachusetts Institute of Technology

Non-aqueous redox flow batteries (NRFBs) are a viable alternative to their aqueous counterparts as they offer a wider range of energy-dense redox motifs for their design.[1] However, suitable membranes that both sustain low cross-over and high electrolyte conductivity in organic media are lacking. Separating the redox components by size-exclusion while allowing unhindered electrolyte transport presents a powerful alternative. The Joint Center for Energy Storage Research (JCESR) originally introduced this concept [2,3] by using highly soluble Redox Active Polymers (RAPs) and Colloids (RACs) in combination with nanoporous separators. RAPs and RACs are highly substituted with redox active pendants that display facile electron transfer and form highly concentrated solutions.

We will present our advances towards creating superior polymers for solution-phase electrochemical energy storage and their use in size-exclusion NRFBs. Critical to this task is the description of newly discovered electrochemical dynamics of RAP solutions. Our collaborative has focused on the creation of both practical and model RAPs and RACs,[3,4] leading to an insightful test platform for understanding charge transfer and transport in redox polymer solutions. We have contributed to modernizing the toolbox for NRFBs including an array of nano-electrode techniques, spectro-electrochemistry, computational analysis, and single-particle analysis. We will discuss how fundamental chemical insight translates into flow battery functionality.

[1] R.M. Darling, et al. *Energy Environ. Sci.* **2014***, 7*, 3459.
[2] G. Nagarjuna, et al. *J. Am. Chem. Soc.* **2014**, *136*, 16309.
[3] M. Burgess, et al. *Acc. Chem. Res.*, **2016**, *49*, 2649.
[4] M. Burgess, et al. *Chem. Mater.* **2016**, *28*, 7362.

1:50 PM

D-IV-2: HIGH-RATE ELECTRICAL ENERGY STORAGE ENABLED BY METALLIC CONDUCTIVITY OF MXENES

[EFRC – FIRST] Maria R. Lukatskaya[1], Mohamed Alhabeb[1], Muhammad Boota[1], Michael Naguib[2], Yu Xie[2], Paul Kent[2], Xiahan Sang[2], Raymond Unocic[2], Jeremy Come[2], Nina Balke[2], David Wesolowski[2], Yury Gogotsi[1]
[1]Drexel University; [2]Oak Ridge National Laboratory

Two-dimensional (2D) transition metal carbides and nitrides known as MXenes (~30 already produced) have received considerable attention for energy storage applications due to their metallic conductivity combined with transition metal oxide-like surfaces capable of reversible redox reactions. Even flowable MXene slurries possess sufficient conductivity for use in flow capacitors. MXenes serve as an excellent model system for fundamental studies of charge transfer and ionic transport in slit pores of tunable width, but also make promising candidates for practical energy storage applications requiring delivery of large amounts of energy at very high rates. When MXenes are fabricated into binder free, free-standing films they have exceptional electronic

conductivity. MXenes are capable of electrochemically intercalating cations of various charges (H^+, Mg^{2+}, Al^{3+}) into the interlayer spaces between their 2D sheets. Furthermore, the reversible intercalation and de-intercalation of organic ions from ionic liquids and solvent-containing electrolytes has been demonstrated. The ability MXenes have for storing and delivering large amounts of energy at high power densities in numerous electrolytes paired with the versatility with which they can be processed into a variety of electrode architectures puts MXenes in a promising position to lead the research and development of the next generation of materials for energy storage and delivery. MXene layers can also be interleaved with monolayers of conductive polymer of nanometer-thin layers of gel electrolyte. This work shows the relation between electronic conductivity, ionic conductivity and charge storage ability of MXenes, offering a new paradigm for development of electrode materials for high-energy, high-power storage.

2:10 PM

D-IV-3: SOLID STATE LI-ION BATTERIES: ADVANCING PERFORMANCE THROUGH FUNDAMENTAL UNDERSTANDING

[EFRC – NEES] Elliot J. Fuller[1], Alex J. Pearse[2], Keith Gregorczyk[2], David Ashby[3], Kim McCelvey[4], Farid El Gabaly[1], Francois Leonard[1], Bruce Dunn[3], Henry S. White[4], Sang Bok Lee[2], Gary Rubloff[2], A. Alec Talin[1]
[1]Sandia National Laboratories; [2]University of Maryland; [3]University of California, Los Angeles; [4]University of Utah

Realization of safe, long cycle life, and simple to package solid-state rechargeable batteries with energy and power density that matches or exceeds those of liquid electrolyte batteries represents a major challenge for the energy storage community. Although solid state electrolytes with Li-ion conductivities $>10^{-3}$ S/cm have now been demonstrated, other factors such as high electrode/SSE interfacial resistances, undesired interfacial reactions, slow Li-ion diffusion in the electrodes, and inhomogeneous current distribution during charging/discharging of 3D electrode structures continue to limit solid state battery performance. In my talk, I will describe several coordinated efforts within the NEES-II EFRC to address these challenges using model materials systems. Some of the topics I will discuss include in situ mapping of the potential distribution across solid electrode/electrolyte interfaces and relating this variation to composition, as well as the fabrication/testing/modeling of 3D SSLIBs using conformal and non-conformal deposition methods and the impact of the resulting structure on performance. I will end my presentation with a brief discussion of how we leveraged our expertise in solid state nanoionics to solve energy challenges beyond storage, such as the need for low power computing.

2:30 PM

D-IV-4: THE MATERIALS PHYSICS OF LITHIUM (DE)INTERCALATION IN LAYERED OXIDE CATHODES

[EFRC – NECCES] Maxwell D. Radin[1], Sunny Hy[2], Mahsa Sina[2], Chengcheng Feng[2], Haodong Liu[2], Julija Vinckeviciute[1], Minghao Zhang[2], M. Stanley Whittingham[3], Ying Shirley Meng[2], Anton Van der Ven[1.]
University of California, Santa Barbara; [2]University of California, San Diego; [3]Binghamton University

Layered oxide cathode materials exhibit complex physical changes during electrochemical cycling because of the many degrees of freedom that couple to lithium intercalation. For example, mechanical deformation, Jahn-Teller activity, and stacking sequence changes are all strongly linked to the insertion or removal of lithium. Despite the importance of layered oxides in state-of-the-art Li-ion batteries, many questions about these phenomena remain unanswered. Here we present computational tools that can be used to simulate the materials physics of lithium (de)intercalation in layered oxides, and discuss how these tools complement experimental characterization in the case of nickel-cobalt-aluminum (NCA) and nickel-manganese-cobalt (NMC) cathodes. Highlights include the local structure of Jahn-Teller distortions, trends in stacking-sequence changes, and factors controlling the migration of cations to tetrahedral sites.

2:50 PM

D-IV-5: CHARACTERIZATION AND MODELING OF OXYGEN REACTIVITY AND STRUCTURAL EVOLUTION DURING ELECTROCHEMICAL CHARGING OF LI-RICH Li_5FeO_4

[EFRC – CEES] Chun Zhan,[1] Jun Lu,[1] Zhenpeng Yao,[2] Liang Li,[1] Fernando Castro,[2] Alper Kinaci,[1,2] Victor A. Maroni,[1] Lu Ma,[1] Tianpin Wu,[1] Lynn Trahey,[1] Jianguo Wen,[1] Yang Ren,[1] Tim Fister,[1] Vinayak Dravid,[2] Chris Wolverton,[2] Maria Chan,[1] Khalil Amine,[1] Christopher Johnson,[1] Michael Thackeray[1]
[1]Argonne National Laboratory, [2]Northwestern University

In the Center for Electrochemical Energy Science (CEES) EFRC, we are investigating a new class of energy storage materials – hybrid Li-ion/Li-oxygen materials – that combine transition metal and oxygen redox to deliver high energy storage capacity and therefore open a new avenue for designing next-generation energy storage devices. For instance, Li_5FeO_4, as a prototypical hybrid material, is found to deliver extremely high charge capacity. In this talk, we will discuss our synthesis, characterization, and first principles modeling efforts on Li_5FeO_4, in an attempt to understand the electrochemical performance and reaction mechanisms. We will report on the in-situ observations of structural changes and phase transformations during electrochemical cycling, via in-situ synchrotron X-ray Diffraction (XRD), high-resolution Transmission Electron Microscope (TEM), and Raman spectroscopy. The charge state and coordination changes of Fe are also quantitatively determined by Mossbauer spectroscopy and first principles studies. The redox reaction is investigated by probing the electronic structure evolution using X-ray Absorption Spectroscopy (XAS) and Electron Energy Loss Spectroscopy (EELS). The origin of the remarkable charge capacity of Li_5FeO_4 is identified and demonstrated by experimental core-level spectra and corresponding first-principles simulations. The challenges and future prospects of hybrid materials will also be discussed.

3:10 PM

D-IV-6: QUANTIFY THE FUNDAMENTAL IRREVERSIBLE STRUCTURAL AND CHEMICAL CHANGES FOR NANOSTRUCTURE DESIGNS IN BATTERY APPLICATIONS

[EFRC – NEES] Yue Qi[1], Kevin Leung[2], Katherine Jungjohann[2], John Cumings[3], Chunsheng Wang[3]
[1]Michigan State University; [2]Sandia National Laboratories; [3]University of Maryland

Understanding the causes of battery degradation requires identifying the “irreversible” chemical and structural changes – from atomic to mesoscale – that appear during battery cycling. To design nanostructures mitigating these degradation mechanisms, will further rely on our ability to quantify and predict these irreversible changes. The Nanostructures for Electrical Energy Storage (NEES), a DOE Energy Frontier Research Center, advances both in situ observations and multiscale modeling techniques to identify, quantify, and predict the fundamental irreversible degradation mechanisms.

This talk will focus on recent modeling methodology developed to compliment in situ observations in order to elucidate the underlying factors contributing to mechanistic failures. For example, most experimental techniques are not sufficiently sensitive to reveal the amorphous Si characteristics change upon cycling. Reactive molecular dynamics, along with a new lithiation and delithiation algorithm, simultaneously tracks and correlates the lithiation-delithiation rate, compositional change, mechanical property evolution, stress distributions, and fracture. The model can quantify the irreversible volume change of Si nanostructure, the amount of trapped Li, the generation and distribution of inner pores and coating delamination, and the atomistic structural difference in the amorphous structures, upon cycling. These findings lead to design criteria for mechanically stable coated Si nanostructures and battery operating guidelines to mitigate capacity loss due to trapped Li and coating delamination.

Such design approaches can extend to other systems, such as optimizing the geometry of CNT encapsulated Sulphur cathodes. The insights gained from these simulations have enhanced our understanding on battery degradation mechanisms and inspired new designs across various length scales.

E. NUCLEAR ENERGY AND WASTE

SESSION I: MONDAY, JULY 24, 2017; 3:00 – 5:00PM; LINCOLN 5

3:00 PM

E-I-1: WAVELENGTH SELECTIVE PHOTOCHEMICAL TRANSFORMATIONS USING ELECTROACTIVE LIGANDS

[EFRC – CAST] Sahan R. Salpage, Shane S. Galley, Thomas E. Albrecht-Schmitt, Kenneth Hanson
Florida State University

Given the similarity in atomic radius and binding affinities, separating actinides using chelating agents or ion exchange resins can sometimes be challenging. In contrast, actinide atoms/complexes have unique and narrow absorption features that may be useful for photochemical separations. Here we share our efforts towards the goal of light driven separations of actinides using photoinduced electron transfer from the metal center to the electroactive, ligands. As a precursor to actinides separations we will first introduce our work coordinating the ligand to Group 8 transition metals Fe(II), Ru(II), and Os(II) and the demonstration of wavelength selective photoreactions. Then we will discuss our more recent progress in generating neodymium and americium complexes and their photoreactivity.

3:20 PM

E-I-2: THE RECENT DEVELOPMENT OF THE DFT/GW + GUTZWILLER SLAVE-BOSON METHOD AND PACKAGE

[CMS – CDMFTS] Yongxin Yao[1], Sangkook Choi[2], Nicola Lanatà[3], Tsung-Han Lee[3], Xiaoyu Deng[4], Cai-Zhuang Wang[1], Kai-Ming Ho[1], Vladimir Dobrosavljević[3], Gabrial Kotliar[2,4]
[1]Ames Lab; [2]Brookhaven National Lab; [3]National High Magnetic Field Lab and Florida State University; [4]Rutgers University

The first-principles simulation of correlated electron systems is a major challenge for the purpose of material discovery and design involving transition metals, lanthanide and actinide elements. In this talk, I will discuss the recent development of the Gutzwiller-Rotationally Invariant Slave-Boson method, including its merger with density functional theory and quasi-particle self-consistent GW method. Ways for further systematically improving the accuracy will be illustrated in 1-band models. The applications of the method for real materials will be demonstrated in the examples of phase diagram of the exotic element Pu, the orbital selectivity and covalent bonding in the nuclear fuel UO_2 and the spectral function of $FeSb_2$.

3:40 PM

E-I-3: WELL-DEFINED ACTINIDE-BASED FRAMEWORKS

[EFRC – CHWM] Natalia B. Shustova[1], Charles Henager, Jr.[2], Ekaterina Dolgopolova[1], Otega Ejegbavwo[1]
[1]University of South Carolina (lead institution); [2]Pacific Northwest National Laboratory

The development of novel materials with enhanced performance is a continuous process driven by technological demands, which are not only to improve various fields in science, but also to ensure environmental safety. Recently, metal-organic frameworks (MOFs), which are porous hybrid materials consisting of organic linkers connected to inorganic secondary building units, were evaluated as promising candidates for a wide range of applications such as heterogeneous catalysis, gas separation, and sensing. Shifting from the more classic use of MOFs, the recent exploration of these well-defined hybrid materials has revealed their high potential for applications in the field of radioactive waste storage and sequestration. Success in the latter area, however, largely depends on effective understanding and utilization of the unique advantages of MOFs: porosity, modularity, and versatility. In this presentation, synthesis, characterization, and analysis of actinide-containing MOFs will be discussed to shed light on the key factors responsible for development of new constituents, architectures, and networks required for effective radioactive waste sequestration and utilization. The specific emphasis will be given to unique role of MOF modularity, which cannot be replicated in any other known system. Furthermore, the synthesis and characterization of MOFs with a high actinide content will be discussed, demonstrating that radioactive wastes can be efficiently trapped in the MOF structure in three different ways: pores, linkers, and metal nodes.

4:00 PM

E-I-4: DESIGN AND PERFORMANCE OF CERAMIC WASTE FORMS FOR IODINE AND CHLORINE SEQUESTRATION WITH HIGH WASTE LOADINGS

[EFRC – WastePD] Spencer M. Scott,[1] Tiankai Yao,[1] Weiguang Zhu,[1] Zelong Zhang,[2] Jianwei Wang,[2] Joseph V. Ryan,[3] John D. Vienna,[3] Jie Lian[1]

[1]Rensselaer Polytechnic Institute; [2]Louisiana State University; [3]Pacific Northwest National Laboratory

Effective management of short-lived Cs and Sr radionuclides as the major heat generators and volatile problematic radionuclides such as long-lived iodine-129 and Tc-99 is critical for the sustainable development of nuclear energy systems. Advanced waste form materials are needed for handling complex environmental wastes including CsCl capsules and high chlorine salts resulting from pyrochemical processing of advanced fuel cycle technologies. It is of significant technological challenge to develop waste forms for sequestration of highly mobile iodine and water soluble chorine, and innovative technologies are required to synthesize and fabricate advanced waste form materials with enhanced waste loadings and confinement of radionuclides. The extremes envisioned for the long-term waste management consisting of temperature, intensive ionizing radiation and water interaction also require waste form materials with extended performance of thermal/radiation stability and corrosion resistance. Within the frame work of the WastePD EFRC, the Ceramics Team targets the development of crystalline host phases to address critical issues of Cs, I and Cl disposition with the emphasis of waste form design and long-term performance evaluation. Promising ceramic waste forms are proposed based upon apatite and defective perovskite structure types showing extensive cation and anion substitutions and crystal structure flexibility. Advanced technologies combining high energy ball milling and spark plasma sintering are being developed for the incorporation and confinement of critical radionuclides and consolidation of the waste form materials into a dense matrix. The thermal stability of the designed waste forms and their chemical durability as evaluated by water dissolution were conducted to achieve mechanistic understanding of waste form performance. The impacts and implication of the designed ceramic waste forms on effective management of environmental wastes, particularly highly volatile iodine and chlorine, are further highlighted.

4:20 PM

E-I-5: Synthesis of Actinide Hydroxylamine Complexes and Characterization of their Electronic Structures

[EFRC – CAST] Thibault Cheisson[1], Alex McSkimming[1], Andrew Gaunt[2], Stosh Kozimor[2], Samantha Schrell[2], Ping Yang[2], Enrique Batista[2], John Gibson[3], Eric J. Schelter[1]
[1]*University of Pennsylvania;* [2]*Los Alamos National Laboratory;* [3]*Lawrence Berkeley National Laboratory*

Hydroxylamine ligands are interesting and noteworthy in studies of *f*-element coordination chemistry due to their excellent donor properties. Complexes of hydroxylamines are stabilized through coordination of their highly anionic oxygen donors. A consequence of the strong donor properties is the concomitant stabilization of higher oxidation states of coordinated metal cations. In this cross-institution effort, we have been applying tailored hydroxylamine ligands to develop coordination chemistry for actinides and especially transuranics. Our goals for this effort are to develop understanding of the stabilities of non-actinyl hydroxylamine complexes, their speciation, their electronic properties and their redox properties. We have used a combination of synthetic chemistry and characterization and computation to achieve these goals. Our results to date indicate the formation of stable complexes of Ce, Th, U, Pu, and Np, and efforts to predict and measure their redox properties are currently underway. These results enable the study and prediction of the redox properties of actinides in contexts of both separations and waste forms.

4:40 PM

E-I-6: – ACTINIDE POLYNUCLEAR SPECIATION AND IMPLICATIONS IN NUCLEAR ENERGY

[EFRC – MSA] May Nyman[1], Peter C. Burns[2], Laura Gagliardi[3], Alexandra Navrotsky[4]
[1]*Oregon State University;* [2]*University of Notre Dame;* [3]*University of Minnesota;* [4]*University of California-Davis*

An(IV) and An(VI) form polynuclear clusters in water that can be exploited in separation chemistries. An(IV) aqueous polycations are poorly soluble except at low pH, while $U(VI)O_2^{2+}$ forms anionic hollow capsules in alkaline-peroxide conditions. The $U(VI)O_2^{2+}$ capsules self-assemble via a bottom-up process from monomers, or a top-down pathway via dissolution of studtite, and the two pathways yield different cluster topologies, which has been investigated by small-angle X-ray scattering (SAXS), Raman spectroscopy and calorimetry. In these studies, we have investigated the effect of counterions and pH on speciation. In two separate studies, we have demonstrated how these cluster forms assemble via dissolution of spent nuclear fuel simulant, followed respectively by solvent-extraction separation or filtration separation. These separation processes are 'atom efficient', in that up to 60 uranium ions are separated as a single molecular unit. Solvent extraction of the $U(VI)O_2^{2+}$ capsules provided the first opportunity to investigate (via NMR and simulations) the behavior of the capsules and their encapsulated species in non-aqueous media. The uranyl peroxide capsules are ideal for X-ray scattering characterization due to the superior scattering power of uranium and the hollow capsule morphologies. We exploit SAXS and Raman to predict the topology of new cluster forms, and follow the evolution of clusters in solution with changing conditions. SAXS is also paramount in identify endohedral clusters; i.e. Bi and Pb oxocations inside uranyl peroxide capsules. These studies also demonstrate exploiting capsules to enable dissolution in alkaline pH where solubility and speciation of Bi and Pb is unknown.

SESSION II: TUESDAY, JULY 25, 2017; 8:30 – 10:10 AM; LINCOLN 5

8:30 AM

E-II-1: INTERFACIAL DYNAMICS OF BOEHMITE & GIBBSITE IN EXTREME ENVIRONMENTS: CONNECTING ACROSS SPATIAL SCALES

[EFRC – IDREAM] Xin Zhang[1], Zhizhang Shen[1], Trenton R. Graham[2], Carolyn I. Pearce[1], Katherine Page[4], Layla Mehdi[1], Micah Prange[1], Sebastien Kerisit[1], Xiaosong Li[3], Jianzhi Hu[1], Nigel Browning[1], Kevin M. Rosso[1], Sue B. Clark[1]

[1]Pacific Northwest National Laboratory, [2]Washington State University, [3]University of Washington, [4]Oak Ridge National Laboratory

In highly alkaline sodium aluminate solutions, interfacial processes underlying nucleation, growth, and dissolution of aluminum (oxy)hydroxides in Hanford tank waste are poorly understood. We are unraveling mechanisms of these processes for gibbsite and boehmite across molecular to mesoscales, using a combined multi-method experiment and simulation approach. We will overview progress in understanding 1) relationships between synthesis conditions and crystallite size, shape, crystallinity, and Al coordination at surfaces; 2) surface-specific mechanisms of gibbsite dissolution; and 3) hydrothermal transformation of gibbsite to boehmite. In all cases a coordination change of Al^{3+} from tetrahedral in solution to octahedral in the solids, and vice versa, is required. By systematically varying temperature, reaction time, pH, and Al-precursor type and concentration, we developed a new method for synthesis of hexagonal nanoplates with high reaction yield. ^{27}Al MAS NMR using high magnetic field allowed quantification of tetrahedral and pentahedral alumina species at surfaces. These transitional alumina site concentrations appear correlated with saturation state, consistent with growth being kinetically controlled by the Al coordination change at the interface. Using classical molecular dynamics simulations and ab initio methods, surface speciation and deprotonation on gibbsite edges at high pH were examined. To explore the dissolution pathway 3-D metadynamics and PMF calculations were used to obtain the detachment free energies and the kinetics of elementary steps of dissolution. Model predictions for rates of microscopic elementary dissolution processes at step edges are being directly compared to AFM studies and multi-method characterization of gibbsite dissolution at high pH from molecular to micron scales.

8:50 AM

E-II-2: MOLECULAR DYNAMICS SIMULATIONS OF CASCADES: EFFECTS OF ION-ELECTRON INTERACTIONS IN IRRADIATED ALLOYS

[EFRC – EDDE] Eva Zarkadoula[1], German Samolyuk[1], William J. Weber[1,2]

[1]Oak Ridge National Laboratory; [2]University of Tennessee-Knoxville

Understanding energy dissipation in materials under ion irradiation is essential to predict and dictate the response of materials in a radiation environment. During irradiation, energy from a fast-moving projectile is lost to lattice atoms (nuclear energy loss) and to electrons (electronic energy loss) of a target material, resulting in different temperature evolutions of the two subsystems. Depending on the local temperature difference, energy between the two subsystems is exchanged via electron-phonon interactions. We investigate the coupled effects of the nuclear and electronic energy loss during irradiation in concentrated solid solution alloys (CSAs) using a coupled two-temperature molecular dynamics (2T-MD) model. We use electronic structure calculations within the coherent potential approximation (CPA) to obtain parameters required to describe the electronic subsystem within the 2T-MD. The effects of the electronic excitation on damage production and defect structures are explored. Compared to the results obtained from classical MD simulations where the electronic effects are ignored, the results, by taking into account both energy loss mechanisms in the 2T-MD simulations, show less damage with smaller defect clusters.

9:10 AM

E-II-3: MULTIMETALLIC NANOPARTICLES: ALLOYS, INTERMETALLICS, AND HETEROSTRUCTURES

[EFRC – CHWM] Hui Wang[1], Scott Misture[2], Simon R. Phillpot[3]
[1]University of South Carolina (lead institution); [2]Alfred University; [3]University of Florida

In the Center for Hierarchical Waste Form Materials (CHWM), the nanoscience team has been developing mechanistic understanding of the structure-composition-property relationships that underpin the formation, deformation, and nanoscale restructuring behaviors of multimetallic nanoparticles comprising both noble metals and less noble transition metals, with the goal of building a central knowledge framework for the rational design of next generation nanostructured nuclear waste storage materials. Au-Cu bimetallic nanoparticles represent a prototypical nanoscale system accommodating two miscible metals. We found that upon thermal heating in polyol solvents, Au@Cu_2O core-shell nanoparticles evolved into Au-Cu disordered alloy nanoparticles, which further transformed into structurally ordered intermetallic phases under appropriate conditions. The structural ordering of the alloy nanoparticles was synergistically maneuvered by multiple intertwining thermodynamic, kinetic, and geometric factors. During dealloying or galvanic replacement reactions, the alloy and intermetallic nanoparticles underwent distinct structural transformations essentially dictated by the diffusion rate of Cu atoms, which strongly depend on both the Au/Cu stoichiometries and the structural ordering. We have also demonstrated the feasibility of depositing an immiscible, lattice-mismatched transition metal on a noble metal nanoparticle using Au-Ni bimetallic nanoparticles as a model system. We showed that despite the large lattice mismatch (>13 %) and poor miscibility between Au and Ni, both cubic- and hexagonal-phase Ni could be controllably deposited on Au nanoparticle surfaces through seed-mediated reduction in polyols to form a variety of Au-Ni heteronanostructures, such as core-shell, core-satellite, and heterodimer nanoparticles. The Ni components in the Au-Ni heteronanostructures were found to be significantly more stable than monometallic Ni.

9:30 AM

E-II-4: UNDERSTANDING THE FORMATION, STRUCTURE, AND STABILITY OF THE PASSIVATING LAYER FORMED ON NUCLEAR WASTE GLASS DURING AQUEOUS CORROSION

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

The glass team of the Center for Performance and Design of Nuclear Waste Forms and Containers (WastePD) aims at attaining a fundamental understanding of the structure chemistry of a thin passivating layer present on nuclear waste glass during aqueous corrosion. A six-component glass called International Simple Glass (ISG) is studied as a model glass, which was selected by the international community to build a consensus on the understanding of corrosion processes of complicated nuclear waste glasses. MD simulations with reactive force fields were employed to investigate atomic scale interactions of the ISG glass with water, which acts as both solvent and reactant at the same time. The elemental compositions and silicate network structures of the passivating layers formed on the ISG in the presence and absence of counter ions were studied with state-of-the-art characterization tools including APT, NMR, ToF-SIMS, XPS, IR, and SFG. Water content and speciation of nano-confined water were determined, and the transport of the water molecules within the passivating layer was assessed using isotopically tagged water molecules and ToF-SIMS depth profiling. The techniques needed for flash-freezing and cryo-FIB have been developed and applied to corroded glass surfaces, which will allow characterization of the surface gel layer without artifacts from sample prep. This talk will present significant progress made in the first seven months of the WastePD Center and how it can be compared with the aqueous corrosion mechanisms of other materials (ceramics and metals) to bring scientific advances that would not otherwise be possible

9:50 AM

E-II-5: RADIATION DRIVEN MODIFICATION OF BOEHMITE AND GIBBSITE

[EFRC – IDREAM] Jay LaVerne[5], Greg Kimmel[1], Thomas Orlando[4], Li Xiaosong[3], Carolyn Pearce[1], and Kevin Rosso[1], Patricia Huestis[5], Nikolay Petrik[1], Alex Alexandrov[4], Sue Clark[2], Anthony Krzysko[2], Shichao Sun[3]
[1]Pacific Northwest National Laboratory, [2]Washington State University, [3]University of Washington, [4]Georgia Institute of Technology, [5]University of Notre Dame

High level radioactive wastes at the Hanford site have been aging in a radiation environment for many years, and little is known about the influence of the radiation on the bulk materials, gibbsite ($Al(OH)_3$) and boehmite ($AlO(OH)$). Research in IDREAM is focused on addressing this knowledge gap. Water surface site energies and kinetics were determined using infrared absorption and temperature programmed desorption of pristine and gamma irradiated powders. Results show strongly chemisorbed water at a variety of sites that are not modified noticeably by gamma radiation. In addition, we are developing low-energy electron radiolysis of more ordered systems to give a complete understanding of water radiolysis processes occurring at these surfaces. Changes in solid phase morphologies as indicated by x-ray diffraction were not observed after gamma radiolysis, possibly due to the relatively low radiation doses used thus far. Chemical modification of the powder surfaces examined using x-ray photoelectron spectroscopy show possible conversion to lower aluminum oxidation states. Raman spectroscopy shows no chemical modification and ongoing x-ray scattering studies will hopefully resolve the issue. Additional computational work is also underway, and will aid in elucidation of mechanisms of radiation driven modification of boehmite and gibbsite.

SESSION IV: TUESDAY, JULY 25, 2017; 1:30 – 3:30PM; LINCOLN 5

1:30 PM

E-IV-1: – ACTINIDE MATERIALS UNDER EXTREME CONDITIONS: LOCAL DEFECT STRUCTURE AND DISORDER

[EFRC – MSA] Maik Lang[1], Rodney C. Ewing[2], Wendy Mao[2]
[1]University of Tennessee, [2]Stanford University

We have investigated several phenomena in nuclear materials induced under intense irradiation, static and dynamic compression, and high temperature by the utilization of state-of-the-art instruments at large user facilities. Examples include the use of intense ultrafast laser pulses (SLAC National Accelerator Laboratory, Stanford) and relativistic heavy ion beams (GSI Helmholtz Center, Darmstadt Germany) to induce high energy densities in materials, which drive the local atomic structure far from equilibrium. This triggers complex structural modifications which require analysis by advanced characterization techniques to obtain fundamental understanding of damage mechanisms, defect behavior, phase transformations, and nanoscale structural alterations. For example, by using complementary neutron total scattering, X-ray diffraction, and calorimetry we have gained new insight into the nature of disorder in complex oxides over a range of length-scales. This experimental effort was supported by DFT calculations confirming the complex disordering mechanism in fluorite-derivative oxide materials. We have further examined how local structural modifications in defective materials affect physical properties by broadband dielectric spectroscopy, revealing a significant increase of ionic conductivity after ion irradiation. This experimental approach has been expanded to actinide compounds by studying the defect structure in uranium oxides with deviations from ideal stoichiometry or doping with lanthanide atoms. Pair distribution function analysis from neutron total scattering shows that the defect structure is governed by complex oxygen defect clustering in these compounds.

1:50 PM

E-IV-2: DEFECT GENERATION, EVOLUTION, AND DYNAMICS IN IRRADIATED CONCENTRATED SOLID SOLUTION ALLOYS

[EFRC – EDDE] Karren L. More[1], Jonathan Poplawsky[1], Xing Wang[1], Hongbin Bei[1], Ian Robertson[2], Lumin Wang[3], Yanwen Zhang[1]

[1]*Oak Ridge National Laboratory;* [2]*University of Wisconsin – Madison;* [3]*University of Michigan*

The random arrangement of multiple elemental species in the ordered lattice structure of binary, ternary, and quaternary concentrated solid solution alloys (CSAs) creates extreme atomic-level chemical complexity, as each atom experiences unique lattice distortions and chemical environments. This complexity can impact and control defect generation and evolution in CSAs under extreme conditions, which in turn dictates their radiation tolerance. For example, the level of radiation-induced damage in NiCo is higher than NiFe, and damage accumulation in both binary CSAs is much lower than in pure Ni, indicating the migration energies of extended defects increase due to the alloying element and/or the chemical complexity. A thorough understanding of inherent lattice-level chemical effects (e.g., elemental and/or interstitial clustering, segregation, compositional complexity) on the type and density of defects (e.g., point defects, stacking faults, loops, etc.) generated and their evolution during irradiation is required to further exploit chemical complexity of CSAs to design structural materials with enhanced radiation tolerance. We are using aberration-corrected scanning transmission electron microscopy imaging and spectroscopy, and atom probe tomography, to identify and quantify atomic-level structure and elemental complexity in Ni-based CSAs, towards understanding how such effects influence defect formation and evolution under ion and electron irradiation conditions.

2:10 PM

E-IV-3: INTEGRATED COMPUTATIONAL MATERIALS DESIGN OF A CORROSION RESISTANT HIGH ENTROPY ALLOY FOR HARSH ENVIRONMENTS: THE SCIENCE BEHIND IT

[EFRC – WastePD] John R. Scully,[1] Jayendran Srinivasan,[1] Christopher Taylor,[2] Pin Lu,[3] James Saal,[3] Gregory B. Olson,[3] Tianshu Li,[2] Orion Swanson,[2] Gerald S. Frankel[2]

[1]*University of Virginia;* [2]*Ohio State University;* [3]*QuesTek Innovations LLC*

The Integrated Computational Materials Engineering (ICME) approach, comprising experimental testing and characterization in synergy with high performance and data-driven computing, is inherently suited to explore the multi-dimensional high entropy alloy (HEA) compositional and processing space. In this work, ICME methods have been used for the design of highly corrosion resistant HEAs (CR-HEAs). Given the difficulty of extrapolating pre-existing metallurgical knowledge into new CR-HEA design, the fundamental mechanisms and key associated parameters describing corrosion resistance must be investigated. Multi-scale/physics modeling has been used to combine knowledge of the atomistic effects and the influences of metal processing to enable predictions of corrosion performances at the macro level. Thermodynamic models have been investigated to explore compositions with desirable characteristics in terms of metal-metal, metal-oxygen and metal-chloride bonding. Three single-phase HEA compositions (FCC, BCC, and HCP) were identified for superior corrosion resistance and adopted for experimental investigation. One of the HEA compositions rich in Ni was successfully synthesized and solutionized on the lab-scale and characterized with respect to microstructure and corrosion. Excellent electrochemical passivity and localized corrosion resistance was observed in a variety of high chloride ion and acidified environments.

2:30 PM

E-IV-4: VOLUME BASED THERMODYNAMICS APPROACH APPLIED TO SALT INCLUSION MATERIALS

[EFRC – CHWM] Theodore M. Besmann[1], Emily E. Moore[1] Gregory Morrison[1] Hans-Conrad zur Loye[1]
[1]*University of South Carolina*

Salt inclusion materials (SIMs) of interest utilize uranyl silicates as frameworks. Thermodynamic stability of these are unknown, however structural information (molar volume) may aid in estimating thermodynamic properties. Estimation techniques developed by L. Glasser et al. allow for direct calculation of standard entropy using correlations that provide constants specific for a given group of framework structures. Lattice potential energy calculated from the ionic strength of various salt and framework components and the Madelung constant can be used in enthalpy calculations. The values are constant with respect to molecular volume for very similar structures, and have a linear relation for more dissimilar species. These principles have been uniquely adapted for SIMs and appear to successfully provide thermodynamic relations that will allow design of stable structures and help predict potential salt inclusion and exchange.

2:50 PM

E-IV-5: HARNESSING THE *f*-ELECTRON STATE IN NOVEL HIGH TEMPERATURE WASTE FORMS

[EFRC – CAST] Ryan Baumbach, Kevin Huang, Dave Graf, You Lai, Lucas William Nelson
Florida State University/National High Magnetic Field Laboratory

Developing new and safe methods for storing nuclear waste has the potential to tremendously impact our growing energy needs. Utilizing new crystalline structures that are stable and built from abundant elements is a promising avenue to accomplish this, but is hindered by the lack of basic knowledge about physical and electronic-magnetic properties - which are intimately related to chemical-environmental properties (e.g., stability in air or water). Our aim is to address these questions using a multi-pronged approach including (1) development of synthesis methods to uncover crystalline structures well suited to actinide elements and (2) characterization of their electrical and thermodynamic properties. For direction (1), we have explored a variety of actinide based intermetallic structures using high melting temperature metal fluxes, chemical vapor transport, and rf-induction furnace heating. We have focused on materials with attractive properties including topological protection and easily tunable electronic ground states relating to unstable *f*-electron valence. Regarding direction (2), we have performed rapid and detailed characterization of multiple 5*f* and related 4*f* materials. In addition to our own CAST projects, we have fully supported other CAST team members: e.g., by characterization of magnetic properties. In this talk we will discuss highlights from these efforts.

3:10 PM

E-IV-6: NEW INSIGHTS INTO THE PHYSICS AND AGING OF PLUTONIUM METAL

[EFRC – MSA] Albert Migliori[1], Boris Maiorov[1], Fedor Balakirev[1], J.B. Betts[1]
[1]*Los Alamos National Laboratory*

Thermodynamic susceptibilities provide some of the most revealing probes of matter. They include heat capacity, thermal expansion, magnetic susceptibility, dielectric susceptibility, and elastic moduli. In order, they include a scalar, three second-rank tensors, and, for elastic moduli, a fourth rank tensor. As the complexity of the susceptibility increases, so does the information it provides. We describe here studies of the elastic moduli of plutonium metal. The technique used is called Resonant Ultrasound Spectroscopy, developed by us, and providing unprecedented absolute accuracy and precision—we can detect under carefully controlled conditions a part in 10^8 change in modulus, and provide absolute accuracies of order 0.1%. Using this technique, we have measured elastic moduli with changing temperature to reveal behavior that has forced electronic structure theories of delta (fcc) plutonium to incorporate new physics that is now becoming important for improving the accuracy of the plutonium equation of state. Using the extreme precision, we observed aging in ^{239}Pu in a matter of hours with surprises that have become a major new focus at Los Alamos for the understanding of the longevity of the main application of this material. For both non-civilian nuclear energy applications and for nuclear weapons, our results have been recognized as of extreme importance. We describe here the results and some implications.

F. QUANTUM MATERIALS

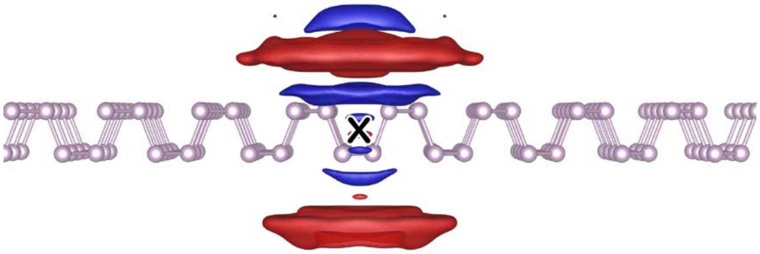
SESSION I: MONDAY, JULY 24, 2017; 3:00 – 5:00PM; LINCOLN 6

3:00 PM – Team Science Finalist

F-I-1: ENVIRONMENTAL SCREENING EFFECTS IN 2D MATERIALS: RENORMALIZATION OF THE BANDGAP, ELECTRONIC STRUCTURE, AND OPTICAL SPECTRA

[CMS – C2SEPEM] Diana Y. Qiu, Felipe H. da Jornada, M. Iqbal B. Utama, Feng Wang, Steven G. Louie
Lawrence Berkeley National Laboratory and UC Berkeley

Few-layer black phosphorus (BP) is a highly promising material for optoelectronic and clean energy technologies. In order to avoid degradation in ambient conditions, it has become common practice to encapsulate these quasi-2D BP devices with wide bandgap insulators. While it is generally assumed that this encapsulation does not significantly affect their electronic and optical properties, we show, in a collaborative effort between ab initio theory and experiment, that the opposite is true [1,2].
We performed the first optical absorption measurements on few-layer BP encapsulated between a sapphire substrate and a boron nitride capping layer. Concurrently, in accordance with the experimental setup, we developed new theoretical and computational techniques to incorporate the screening environment from the substrate and the capping layer in our *ab initio* GW and GW-BSE calculations. We find that, contrary to previous belief, BP is exceptionally sensitive to environmental screening. We showed for the first time that encapsulation reduces the exciton binding energy by as much as 70%, and dramatically changes the nature of the excited states and the qualitative features of the absorption spectrum. This can be seen in the figure below, where we plot the difference between the induced charge density for encapsulated monolayer BP and isolated BP, given an external test charge at "X"



Our discovery and understanding of large environmental screening effects open new pathways for tuning the properties of low-dimensional materials by treating screening and confinement as separately tunable degrees of freedom. Furthermore, the new methods we developed for including substrate screening push the frontiers of state-of-the-art many-body GW and GW-BSE calculations, allowing us not only to accurately account for the experimental environment, but also to calculate excited-state phenomena in incommensurate, layered heterostructures. Finally, in a similar synergetic setup between experiment and theory, we are now studying the role of substrates in the electronic properties of few-layer transition metal dichalcogenides (TMDs).

References: [1] L. Li, J. Kim, C. Jin, G. J. Ye, D. Y. Qiu, F. H. da Jornada, Z. Shi, L. Chen, Z. Zhang, F. Yang, K. Watanabe, T. Taniguchi, W. Ren, S. G. Louie, X. H. Chen, Y. Zhang, F. Wang, *Nature Nanotechnology* **12**, 21 (2016). [2] D.Y. Qiu, F.H. da Jornada, and S. G. Louie, submitted to *Nano Letters*.

Contributions: D.Y.Q., F.H.J., S.G.L. developed the theory and performed *ab initio* calculations. M.I.B.U. and F. Wang fabricated and characterized the (TMDs) samples and analyzed the absorption spectra.

3:20 PM

F-I-2: THE SCAN DENSITY FUNCTIONAL: SUCCESS STORIES FOR 2D, LAYERED AND 3D MATERIALS

[EFRC – CCDM] A. Bansil[1], M. Haataja[2], M. L. Klein[3], J. P. Perdew[3], A. Ruzsinszky[3], G. E. Scuseria[4], D. J. Srolovitz[5], J. Sun[6], X. Wu[3], Q. Yan[3], W. Yang[7]

[1]*Northeastern University,* [2]*Princeton University,* [3]*Temple University,* [4] *Rice University,* [5]*UPenn,* [6]*University of Texas-El Paso,* [7]*Duke University*

I will discuss how the SCAN (Strongly Constrained and Appropriately Normed)-based functionals are providing an efficient scheme for a new generation of improved understanding of electronic structures and properties of wide classes of materials with focus on 2D and layered systems. [1, 2] Ground-state electronic and geometric structures of monolayers of graphene and a number of 'beyond graphene' compounds, including films of transition-metal dichalcogenides (TMDs) are considered. The GGA (Generalized Gradient Approximation) yields expanded lattices and softened bonds in relation to the LDA (Local Density Approximation), but the SCAN meta-GGA systematically improves the agreement with experiment. Our analysis suggests the efficacy of the SCAN functional for accurate modeling of electronic structures of layered materials in high-throughput calculations. I will also comment on the viability of SCAN for diversely bonded systems more generally. Work supported by the U.S.D.O.E.

[1] Buda, I.G.; Lane, C.; Barbiellini, B.; Ruzsinszky, A.; Sun, J.; and Bansil, A.: *Nature Scientific Reports* 7, 44766 (2017).
[2] Sun, J.; Remsing, R. C.; Zhang, Y.; Sun, Z.; Ruzsinszky, A.; Peng, H.; Yang, Z.; Paul, A.; Waghmare, U.; Wu, X.; Klein, M. L.; and Perdew, J. P.: *Nature Chemistry* 8, 831 (2016).

3:40 PM

F-I-3: TOWARDS EXPERIMENTALLY VALIDATED, PREDICTIVE QUANTUM SIMULATIONS OF VANADIUM AND NICKEL OXIDES

[CMS – CPSFM] Janakiraman Balachandran[1], Anouar Benali[2], Anand Bhattacharya[2], Panchapakesan Ganesh[1], Olle Heinonen[2], Paul Kent[1], Jaron Krogel[1], Ho Nyung Lee[1], Ye Luo[2], Yogesh Sharma[1], Hyeondeok Shin[2], Friederike Wrobel[2]

[1]*Oak Ridge National Laboratory;* [2]*Argonne National Laboratory*

One central aim of the Center for Predictive Simulations of Functional Materials is to explain and predict the properties of strongly correlated oxides such as vanadium dioxide (VO_2) and nickel oxide (NiO). This will enable control of properties such a metal-insulator transitions (MIT) through variation in doping and composition and by external stimuli such as strain, temperature and electric field. We have performed a series of closely coupled experiments and calculations to establish a proof of principle. We study electrochemical and mechanical modification of the MIT in VO_2 thin films epitaxially grown on (001) TiO_2 substrates, using scanning probe microscopy (SPM). Applied electric voltage and mechanical pressure through the SPM-tip were shown to locally modulate VO_2 film's conductivity. Surface chemical potential and conductivity variations were measured as a function of temperature near the MIT. Our results could be attributed to the local change in the oxygen stoichiometry in VO_2 films. We quantified these changes in oxygen stoichiometry and their strain dependence using density functional theory (DFT) informed by Quantum Monte Carlo (QMC) calculations to better account for correlations. The calculations provide the basis for role of oxygen vacancies towards control of MIT in VO_2 thin films. We have also performed DFT and QMC calculations of K-doped NiO, with a goal of understanding and

controlling the evolution of the electronic structure on doping. Our calculations will be correlated with measurements on MBE-grown systems currently underway.

4:00 PM

F-I-4: ULTRAFAST EXPERIMENTS AND QUANTUM DYNAMICS OF LAYERED MATERIALS

[CMS – MAGICS] David Fritz[1], Uwe Bergmann[1], Priya Vashishta[2], Rajiv K. Kalia[2], Aiichiro Nakano[2], Oleg Prezhdo[2], David J. Singh[3]

[1]*SLAC National Accelerator Laboratory, Stanford University*; [2]*University of Southern California*; [3]*University of Missouri*

We have used joint experimental-computational studies to examine phononic, electronic, mechanical and thermal properties of various LMs. Pump-probe experiments are carried out using ultrafast electron diffraction at SLAC. The salient accomplishments include: (1) sub-picosecond photo-induced lattice dynamics probed by mega-electron volt femtosecond electron beam at SLAC and non-adiabatic quantum molecular dynamics (NAQMD) simulations to study light-driven phonon softening due to ultrafast electronic-to-lattice energy transfer; (2) studies of electron-phonon coupling and fracture in heterostructures of MoS_2/WS_2 and $MoSe_2/WSe_2$; and (3) NAQMD to screen transition of transition metal dichalcogenides (TMDs) with and without chemical defects for predicting charge cooling and recombination rates.

4:20 PM

F-I-5: ADVANCES IN MANY-BODY SIMULATIONS OF MATERIALS

[CMS – CPSFM] Luke Shulenburger[1], Luning Zhao[2], Eric Neuscamman[2], Miguel Morales[3], Cody Melton[4], Chandler Bennett[4], Lubos Mitas[4]

[1]*Sandia National Laboratories;* [2]*University of California Berkeley;* [3]*Lawrence Livermore National Laboratory;* [4]*North Carolina State University*

One of the primary attractions of the quantum Monte Carlo family of methods is that in theory all their approximations can be systematically converged, yielding ever more accurate predictions. In practice, several computationally expedient approximations remain that must be improved upon to predict the properties of materials with high confidence and with a minimum of empirical data. This talk will detail progress made by the Center for Predictive Simulation of Functional Materials to determine where these approximations lead to a significant source of error and then to develop improved techniques to control them. This includes developments in our ability to parameterize and optimize wavefunctions and in the generation and use of pseudopotentials. To allow progress to be measured, we have identified a test set of materials chosen specifically to challenge the methods.

4:40 PM

F-I-6: BAND GAPS FROM HYBRID DENSITY FUNCTIONALS FOR 1D, 2D, AND 3D SOLIDS: THE RIGHT ANSWER FOR THE RIGHT REASON

[EFRC – CCDM] J.P. Perdew[1], H. Peng[1], A. Ruzsinsky[1], G. E. Scuseria[2], J. Sun[3] and W. Yang[4]
[1]*Temple University,* [2]*Rice University,* [3]*University of Texas-El Paso,* [4]*Duke University*

Realistic band gaps of semiconductors extended in 1D, 2D, or 3D are found within density functional calculations only from hybrid functionals that mix in a fraction of exact exchange, and then only in a generalized Kohn-Sham (GKS) scheme that employs a non-multiplicative exchange-correlation potential. The present work moves the justification for this standard approach from empiricism to first principles. The experimental gap is a ground-state energy second difference (ionization energy minus electron affinity). Under rather general conditions, it is proved analytically and numerically [1] that the GKS gap in the band structure for a given approximate functional is equal to the ground-state energy second difference for the same approximate functional, and thus has a physical interpretation in ground-state density functional theory, improving up the ladder from the local density approximation to the generalized gradient approximation (GGA), the meta-GGA, and the hybrid. Although the SCAN meta-GGA often performs as well as a hybrid, this is not so for the band gap, because only the hybrid includes the long-range partly-screened exchange present in semiconductors.

[1] Perdew, J.P.; Yang, W.; Burke, K.; Gross, E.K.U.; Scheffler, M.; Scuseria, G.E.; Yang Z.; Ruzsinszky, A.; Peng, H.; Sun, J.; Zhang, I.Y.; Henderson, T.M; Trushin, E.; and Goerling, A.: *Proceedings of the National Academy of Sciences (USA)* 114, 2801 (2017).

SESSION III: TUESDAY, JULY 25, 2017; 10:40 AM – 12:00PM; LINCOLN 6

10:40 AM

F-III-1: EXPLOITING SPIN-CHIRAL TOPOLOGICAL SURFACE STATES IN KONDO INSULATOR SmB_6 THIN FILMS

[EFRC – SHINES] Yufan Li[1], Tao Liu[2], Mingzhong Wu[2], C. L. Chien[1]
[1]*Johns Hopkins University;* [2]*Colorado State University*

The unique topological spin-chiral surface state of topological insulators (TIs) can benefit new applications in spintronics. A new class of TIs of strongly-correlated Kondo insulators, SmB_6 in particular, in addition to bismuth chalcogenides, has been proposed. These new TIs may possess truly insulating interior that has eluded their Bi-based counterparts. However, experimental verifications of the topological nature in SmB_6 resulted in conflicting verdicts. Moreover, exploiting the proposed surface state for spintronic applications have never been experimentally carried out. We have developed methods to synthesize high-quality SmB_6 thin films that allowed us to demonstrate spin-charge conversion with high efficiency in accordance with the proposed topological surface state. We have exploited strong pure spin current from SmB_6 to switch an adjacent ferromagnet via spin-orbit torque. We have observed a strong inverse spin Hall effect confirming SmB_6 as a spin current detector. Spin-pumping experiments revealed unique temperature and thickness dependence of the spin-charge conversion that evidently demonstrates the spin-chiral surface state. What's more, we have also observed very long spin diffusion length, an order of magnitude longer than those reported in elemental heavy metals, and determined the depth of the non-trivial surface states.

11:00 AM

F-III-2: NATURE OF THE CHARGE DENSITY WAVES IN CUPRATE SUPERCONDUCTORS

[EFRC – CES] Mark P. M. Dean[1], Hu Miao[1], John M. Tranquada[1], Ruidan.D. Zhong[1] Genda.D. Gu[1]
[1]*Brookhaven National Laboratory*

Understanding the nature of the normal state from which high temperature superconductivity in the cuprates emerges is widely believed to be a crucial prerequisite to solving the problem. This state, however, hosts multiple intertwined charge and spin orders, which appear to have different properties in different cuprates materials making the task of identifying universal phenomenology particularly challenging. Here we use ultra-sensitive inelastic x-ray scattering to measure charge and spin fluctuations in $La_{2-x}Ba_xCuO_4$ and track the transition between the long-range stripe-ordered state and the high temperature precursor phase. We find that the precursor charge correlations unlock from the spin correlations above the ordering transition to form a state that helps identify the universal properties of charge and spin stripe correlations in all underdoped cuprates.

11:20 AM

F-III-3: LONG-DISTANCE SPIN TRANSPORT THROUGH A GRAPHENE QUANTUM HALL ANTIFERROMAGNET

[EFRC – SHINES] Petr Stepanov[1,2], Shi Che[1,2], Dmitry Shcherbakov[1,2], Jiawei Yang[1,2], Kevin Thilahar[1], Greyson Voigt[1], Marc W. Bockrath[1,2], Dmitry Smirnov[3], Kenji Watanabe[4], Takashi Taniguchi[4], Roger K. Lake[5], Yafis Barlas[1], Allan H. MacDonald[5], Chun Ning Lau[1,2]
[1]University of California, Riverside; [2]The Ohio State University; [3]National High Magnetic Field Laboratory, Tallahassee; [4]National Institute for Materials Science, Japan; [5]University of California, Riverside; University of Texas at Austin

Antiferromagnetic insulators (AFMI) are robust against stray fields, and their intrinsic dynamics could enable ultrafast magneto-optics and ultrascaled magnetic information processing. Low dissipation, long distance spin transport and electrical manipulation of antiferromagnetic order are much sought-after goals of spintronics research. Here, we report the first experimental evidence of long-distance, spin transport through an AFMI, in our case the gate-controlled, canted antiferromagnetic (CAF) state that appears at the charge neutrality point of graphene in the presence of an external magnetic field. Utilizing gate-controlled quantum Hall (QH) edge states as spin-dependent injectors and detectors, we observe large, non-local electrical signals across a 5 μm-long, insulating channel only when it is biased into the $\nu=0$ CAF state. Among possible transport mechanisms, spin superfluidity in an antiferromagnetic state gives the most consistent interpretation of the non-local signal's dependence on magnetic field, temperature and filling factors. This work also demonstrates that graphene in the QH regime is a powerful model system for fundamental studies of ferromagnetic and antiferromagnetic spintronics.

11:40 AM

F-III-4: POTENTIAL NEW HYDRIDE SUPERCONDUCTORS

[EFRC – EFree] Maddury Somayazulu[1], Muhtar Ahart[1], Ajay Mishra[1], Maria Baldini[1], Zachary Geballe[1], Hanyu Liu[1], Zhenxian Liu[1], Viktor Struzhkin[1], Roald Hoffmann[2], Neil Ashcroft[2], Russell Hemley[3]
[1]Carnegie Institution of Washington, [2]Cornell University, [3]George Washington University

Theoretical predictions of superconductivity in hydrogen-rich systems have received a boost with the discovery of superconductivity above 200 K (when above 160 GPa) in H_2S. Starting from the earliest predictions of superconductivity in metallic, atomic hydrogen and possibility of reducing the transition pressure by doping as well as tailoring metal hydrides that would apply the optimal chemical pressure, the interplay between theory and experiment has been the hallmark of these studies. The fact that H_3S (identified as the superconducting phase that results from pressurizing H_2S), shows evidence of being a classic, BCS superconductor further confirms the theoretical predictions regarding the possibility of other hydrides showing similar behavior. In particular, hydrides of calcium, yttrium and lanthanum are predicted to have very high transition temperatures. Correspondingly, theory predicts that the formation pressure for these 'superhydrides' also increases appreciably. Using theory as a guiding tool, we have investigated the pressure-temperature-composition phase space of Ca-H_2; Y-H_2; Pd-H_2 and La-H_2. In addition, we have undertaken a systematic survey of the S-Se-P-H_2 system. These experiments requiring megabar pressures and heating metals in hydrogen-rich environments require *in situ* laser heating and synchrotron micro-diffraction. Synthesized samples were characterized by a number of methods including Raman and IR spectroscopy, optical absorption (UV-Vis-NIR-MIR) and reflection both at ambient as well as low temperatures followed by magnetic susceptibility measurements. We report synthesis of $CaH_{2.5}$, CaH_4, CaH_6, YH_x, PdH_x as well as $(H_2S_xSe_{1-x})_2H_2$ and $(H_2S_xP_{1-x})_2H_2$ in addition to $(H_2Se)_2H_2$ that transform to H_3Se above 120 GPa when held below 100 K.

SESSION IV: TUESDAY, JULY 25, 2017; 1:30 – 3:30PM; LINCOLN 6

1:30 PM – Team Science Finalist

F-IV-1: MAGNETIC SKYRMIONS IN FERROMAGNETIC/HEAVY-METAL MULTI-LAYERS

[EFRC – SHINES] Gen Yin[1], Xin Ma[2], Kang L. Wang[1] and Xiaoqin Li[2]
[1]*University of California, Los Angeles,* [2]*University of Texas at Austin*

Magnetic skyrmions are circular, bubble-like magnetic domains in which the spins on the periphery are polarized vertically, the central spin is polarized in the opposite direction, and, in between, the spins smoothly transition between the two opposite polarizations [Fig. 1(a)]. Due to their amazing properties, magnetic skyrmions are considered to be a competitive candidate to replace the traditional magnetic recording technology used in hard disk drives for higher data density, lower power and faster input/output. The size of skyrmions observed in different material systems varies from ~3nm to ~1000nm, which is mainly determined by the intricate competition between different magnetic interactions. Among all these interactions, Dzyaloshinskii-Moriya interaction (DMI) is an important one. When ferromagnetic (FM) thin films are interfacing with metals (HMs), DMI can be induced in the FM layer. The magnitude of this DMI is strongly determined by the structural and chemical details at the interface, providing a cornucopia of engineering degrees of freedom to fine tune the size, the stability, and the switching difficulty of magnetic skyrmions.

Within SHINES, Dr. Kang L. Wang's research group at UCLA has been pioneering in the field of magnetic skyrmions. The team has demonstrated one of the first multilayer devices that operate magnetic skyrmion bubbles at room temperature, namely, MgO/CoFeB/HM thin films [Fig. 1(b)] [1]. Although these devices function at room temperature, the diameter of skyrmions is typically ∼700 nm, which is too large for memory or recording applications. To optimize the interfacial DMI and to further reduce the size, with their world-leading expertise in Brillouin light scattering (BLS) spectroscopy, Dr. Xiaoqin Li's research team at UT Austin carried out systematic investigations in the interfacial DMI at FM/HM interfaces [2]. This technique measures the spectrum of solid-state elementary excitations (in the present case, spin-wave modes, or magnons) through their interaction to incident phonons [Fig. 1(c)]. Due to DMI, the spectrum shifts its frequency in opposite directions [Fig. 1(e)], therefore the DMI magnitude can be quantitatively extracted [Fig. 1(d)].

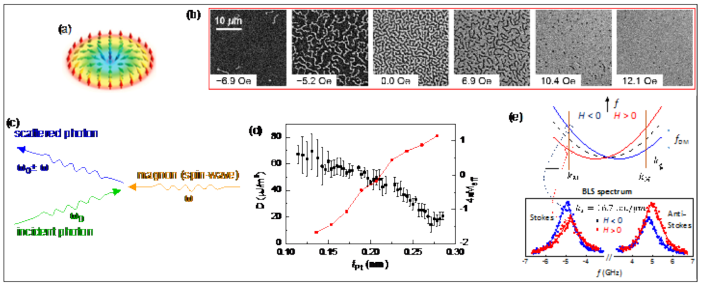


Figure 1: Magnetic skyrmions in ferromagnetic/heavy-metal multilayers. (a) The spin texture of skyrmions in heavy-metal multi-layers. (b) Spin-texture evolution at different magnitudes of applied magnetic fields. (c) Schematic setup of Brillouin-light scattering (BLS) measurement. (d) DMI magnitude at different thickness of HM layers. (e) Rashba-like shift of spin-wave modes and the BLS spectroscopy

Driven by the collaborative platform provided by SHINES, experimental and theoretical resources of different areas were able to combine to systematically investigate the interplay between spin, charge, magnons and phonons. In close collaboration, Wang and Li's research groups were able to design a multilayer structure with two active interfaces and change the magnitude of DMI systematically. Based on these results, the FM/HM material system has been further optimized. Small magnetic skyrmion bubbles of ∼ 70nm have been experimentally observed.

References: [1] G. Yu, P. Upadhyaya, X. Li, W. Li, S. K. Kim, Y. Fan, K. L. Wong, Y. Tserkovnyak, P. K. Amiri, and K. L. Wang. Nano Lett. 17, 261 (2017); [2] X. Ma, G. Yu, X. Li, T. Wang, D. Wu, K. S. Olsson, Z. Chu, K. An, J. Q. Xiao, K. L. Wang, and X. Li. Phys. Rev. B 94, 180408(R) (2016).

Contributions: The UCLA team (G.Y. and K.L.W) modeled, fabricated and tested the skyrmion hosting multi-layer devices. The UT Austin team (X.M. and X.L.) carried out BLS measurements. All team members contributed to the design of the experiment and data analysis.

1:50 PM

F-IV-2: SUPERCONDUCTIVITY IN THE TOPOLOGICAL INSULATOR BI2SE3

[EFRC – CES] James Eckstein[1], Yang Bai[1], Can Zhang[1], David Floetotto[1], Tai Chiang[1], J. C. Seamus Davis[2], Ivan Bozovic[2], Y. Ota[3], T. Hashimoto[3], S. Shin[3]

[1]*University of Illinois, Urbana Champaign,* [2]*Brookhaven National Laboratory,* [3]*University of Tokyo*

By combining materials growth, fabricated transport devices, and angle resolved photoemission spectroscopy we have explored how superconducting pairs propagate in the topological insulator Bi_2Se_3. In regular arrays of niobium islands we find that a zero resistance state occurs via a BKT transition at low temperatures, and that this strongly depends on the contact conductance between the underlying Bi2Se3 film and the islands. The ratio of the carrier mean free path to the island spacing appears to control the temperature at which the array becomes coherent. We've also developed a novel method of preparing samples for ARPES studies. We've made Bi_2Se_3 films of different thicknesses ranging from 4 to 10 molecular layers thick on top of superconducting niobium substrates and studied how the superconductivity from the substrate propagates through the film to the surface which is studied by ARPES at 1.5K. We find that if the Bi_2Se_3 layer is 4 quint layers thick, a strong gap is evident in the ARPES spectrum. However this attenuates rapidly as the films are made thicker. Combining these studies a picture emerges of a strongly anisotropic proximity effect in which the layers in closest contact with the superconductor are strongly proximity coupled and the induced pairs propagate easily in plane but not between planes.

2:10 PM

F-IV-3: TOPOLOGICAL SPINTRONIC HETEROSTRUCTURES AND THEIR PROPERTIES – EXAMPLES OF THE COLLABORATIVE RESEARCH IN SHINES

[EFRC – SHINES] Kang L. Wang[1], Xiaoqin(Elaine) Li[2], Allan MacDonald[2]

[1]*University of California, Los Angele;* [2]*University of Texas at Austin*

Due to the interfacial electron wave hybridization, fascinating and rich spintronic physics can be introduced via proximity effects. Provided by the collaborative platform of SHINES, complex interfaces with non-trivial topology are systematically investigated. Collaborating with Dr. Allan McDonald's team at UT Austin, Wang's research group at UCLA have systematically investigated the gigantic spin-orbit-torque (SOT) ratio observed in the heterostructure formed by magnetic and regular TI bi-layer structures. A plausible explanation of the large SOT ratio has been uncovered. Unlike regular heavy-metal/ferromagnet interfaces, Dirac fermions away from the Fermi level contributes an extra torque originated from the Berry phase, which works together with the k-s locking, resulting in the large SOT ratio. Also, in collaboration with Dr. Xiaoqin Li's group at UT Austin, Wang's group carried out systematic research in the interfacial Dzyaloshinskii-Moriya interaction (DMI) in magnetic heavy-metal multilayers. This interaction is the essential mechanism that maintains the chirality of the domain wall in each magnetic skyrmion, stabilizing

its topological order. Combined with the world-leading Brillouin light scattering technique provided by Li's team, interfacial DMI in the system is now quantitatively understood. By inserting another DMI-active insertion layer, the DMI in the system has been enhanced by a factor of 3. Furthermore, this collaborative project also led to the discovery of the DMI at antiferro-/ferro-magnet heterostructures. The exchange bias of this heterostructure exerts an internal exchange field to the skyrmion hosting layer, such that room-temperature, zero-field skyrmions have been demonstrated experimentally for the first time.

2:30 PM

F-IV-4: OPTICAL PROPERTIES OF THE NARROW-GAP SEMICONDUCTOR FESB$_2$

[CMS – CDMFTS] Christopher C. Homes[1], Qianhang Du[1,2], Cedomir Petrovic[1], Kristjan Haule[3] Sangkook Choi[1,3], Gabriel Kotliar[1,3]
[1]Brookhaven National Lab;[2] Stony Brook University; [3]Rutgers University

The iron antimonide $FeSb_2$ has the highest thermoelectric power factor ever measured. At room temperature this material is a poor metal. As the temperature is reduced, the resistivity either increases (activated response), or decreases (metallic behavior), before increasing dramatically below about 100 K; the thermoelectric power factor is highest in the latter samples, which are said to possess a metal-insulator transition (MIT). The original optical studies revealed a material with broad phonon features and rather ordinary semiconducting behavior at low temperature with an optical gap of $2\Delta \sim 38$ meV. The optical properties have been reinvestigated along all three lattice directions in samples with and without the MIT. At room temperature, an anisotropic optical response is observed; at low temperature, one-dimensional semiconducting behavior is clearly seen along the *b* axis with $2\Delta \sim 76$ meV. The infrared-active lattice modes have also been studied in detail. At low temperature the modes along *b* and *c* axes are extremely narrow, suggesting quasi-ballistic phonons. In addition, several *a* axis lattice modes undergo significant changes below about 100 K, hinting at possible structural changes. Perhaps most surprising is that the optical response is observed to be nearly identical in both types of crystals, which is unexpected given their dramatically different behavior. This suggests that the differences in the transport are likely due to an impurity band, which may also be responsible for the large thermoelectric power factor.

2:50 PM

F-IV-5: THERMAL TRANSPORT ON EXPERIMENTALLY IMPOSED LENGTH SCALES: NON-DIFFUSIVE KINETICS, PHONON MEAN FREE PATHS, AND FIRST-PRINCIPLES MODELING

[EFRC – S3TEC] Vazrik Chiloyan[1], Samuel Huberman[1], Ryan A. Duncan[1], Mojtaba Forghani[1], Lingping Zeng[1], Alexei A. Maznev[1], Nicolas G. Hadjiconstantinou[1], Evelyn Wang[1], Gang Chen[1], Keith A. Nelson[1]
[1]*Massachusetts Institute of Technology*

We have developed time-resolved optical methods to study the fundamentals of microscale and nanoscale phonon transport. Transient thermal grating (TTG) measurements, in which crossed laser pulses generate a sinusoidal heating pattern, reveal transport kinetics far outside of the Fourier "thermal diffusion" limit, highlighting the role of phonons with mean free paths comparable to the experimentally imposed transport length scale. Experiments on prototype semiconductors and alloys, graphite, diamond, and nanopatterned materials, using visible light and extreme UV pulses from FEL sources to reach shorter length scales, reveal the interplay among phonon densities of states, mean free paths, and wavevector-dependent scattering mechanisms that together dictate integrated thermal transport kinetics. The experimental approach is amenable to first-principles modeling with a minimum of assumptions. We developed efficient methods to solve the phonon Boltzmann Transport Equation (BTE), including a variational approach using trial solutions guided by experimental results and the deviational Monte Carlo technique, enabling accurate simulations of thermal transport in complex nanostructured geometries. Good agreement between TTG experiments and first-principles-based BTE calculations was demonstrated. Our experimental data from graphite and diamond posed new challenges for theory and stimulated the development of methods for solving the BTE with the full scattering matrix in nanostructured geometries, which will also be instrumental for analyzing thermal transport in 2D materials such as graphene. We look forward to using x-ray FEL sources for measurements of both thermal transport and mode-specific phonon properties on all length scales to enable comprehensive first-principles modeling of a wide range of materials and structures.

3:10 PM

F-IV-6: TRANSPORT PROPERTIES OF CORRELATED FESB$_2$: FIRST PRINCIPLES COMBINED WITH DYNAMICAL MEAN FIELD THEORY

[CMS – CDMFTS] Sangkook Choi[1], Walber Hugo Brito[1], Christopher C. Homes[1], Cedomir Petrovic[1], Gabriel Kotliar[1,2]
[1]Brookhaven National Lab; [2]Rutgers University

Over the past decade, thermoelectric materials are of revived interest due to increasing social needs for renewable energies. In 2007, a German group made the surprising discovery that at low temperatures, the correlated semiconductor $FeSb_2$ with the marcasite crystal structure exhibits a giant thermoelectric power factor of 2300 $\mu WK^{-2}cm^{-1}$, more than 65 times the value for state-of-the art thermoelectric materials such as Bi_2Te_3. From the standpoint of basic science, correlated material $FeSb_2$ raises interesting questions: the mechanism for the giant thermoelectric power factor. In this talk, I'll discuss the role of electronic correlation on the charge and heat transport properties of $FeSb_2$ by calculating transport properties of $FeSb_2$ within various theories (DFT, GW, LDA+DMFT and MQSGW+DMFT) with different level of approximations to the electronic correlation.

G. SEPARATION SCIENCE

SESSION II: TUESDAY, JULY 25, 2017; 8:30 – 10:10 AM; THURGOOD MARSHALL WEST

8:30 AM

G-II-1: ENGINEERING NANOPOROUS MATERIALS WITH INCREASED ACID GAS RESISTANCE

[EFRC – UNCAGE-ME] Guanghui Zhu[1], Simon H. Pang[1], Yang Liu[1], Uma Tumuluri[2], Zili Wu[2], David S. Sholl[1], Sankar Nair[1], Christopher W. Jones[1], Ryan P. Lively[1]
[1]Georgia Institute of Technology, [2]Oak Ridge National Laboratory

Microporous materials such as metal-organic frameworks (MOFs), zeolitic imidazolate frameworks (ZIFs) and porous organic cages (POCs) have significant potential to enhance and revolutionize molecular separation processes. The stability of the material in the face of aggressive contaminants such as H_2S, SO_X, NO_X, and water, is an important challenge not often discussed in the literature. Here, we assess the resistance of ZIF-8 and the POC CC3 to SO_2 exposure. The chemical and physical degradation mechanism of the two materials is discussed, and promising routes to engineering improved acid gas resistance are developed.

8:50 AM

G-II-2: DETERMINING MECHANISMS OF GAS ADSORPTION IN MOFS BY COMBINING X-RAY SPECTROSCOPY AND THEORY

[EFRC – CGS] Walter S. Drisdell[1], Christopher M. McGuirk[2], Liwen F. Wan[1], Gregory Su[1], Rebecca L. Siegelman[2], Philip J. Milner[2], David Prendergast[1], Jeffrey R. Long[1,2]
[1]Lawrence Berkeley National Laboratory (LBNL); [2]University of California, Berkeley

In order to enable directed design of porous materials for efficient gas separations such as carbon capture, we must understand (and tune) mechanisms for chemisorption of gases in such materials. A combined X-ray spectroscopy and first principles theory approach played a key role in determining a novel insertion mechanism for chemisorption of CO_2 in diamine-appended metal-organic frameworks (MOFs) that produces step-shaped adsorption isotherms with the potential for significantly increased separation efficiency. We now apply this approach towards understanding how to extend and tune this chemistry. We demonstrate that a similar diamine-appended MOF is capable of chemisorbing CS_2, a toxic by-product of Rayon and cellophane production that also contributes to acid rain, via an analogous insertion mechanism. We also explore ways to increase CO_2 capture efficiency by employing different diamines to tune the position of the “step” in the isotherm. We find that a promising candidate material exhibits competing adsorption mechanisms, one by insertion and the other by formation of hydrogen bonded carbamic acid pairs. By probing the dominant adsorption pathway as a function of CO_2 pressure, we aim to determine if the pairing mechanism is purely parasitic, and if so, how suppress it in favor of the insertion mechanism.

9:10 AM

G-II-3: LINKING MORPHOLOGY AND INTERFACIAL INTERACTIONS TO ACID GAS UPTAKE

[EFRC – UNCAGE-ME] Bobby G. Sumpter[1], Jan-Michael Y. Carrillo[1], Matthew E. Potter[2], Miles A. Sakwa-Novak[3], Simon H. Pang[2], Guanghui Zhu[2], Gernot Rother[1], Ryan P. Lively[2], Zili Wu[1], Kuan Huang[1,4], Sheng Dai[1,5], Christopher W. Jones[2]

[1]*Oak Ridge National Laboratory,* [2]*Georgia Institute of Technology,* [3]*Global Thermostat, LLC,* [4]*University of Tennessee*

Composite gas sorbents, formed from an active polymer phase and a porous support, are promising materials for the separation of acid gasses from a variety of gas streams. Significant changes in sorption performance (capacity, rate, stability etc.) can be achieved by tuning the properties of the polymer and the nature of interactions between polymer and support. In this regard, by using an integrated computational and experimental approach we have developed an understanding for the effect of silica support morphology on polymer dynamics and CO_2 adsorption capacities in aminopolymer/silica composites. Different morphologies of the mesoporous silica supports ranging from hexagonally packed cylindrical pores of SBA-15, double gyroids of KIT-6 and MCM-48, and cage-like structures of SBA-16 were used to form composites with poly(ethyleneimine) (PEI). Large-scale molecular-based simulations predicted that a 3D pore morphology, such as that of KIT-6, MCM-48, and SBA-16 have a lower probability of primary amine and surface silanol associations and thus would have faster segmental mobility of the PEI, which translates to higher CO_2 uptake in comparison to a 2D pore morphology such as that of SBA-15. Indeed, it is found that KIT-6 has higher CO_2 uptake than SBA-15 at equivalent PEI loading, even though both supports have similar surface area and pore volume. Other types of PEI supports were studied utilizing the basic design concept of optimizing interfacial interactions and pore morphology. In particular Boron Nitride-PEI and Amorphous Scrambled Porous Organic Cage (ASPOC)-PEI composites show interesting acid gas uptake behavior.

9:30 AM – Team Science Finalist

G-II-4: RATIONAL DESIGN OF NEW MATERIALS FOR CARBON DIOXIDE CAPTURE

[EFRC – CGS] Rebecca L. Siegelman,[1] Alexander C. Forse,[1] Phillip J. Milner,[1] Thomas M. McDonald,[1] Miguel I. Gonzalez,[1] Tomče Runčevski,[1] Jeffrey D. Martell,[1] Jarad A. Mason,[1] Jung-Hoon Lee,[1,2] Bess Vlaisavljevich,[1] Walter S. Drisdell,[2] Jeffrey B. Kortright,[2] David Prendergast,[2] Jeffrey B. Neaton,[1,2,3] Berend Smit, Jeffrey A. Reimer,[1] Jeffrey R. Long[1,2]

[1]University of California, Berkeley; [2]Lawrence Berkeley National Laboratory; [3]Kavli Energy NanoSciences Institute at Berkeley

The capture of CO_2 from point-source emitters such as coal-fired power plants has been proposed as a promising strategy to mitigate greenhouse gas emissions. Toward that end, the Center for Gas Separations (CGS) is developing new adsorbents to minimize the energetic costs of CO_2 separations. Initial efforts coupled computation and experiment to study MOF-74 metal–organic frameworks, which bind gases at unsaturated metal(II) sites in the pore interior. These studies showed that high CO_2 capacity and selectivity could be achieved from dry gas streams, but H_2O outcompetes CO_2 at equilibrium. To address this, amine-appended adsorbents capable of maintaining CO_2 capacity under humid conditions were developed. In particular, adsorbents of the form M_2(dobpdc)(diamine)$_2$ (M = Mg, Mn, Fe, Co, Ni, Zn; dobpdc^{4-} = 4,4′-dioxidobiphenyl-3,3′-dicarboxylate) feature step-shaped CO_2 adsorption isotherms. This switch-like adsorption enables the full CO_2 working capacity to be achieved with a minimal pressure or temperature swing. By combining computation, XRD, XAS, IR, and NMR, a co-operative mechanism involving the formation of ammonium carbamate chains was found (Figure 1).

The adsorption thermodynamics of amine-appended MOFs can be tuned by modifying the constituent metal or diamine, enabling rational design of adsorbents for specific CO_2 separations. In this manner, a new material was designed to minimize the energetic cost of CO_2 capture from the flue gas of coal-fired power plants. This material is stable to over 1000 cycles with a high CO_2 working capacity of 2.4 mmol/g and modest regeneration temperature of 100 °C. *In situ* diffraction and NMR methods were developed to characterize the unusual CO_2 adsorption properties of this material and revealed a complex mechanism involving formation of a mixture of ammonium carbamate and carbamic acid pairs. In future efforts, next-generation adsorbents will be designed with the support of computational screening, and diamine-appended frameworks will be incorporated within mixed-matrix membranes.

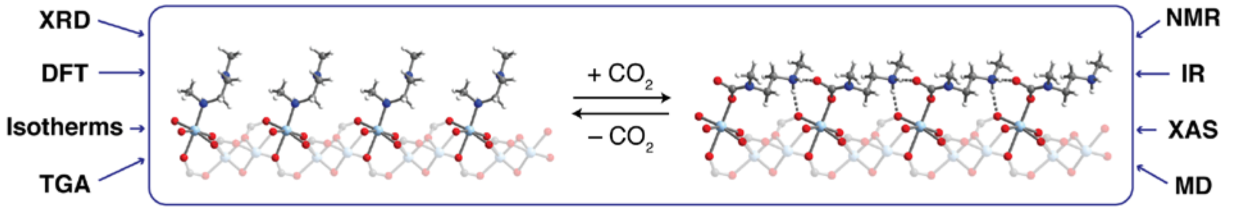


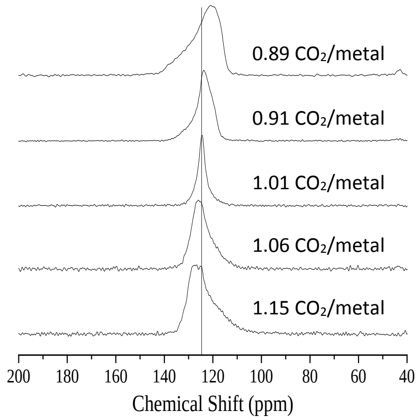
Figure 1. Multidisciplinary approach employed in the CGS to rationally design new materials for energy-efficient CO_2 sorption.

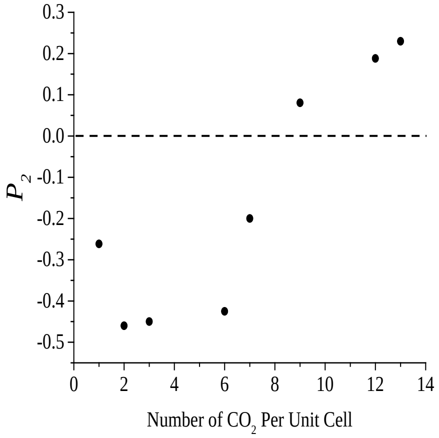
Contributions: R.L.S., P.J.M, J.D.M., T.M.M., and J.A.M. designed, synthesized, and characterized the adsorbents under the advisement of J.R.L. A.C.F. collected and analyzed NMR data with support from J.A.R. R.L.S., M.I.G., T.R., and J.A.M. collected and analyzed the diffraction data. J.-H.L., B.V., J.B.N., and B.S. performed the computational work. W.S.D. and J.B.K. collected and analyzed the XAS data.

9:50 AM – Team Science Finalist

G-II-5: UNDERSTANDING STRUCTURE AND DYNAMICS OF CO_2 ADSORBED IN OPEN-SITE METAL-ORGANIC FRAMEWORKS

[EFRC – UNCAGE-ME] Robert M. Marti[1], Joshua D. Howe[2], Cody R. Morelock[2], Krista S. Walton[2], Mark S. Conradi[1,3] , David S. Sholl[2], Sophia E. Hayes[1]
[1]Washington University, [2]Georgia Institute of Technology, [3]ABQMR





Metal-organic frameworks are crystalline organic-inorganic hybrid materials that have been of interest for adsorption applications for their tunability, high crystallinity, and high surface areas. Mg-MOF-74 has long been of interest for its exceptional gravimetric uptake of CO_2 at flue-gas relevant conditions. CO_2 adsorption in Mg-MOF-74 is well studied, but most work has focused on understanding adsorption at the undercoordinated open-metal sites that line the pores. Despite this, loadings of CO_2 in Mg-MOF-74 at even modest partial pressures can exceed one CO_2 per open-metal site, requiring a more nuanced picture to understand the behavior and loading of CO_2. Recent neutron diffraction studies have shown that CO_2 occupies not only these primary adsorption sites, but also "secondary" and even "tertiary" sites that exist within the MOF pore.[1]

Here we present a joint experimental NMR and theory study that demonstrates that higher CO_2 loadings qualitatively alter the structure of adsorbed CO_2 within the MOF pore. Constructing special NMR hardware to deliver gases at variable temperature and pressure, we have found that the ^{13}C NMR lineshape evolves in a predictable fashion as these different sites become occupied. We show that the time-averaged value of the second Legendre polynomial, P_2, which maps to the alignment of CO_2 with respect to the MOF pore axis, allows understanding of the so-called "sign" of the NMR lineshape—which shifts in appearance with loading in a highly sensitive and informative manner. The evolution of the NMR lineshape with CO_2 loading, which probes the aggregate dynamics and structure of adsorbed CO_2, agrees exceptionally well with the DFT-predicted loading-dependent structures of CO_2 within the Mg-MOF-74 pore through analysis in terms of P_2. NMR experiments also point to qualitative differences between the behavior of CO_2 in Mg-MOF-74 and Mg-Cd-MOF-74, which we rationalize in terms of theoretical calculations for mixed-metal MOF-74 systems[2] and our calculations on Mg-MOF-74. Importantly, the NMR spectra are difficult to interpret without the detailed picture of adsorption sites provided by DFT, and the combined effect demonstrates how experiments can reinforce the DFT models of collective CO_2 behavior.

Contributions: CRM and KSW performed materials synthesis and characterization. RMM, MSC and SEH performed NMR experiments. JDH and DSS conducted DFT calculations. All authors contributed to data analysis and interpretation.

References: [1] Queen, W. L.; Hudson, M. R.; Bloch, E. D.; Mason, J. A.; Gonzalez, M. I.; Lee, J. S.; Gygi, D.; Howe, J. D.; Lee, K.; Darwish, T. A.; James, M.; Peterson, V. K.; Teat, S. J.; Smit, B.; Neaton, J. B.; Long, J. R.; Brown, C. M. *Chem. Sci.* **2014**, *5,* 4569. [2] Howe, J. D.; Morelock, C. R.; Jiao, Y.; Chapman, K. W.; Walton, K. S.; Sholl, D. S. *J. Phys. Chem. C* **2017**, *121*, 627–635.

H. SOLAR ENERGY CONVERSION

SESSION I: MONDAY, JULY 24, 2017; 3:00 – 5:00PM; THURGOOD MARSHALL SOUTH

3:00 PM

H-I-1: MOLECULAR AND POLYMER CHROMOPHORE-CATALYST ASSEMBLIES FOR SOLAR FUELS PRODUCTION

[EFRC – UNC] Junlin Jiang[1], Gyu Leem[1], Zachary A. Morseth[2], Toan Pho[3], Benjamin D. Sherman[2], Thomas J. Meyer[2], John M. Papanikolas[2], John R. Reynolds[3], Kirk S. Schanze[1]
[1]University of Texas at San Antonio; [2]University of North Carolina at Chapel Hill; [3]Georgia Institute of Technology

Supramolecular assemblies of visible light-harvesting chromophores and metal-complex based catalysts for multi-electron oxidation and reduction are the subject of investigation within the Center for Solar Fuels EFRC with the goal of developing artificial photosynthesis systems. Molecular and polymeric assemblies are constructed using several approaches, including covalent assembly, templated self-assembly, and polyelectrolyte layer-by-layer assembly. The chromophore-catalyst assemblies are mounted at the interface of wide-bandgap metal oxide semiconductors where light-induced charge transfer and catalysis takes place. Mechanistic investigations using electrochemistry, photoelectrochemistry and time-resolved spectroscopy provide detailed insight concerning the dynamics and efficiency of light-induced charge transfer and catalytic water oxidation. This talk will highlight recent accomplishments in the Center focused on self-assembled systems at SnO_2/TiO_2 core/shell and nano-ITO mesoporous electrodes.

3:20 PM

H-I-2: COHERENT WAVEPACKETS IN THE FMO COMPLEX ARE ROBUST TO SPECTRAL PERTURBATIONS BY MUTAGENESIS

[EFRC – PARC] Margherita Maiuri[1], Evgeny Ostroumov[1], Rafael G. Saer[2], Robert E. Blankenship[2], Gregory Scholes[1]
[1]Princeton University; [2]Washington University

Nature has developed sophisticated ways to control photosynthetic complexes where the arrangement of the individual pigments is engineered to funnel the absorbed energy and transfer it to reaction centers with evolutionary efficiency (> 95%). In the last decade, it has been discovered that light-harvesting in Nature may involve quantum-coherence. The early observation of long-lived coherent oscillations at cryogenic and ambient temperatures in the photosynthetic complexes of a green sulfur bacteria, the Fenna-Matthews-Olson (FMO) complex, has generated deep interest in the role of such beatings in energy transfer. Theoretical studies have now predicted that the coherent oscillations observed in many ultrafast experiments are assigned to vibronic coherence, a quantum mechanical mixture of vibrational levels and excited electronic states.

Here we study the coherent oscillations in FMO complex by exploiting the combination of femtosecond spectroscopy and biological mutagenesis. We report a pump-probe investigation of a series of FMO complexes, where site-mutagenesis enabled us to perturb the energies of selected chromophores, thereby changing their electronic interactions, and compare the generated coherences. Our experiments reveal two oscillations dephasing on a picosecond time scale—both at 77K and room temperature, which are surprisingly insensitive to the spectral

mutations. By studying these coherences with selective excitation of the lowest excitonic state, we assign them to ground state vibrational oscillations. Furthermore, we explicitly observe delocalization of the electronic excitation over several light-harvesting chromophores. This discovery contributes to the discussion about the influence of vibronic coupling in light-harvesting and how artificial systems should be designed.

3:40 PM

H-I-3: CONTROLLING ENERGY TRANSFER IN DNA-BASED EXCITONIC CIRCUITS

[EFRC – CE] James Banal[2], Toru Kondo[2], Nicolas Sawaya[1], Remi Veneziano[2], Wei Jia Chen[2], Alan Aspuru-Guzik[1], Mark Bathe[2], Gabriela Schlau-Cohen[2]
[1]Harvard University; [2]Massachusetts Institute of Technology

Photosynthetic light harvesting converts absorbed photoenergy to chemical energy with a remarkable near-unity quantum efficiency. This remarkable efficiency arises through the organization of the dense chromophore units that are held by protein scaffolds. The close packing of these chromophores leads to electronic interactions that optimize the photophysical properties to produce a manifold of excited states that facilitates energy transfer. Synthetic mimics of these chromophore structures rely on supramolecular assembly of dyes, driven by hydrophobic interactions, resulting to nanostructures that are physically difficult to control, which has previously been a major limitation for designing artificial light-harvesting systems with controlled energy transport. We overcome this limitation through the use of DNA origami as a scaffold to control the nanoscale assembly of chromophores. In our investigations, we leverage the innate property of a dye, pseudoisocyanine (PIC), to bind selectively on specific DNA sequences to form superradiant aggregates. Through this specificity, we control the formation and size of these superradiant aggregates. Furthermore, we demonstrate that these superradiant aggregates facilitate energy transfer more efficiently than randomly bound, monomeric dyes. Using this building block, we have explored the use of superradiant PIC aggregates in exciton circuits assembled on double-crossover (DX) tile DNA assemblies. The DX tiles are an enabling toolbox for the construction of designer exciton circuits that are useful for a myriad of applications, including solar energy conversion.

4:00 PM

H-I-4: ULTRAFAST INJECTION AND RECOMBINATION DYNAMICS AT SnO_2/TiO_2 CORE/SHELL AND NIO INTERFACES FOR SOLAR FUELS PRODUCTION

[EFRC – UNC] Melissa K. Gish, Robert J. Dillon, Lenzi J. Williams, David F. Zigler, M. Kyle Brennaman, Alexander M. Lapides, Leila Alibabaei, James F. Cahoon, Thomas J. Meyer, John M. Papanikolas
University of North Carolina at Chapel Hill

One of the great challenges in the development of light-driven solar fuels production is the formation of a long-lived charge-separated state that enables catalytic water oxidation and carbon dioxide reduction in a tandem dye sensitized photoelectrosynthesis cell (DSPEC). While electron-hole recombination times on TiO_2 are sufficient for dye sensitized solar cell function, they are far too short for efficient water oxidation at the DSPEC photoanode. The fabrication of core/shell nanoparticles that localize the injected electron in the core of the particle is one strategy for extending the charge separation lifetime. We have used time-resolved absorption methods, on time scales ranging from femtoseconds to milliseconds, to follow the interfacial electron injection and recombination dynamics from photoexcited Ru(II) chromophores into SnO_2/TiO_2 core/shell nanoparticles. Our results show that while charge separation can be extended, the presence of the TiO_2 shell also gives rise to a sub-nanosecond recombination component that impacts a significant fraction of the injected electrons. Furthermore, the tandem DSPEC device requires the coupling of a photoanode to a photocathode. The charge separated state at the photocathode is created by hole injection into a *p*-type metal oxide, such as NiO, which typically exhibits fast sub-nanosecond recombination. Transient absorption measurements on the Ru(II)/NiO photocathodes under bias reveal that the short-lived charge-separated state is the result of a non-geminate recombination process involving holes present in the unfilled valence band.

4:20 PM

H-I-5: MODELING, SIMULATION AND PROTOTYPING OF SOLAR-FUEL DEVICES

[Hub – JCAP] Chengxiang Xiang[1]
[1] *California Institute of Technology*

Efficient solar-fuel devices require synergistic assembly of light absorbers, electrocatalysts, membrane separators and electrolytes. Over the past years, we have developed a robust multi-physics, multi-dimensional, solar-fuel device model that accounts for all key photoelectrochemical processes to guide the materials discovery, to define operational conditions and constraints and to optimize and explore viable device architectures for solar-driven water-splitting devices as well as solar-driven CO_2 reduction devices. In particular, the modeling revealed the local pH and CO_2 concentration at the electrode surface spatially and defined operational constraints and conditions for systems to perform sustainable and efficient solar-driven CO_2 reduction.

Through the modeling guided device development, integrated solar-hydrogen devices with conversion efficiency exceeded 10% and device stability exceeded 100 hours have been demonstrated at the laboratory scale (~ 1 cm^2) with product separations. Various device configurations have been implemented by the prototyping team including photocathode devices and photoanode devices, as well as devices that operated at alkaline conditions, at acidic conditions and at near-neutral pH conditions. Leveraging the solar water-splitting work, we have recently constructed a proof of concept, a bipolar-membrane based solar-driven CO_2 reduction device with a high solar-to-fuel conversion efficiency of 10% under 1.0 sun illumination. The device operated in two electrolytes with different pHs to achieve the optimal performance and the lowest overpotentials for oxygen evolution reaction and CO_2 reduction to formate with robust product separations.

4:40 PM – Team Science Finalist

H-I-6: THE PYRIDINE ALKOXIDE LIGAND WORKS FOR WATER OXIDATION CATALYSTS BOTH IN THEORY AND IN PRACTICE

[EFRC – ANSER] Benjamin Rudshteyn,[1] Kelly L. Materna,[1] Nathan T. La Porte,[2] Katherine J. Fisher,[1] Ke R. Yang,[1] Svante Hedstrom,[1] Jose F. Martinez,[2] Gihan Kwon,[3] Jiyun Hong,[2] David M. Tiede,[3] Lin X. Chen,[2,3] Michael R. Wasielewski,[2] Robert H. Crabtree,[1] Gary W. Brudvig,[1] Victor S. Batista[1]
[1]Yale University, [2]Northwestern University, [3]Argonne National Laboratory

Catalytic water oxidation is a critical bottleneck in the generation of solar fuels, a challenging reaction that requires active and robust catalysts. Efficient transition metal catalysts require ligands that can stabilize high oxidation states, as necessary for oxidative catalysis and at the same time resist degradation under the harsh oxidative conditions. We find that the ligand 2-(2′-pyridyl)-2-propanoate (pyalk) is an exceptional chelating group that fulfills the necessary requirements. Through collaborative theoretical and experimental efforts of research groups working within the ANSER Center, we have determined the structures and mechanisms for pyalk-containing water-oxidation catalysts. Combining computational modeling and X-ray spectroscopy, we have determined the structure of an active Ir-pyalk dimeric species in solution (Figure 1),[1] and determined the underlying water-oxidation mechanism. Furthermore, we have developed and characterized a catalytic surface-bound species using IR spectroscopy.[2] We have also developed a $Cu^{II}(pyalk)_2$ electrocatalyst and characterized its water-oxidation mechanism.[3] This same suite of collaborative theoretical and experimental methods is now being applied to understanding CO_2 reduction via super-reducing Re-perylenedimiide systems driven with near-infrared light.[4]

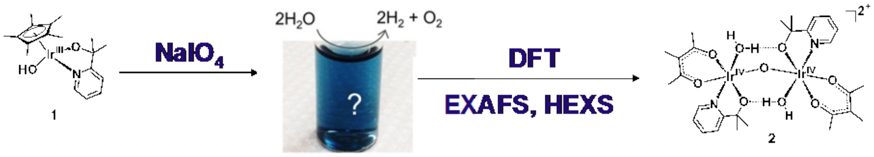


Figure 1. Precatalyst **1** is chemically activated to give an active water-oxidation catalyst. Combined theoretical calculations and experimental X-ray spectroscopies provided the structure of the catalyst, **2**.

[1]Ke R. Yang, et al. *J. Am. Chem. Soc.* **2016**, *138*, 5511. [2]Kelly L. Materna, et al. *ACS Catal.* **2016**, *6*, 5371. [3]Katherine J. Fisher, et al. *ACS Catal.* **2017**, *7*, 3384. [4]Nathan T. La Porte, et al. *Chem. Sci*. **2017**, *Advance*: DOI: 10.1039/c6sc05103k.

Contributions: BR, SH, and KRY performed theoretical density functional theory calculations and modeling of spectroscopy. KLM and KJF performed synthesis and characterization by electrochemistry and UV-Vis/IR spectroscopy. NTLP and JFM performed experiments for the Re-PDI project. GK and JH conducted EXAFS experiments. DMT, LXC, MRW, RHC, GWB, and VSB supervised the work. All authors contributed to the discussion and contributed to their respective manuscripts.

SESSION II: TUESDAY, JULY 25, 2017; 8:30 – 10:10 AM; THURGOOD MARSHALL SOUTH

8:30 AM

H-II-1: LEAD-FREE PEROVSKITE FILMS FOR HETEROJUNCTION DEPLETED PEROVSKITE SOLAR CELLS

[EFRC – ANSER] Feng Hao[1], Weijun Ke[1], Duyen H. Cao[1], Michelle Chen[1], Chan Myae Myae Soe[1], Tobin J. Marks[1], Michael R. Wasielewski[1], Mercouri G. Kanatzidis[1]
[1]*Northwestern University*

Organo-lead halide perovskite solar cells have gained enormous significance and have now achieved power conversion efficiencies of similar to 20%. However, the potential toxicity of lead in these systems raises environmental concerns for widespread deployment. We have investigated solvent effects on the crystallization of the lead-free methylammonium tin triiodide ($CH_3NH_3SnI_3$) perovskite films in a solution growth process. Highly uniform, pinhole-free perovskite films are obtained from a dimethyl sulfoxide (DMSO) solution via a transitional $SnI_2{\cdot}3DMSO$ intermediate phase. This high-quality perovskite film enables the realization of heterojunction depleted solar cells based on mesoporous TiO_2 layer but in the absence of any hole-transporting material with an unprecedented photocurrent up to 21 mA cm^{-2}. Charge extraction and transient photovoltage decay measurements reveal high carrier densities in the $CH_3NH_3SnI_3$ perovskite device which are one order of magnitude larger than $CH_3NH_3PbI_3$-based devices but with comparable recombination lifetimes in both devices. The relatively high background dark carrier density of the Sn-based perovskite is responsible for the lower photovoltaic efficiency in comparison to the Pb-based analogues. These results provide important progress toward achieving improved perovskite morphology control in realizing solution-processed highly efficient lead-free perovskite solar cells.

8:50 AM

H-II-2: LUMINESCENT 2D METAL HALIDE PEROVSKITE NANOPLATELETS

[EFRC – CE] Mark Weidman[1], Daniel Congreve[1], Michael Seitz[1], Marc Baldo[1], William Tisdale[1]
[1]*Massachusetts Institute of Technology*

Colloidal perovskite nanoplatelets are a promising new class of semiconductor nanomaterials, exhibiting bright luminescence, tunable and spectrally narrow absorption and emission features, strongly confined excitonic states, and facile colloidal synthesis. These new nanomaterials, which are only a few unit cells in thickness, experience the effects of strong dielectric and quantum confinement – leading to narrow and blue-shifted absorption / emission as compared to the bulk state – allowing lead bromide and lead iodide nanoplatelets to cover the entire visible range. In this talk I will present an overview of colloidal perovskite nanoplatelets: how they are made, what are their capabilities, why 2D is beneficial, and where these materials are headed. We draw analogues to solid phase layered perovskites, cadmium selenide nanoplatelets, and 2D transition metal dichalcogenides to emphasize some of the most promising attributes of 2D materials such as their penchant for directional emission, fast /directional energy transfer, strong exciton binding energy, and reduced dielectric screening effects. We discuss the interesting physics present in these materials, remaining stability issues, and the future applications for nanoplatelets in LEDs, photovoltaics, photodetectors, and lasers.

9:10 AM

H-II-3: NOVEL HIGH PERFORMANCE P- AND N-TYPE ZINTL THERMOELECTRICS

[EFRC – S3TEC] Jing Shuai[1], David J. Singh[2], Jifeng Sun[2], Jun Mao[1], Shaowei Song[1], Qing Zhu[1], Yumei Wang[1], Ran He[1], Jiawei Zhou[3], Gang Chen[3], Zhifeng Ren[1]
[1]University of Houston; [2]University of Missouri, Columbia; [3]Massachusetts Institute of Technology

> We report the discovery of new Zintl phase p- and n-type thermoelectrics with very high performance including unprecedented combinations of high peak ZT, high power factor and high average ZT. These materials were discovered by a synergistic approach combining experimental synthesis and characterization, computational screening, modeling based on combinations of first principles and experimental data, and detailed theoretical/experimental transport studies. We report new strategies for producing high performance in thermoelectric materials discovered during this research, for example manipulation of the scattering mechanisms to increase mobility while at the same time reducing thermal conductivity. We find an n-type Mg_3Sb_2 based composition, nominally $Mg_{3.2-x}Nb_xSb_{1.5}Bi_{0.5}Te_{0.01}$ that has a peak ZT in excess of 1.5 with an unprecedented high average ZT~1.1 over the technologically important range 298-773 K, which would enable over 15% energy conversion efficiency when operated over this temperature range. We report p-type compositions based on the same structure type with ZT ~ 1.3.

9:30 AM

H-II-4: LUMINESCENT CONCENTRATORS AS LIGHT COMPRESSORS

[EFRC – LMI] A. Paul Alivisatos[1,2]
[1]University of California, Berkeley; [2]Lawrence Berkeley National Laboratory

> How tightly can we focus light? This presentation will explore the limits of concentration of sunlight with luminescent concentrators. The underlying thermodynamic limits will serve as a reference point and challenge for the fabrication of atomically precise light emitters and photonic cavities.

9:50 AM

H-II-5: TRANSPORT IN 2D METAL-ORGANIC FRAMEWORKS

[EFRC – CE] M. Dinca[1], G. Skorupskii[1], L. Sun[1], M. Baldo[1], J. Li[1], W. Li[1], W. Tisdale[1]
[1]Massachusetts Institute of Technology

> Metal-Organic Frameworks (MOFs) are more well-known for their high surface area, porosity, and potential applications in gas storage or capture, which are at odds with applications in optoelectronics that require efficient charge and/or exciton transport. Inspired by strongly coupled molecular systems with singlet biradical ground states, we have recently devised new MOFs that exhibit semiconductor or even metallic behavior. These are made primarily from two-dimensional honeycomb lattices self-assembled from trigonal organic radical ligands and square-planar metal ions. We will discuss the fundamental properties of these materials as they relate to charge transport and their potential applications in optics.

SESSION III: TUESDAY, JULY 25, 2017; 10:40 AM – 12:00PM; THURGOOD MARSHALL SOUTH

10:40 AM

H-III-1: NANOPHOTONICS FOR TAILORING EMISSION AND ABSORPTION OF LIGHT

[EFRC – S3TEC] Nicholas Rivera[1], Ognjen Ilic[3], Arny Leroy[1], Bikram Bhatia[1], Kyle Wilke[1],
Peter Bermel[2], Ivan Celanovic[1], Ido Kaminer[1], Bo Zhen[1], John D. Joannopoulos[1],
Evelyn N. Wang[1], Gang Chen[1], and Marin Soljacic[1].
[1]*Massachusetts Institute of Technology,* [2]*Purdue University;* [3]*Caltech*

Nanophotonics offers many different opportunities for tailoring absorption, or emission of light; in turn this could of course be potentially very useful for many energy conversion applications. We will present our recent work on exploring nanophotonics for tailoring emission from incandescent light sources (at T~3000K): for example, emission into infrared can be dramatically reduced compared to emission into visible. We will also present our recent work in which we consider spontaneous emission of quantum emitters (e.g. atoms, or quantum dots) in the presence of 2D-material plasmons. Wavelength of these plasmons is dramatically smaller than the wavelength of corresponding light in air. As a result, many "forbidden" transitions can now be allowed.

11:00 AM

H-III-2: QUANTUM DOT DEVICE STRUCTURES FOR HIGH EFFICIENCY PHOTOCONVERSION

[EFRC – CASP] Joseph M. Luther[1], Jun Du[2], Tianshuo Zhao[3], Erin M. Sanehira[1,4], Ashley R. Marshall[1,5], Abhishek Swarnkar[1,6], Jeffrey A. Christians[1], Greg F. Pach[1,5], Hyeong Jin Yun[2], Tianshuo Zhao[3], Earl D. Goodwin[3], Jiacen Guo[3], Han Wang[3], Benjamin T. Diroll[3], Christopher B. Murray[3], Cherie R. Kagan[3], Matthew C. Beard[1], Victor I. Klimov[2]
[1]*National Renewable Energy Laboratory;* [2]*Los Alamos National Laboratory;* [3]*University of Pennsylvania;*
[4]*University of Washington;* [5]*University of Colorado;* [6]*Indian Institute of Science Education and Research*

Advanced architectures are required to exploit the novel properties of quantum dots (QDs) in devices. We will discuss recent work involving QD-specific photovoltaic (PV) architectures for various material systems. For instance, CASP has an established effort in QD-sensitized TiO_2 PVs, devices that specifically take advantage of the strong light harvesting of near-IR-active QDs based on toxic-element-free $CuInSe_{2-x}S_x$. Through optimization of both the QDs and the fabrication methods, we have recently achieved efficiencies greater than 10%, approaching the record values for dye-sensitized PVs. Meanwhile, in more conventional thin-film devices, we have introduced the use of CdSe QD buffer layer in PbS QD solar cells. Because the surface- and size-tunable electronic properties of CdSe can be used to optimize carrier concentration and energy band positions, the buffer layer suppresses interface recombination *while contributing additional photogenerated carriers*, leading to a 25% increase in the overall efficiency.

Finally, we will discuss our new effort in $CsPbI_3$ QD PV cells. The cubic phase of bulk $CsPbI_3$—the variant with desirable bandgap for PVs—is typically only stable at elevated temperatures. We describe α-$CsPbI_3$ QD films that retain the cubic phase at room temperature, an important advance over the bulk thin-film form that gives this customizable new material system incredible potential for many applications ranging from PVs to light-emitting diodes (LEDs), displays and lasers. In this talk, we will present PV devices with record-high V_{OC} of 1.23 V, and NREL-certified efficiency of 13.4%, as well as LED operation with low turn-on voltage and bright, tunable emission.

11:20 AM

H-III-3: 3D GRADIENT REFRACTIVE INDEX MICRO-OPTICS FOR ENHANCED CONTROL OF LIGHT

[EFRC – LMI] Paul V. Braun[1], Christian Ocier[1], Neil Krueger[1], John A. Rogers[1], A.L. Holsteen[2], Mark L. Brongersma[2]
[1]University of Illinois at Urbana-Champaign, [2]Stanford University

Microscale photonic elements with complex 3D distributions of internal optical constants are challenging to fabricate, yet offer unique opportunities for both refractive and diffractive control of light propagation. We have now developed a platform starting with the electrochemical formation of porous silicon, followed by materials conversion to the wide set of materials that can be grown via gas-phase deposition strategies, to form 3D gradient refractive index micro-optics including flat lenses, Bragg mirrors, polarization sensitive optical splitters and even complex structures with nearly arbitrary refractive index distributions. In this work, we have a particular focus on micro-optics important for solar energy harvesting. For solar applications, the conversion of porous silicon to silica and titania enabled the optics to operate in the visible with minimal loss. This approach for example enables formation of structures with integrated antireflection coatings (or index matched layers). A detailed inverse design strategy was developed, starting with the desired optical properties, which was then used to generate a refractive index profile, which in turn was used to generate the required time-varying electrochemical etch parameters necessary to form the complex structure of interest.

11:40 AM – Team Science Finalist

H-III-4: TAILORING THERMAL EMISSION FOR HIGH PERFORMANCE SOLAR THERMOPHOTOVOLTAIC DEVICES

[EFRC – S3TEC] David M. Bierman[1], Veronika Stelmakh[1], Andrej Lenert[1,2], Veronika Rinnerbauer[1,3], Walker R. Chan[1], Ivan Celanovic[1], Marin Soljacic[1], and Evelyn N. Wang[1]

[1]Massachusetts Institute of Technology; [2]Currently at University of Michigan – Ann Arbor; [3] Currently at Johannes Kepler University Linz

Solar thermophotovoltaics (STPVs) present an enormous opportunity for the efficient conversion of high-grade thermal energy to electricity. These solid-state devices rely on a heat source to generate a tailored thermal emission spectrum which illuminates a photovoltaic cell. The required high temperature operation presents substantial scientific and engineering challenges which have prevented these devices from unlocking their full potential. In this talk, we discuss our development of high temperature stable spectrally engineered surfaces towards the realization of high performance STPV devices (Fig. 1).

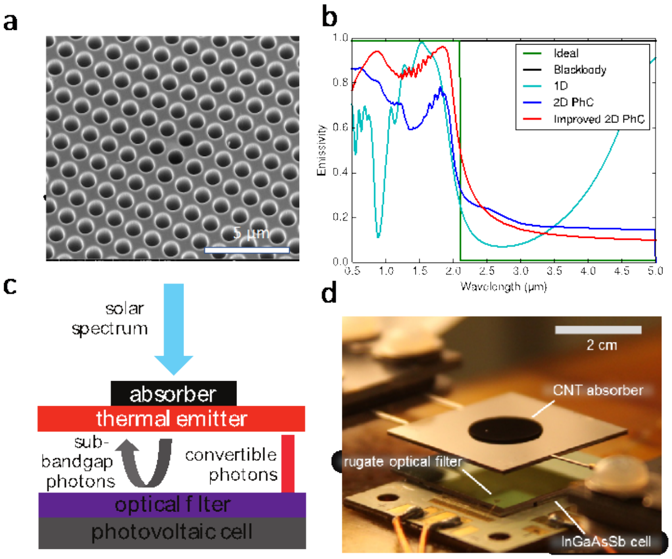


Figure 2: a) SEM of two-dimensional photonic crystal. b) Spectral properties in STPV. c) schematic of STPV energy flow. d) optical image of STPV device

For efficient conversion, the radiative exchange between all components must have a strong spectral dependence. We developed photonic crystal based absorbers and emitters that can withstand temperatures >1200 °C and provide excellent spectral control. We explored different approaches including one-dimensional and two-dimensional photonic crystals to achieve this spectral selectivity (Fig. 1a-b). These consisted of alternating layers of Si and SiO_2 films[1], and patterned refractory metals with arrays of nano-cavities[2], respectively.

We incorporated these photonic crystals for proof-of-principle STPV demonstrations (Fig.2c-d). By coupling a selective emitter with a rugate filter, we demonstrated unprecedented solar-to-electricity conversion efficiencies of 6.8%, exceeding the performance of the same PV cell directly placed under identical solar flux[3]. We also showed that the performance of the device can be improved, and the architecture simplified by incorporating our two-dimensional photonic crystal for both selective solar absorption and thermal emission[4]. Our work suggests a promising route to develop STPVs as a feasible technology to address our sustainable energy needs. We are currently pursuing technology transition opportunities based on this work, including our successful entry into the Cyclotron Road program at Lawrence Berkeley National Laboratory.

Contributions: V.S. and V.R. fabricated the 2-D photonic crystals, W.R.C. designed the 1-D photonic crystals, D.M.B. and A.L. envisioned, designed, and performed experiments for the solar TPV device. I.C., M.S., and E.N.W. supervised all research.

References: [1] Chan, W. R. *et al. Proc. Natl. Acad. Sci. U. S. A.* **110,** 5309–14 (2013); [2] Stelmakh, V. *et al. Appl. Phys. Lett.* **103,** 123903 (2013); [3] Bierman, D. M. *et al. Nat. Energy* **1,** 16068 (2016); [4] Rinnerbauer, V. *et al. Adv. Energy Mater.* **4,** (2014).

SESSION IV: TUESDAY, JULY 25, 2017; 1:30 – 3:30PM; THURGOOD MARSHALL SOUTH

1:30 PM – Team Science Finalist

H-IV-1: IDENTIFICATION AND PASSIVATION OF THE DEFECT STATES IN NIO FOR PHOTOVOLTAIC AND SOLAR FUEL APPLICATIONS

[EFRC – UNC] Taylor H. Moot[1], Lesheng Li[1], Aaron D. Taggart[1], Bing Shan[1], Shannon M. McCullough, Carrie L. Donley[1], Thomas J. Meyer[1], Yosuke Kanai[1], James F. Cahoon[1].
[1]*University of North Carolina at Chapel Hill.*

Nickel oxide (NiO) is one of the most common wide-bandgap p-type semiconductors, and it is often used in photovoltaic devices as either a hole-transporting layer or a photocathode. Despite its ubiquitous use, NiO is plagued with a large trap-state density, which turns this wide band gap material black, gives rise to fast recombination, and lowers solar-cell efficiency. These problems are of particular concern for the use of NiO as a photocathode, such as in p-type dye sensitized solar cells (p-DSSCs) or in tandem solar fuel devices for water splitting or CO_2 reduction.

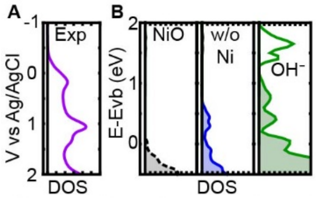


Figure 1. Density of states of A) experimental NiO and B) DFT calculations as labeled.

Although the problem of trap states in NiO has been anecdotally known for years, the exact character and number of trap states has been widely debated. We first focused on the fundamental question of what defects may be responsible for the experimentally-resolved trap states. To identify plausible defects, first-principles calculations were performed. Realizing the well-known failure of density-functional theory (DFT) for later-transition metal oxides, a DFT+*U* scheme was employed, where a local Hubbard correction augments the DFT Hamiltonian to correct erroneous electron delocalization in DFT. From these calculations, it was determined that defects, which give rise to a majority of the trap states, likely arise from a combination of Ni vacancies with and without a hydroxyl group that give rise to oxygen-localized electronic states.[1,2]

Beyond identifying plausible trap states, the calculated density of states (DOS) also shows states directly above the valence band edge of the semiconductor, which matches experimental measurements and explains the black color of NiO. With an understanding of the character and implications of the trap states, subsequent work to minimize the trap-state density was undertaken. By using a low-temperature, vapor-phase method termed targeted atomic deposition (TAD),[2] aluminum was placed at the most reactive, defect sites of NiO. As predicted by the first-principles calculations, the TAD Al-treated NiO turned white, indicative of minimizing trap states. The power conversion efficiency of fabricated p-DSSCs nearly tripled, primarily driven by an increase in V_{OC} to ~300 mV.[2]

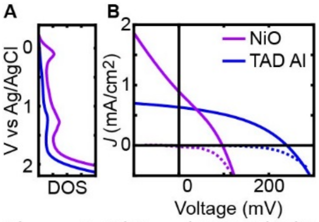


Figure 2. NiO and TAD Al NiO A) DOS and B) JV curves.

1. **Moot, T.H.**; **Li, L.**; Shan, B.; McCullough, S. M., Taggart, A. D.; Donley, C.L.; Meyer, T.J.; Kanai, Y.; Cahoon, J. F. Probing the Valence Band Density of States of NiO to Understand Photovoltaic Performance. *In Preparation.*
2. Flynn, C. J.; McCullough, S. M.; Oh, E. E.; **Li, L.**; Mercado, C. C.; Farnum, B. H.; Li, W.; Donley, C. L.; You, W.; Nozik, A. J.; McBride, J. R.; Meyer, T. J.; Kanai, Y.; Cahoon, J. F. Site-Selective Passivation of Defects in NiO Solar Photocathodes by Targeted Atomic Deposition. *ACS Appl. Mater. Interfaces* **2016,** *8* (7), 4754-4761. DOI: 10.1021/acsami.6b01090

Contributions: T. Moot, A. Taggart, C. Flynn, B. Shan, and C.L Donley collected the experimental data and L. Li was responsible for all computational work.

1:50 PM

H-IV-2: SOFT MATTER AND HYBRID SOLAR CELL INTERFACIAL SCIENCE

[EFRC – ANSER] Tobin J. Marks[1], Lin X. Chen[1,2], Robert P. H. Chang[1], Mercouri G. Kanatzidis[1], Luping Yu[3], Mark A. Ratner[1], Michael R. Wasielewski[1]
[1]Northwestern University, [2]Argonne National Laboratory, [3]University of Chicago

Molecularly tailoring interfaces with atomistic precision offers an effective and informative means to selectively modulate charge transport, molecular self-assembly, and exciton dynamics at hard matter-soft matter and soft-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 four interrelated challenge areas: 1) modulating charge transport across hard matter-soft matter interfaces in polymer and perovskite solar cells, 2) controlling charge transport by specific active layer atomistic/microstructural organization in active layers and on electrodes, 3) controlling exciton dynamics and carrier generation at active layer donor-acceptor interfaces, 4) designing transparent electrodes and interfacial layers with enhanced properties. It will be seen that rational interface engineering along with improved donor and acceptor structures, guided by theoretical/computational analysis, affords exceptional fill factors, power conversion efficiencies, and enhanced solar cell durability. The symbiosis of green materials creation, computational modeling and simulation, materials characterization, and device fabrication and evaluation, are central to this program.

2:10 PM

H-IV-3: DISCOVERY OF NEW SOLARFUELS PHOTOANODE MATERIALS WITH A COMBINATION OF HIGH-THROUGHPUT THEORY AND EXPERIMENT

[Hub – JCAP] Qui Yan[1], Ji Yu[1], Santosh K. Suram[2], Lan Zhou[2], Aniketa Shinde[2], Paul F. Newhouse[2], Wei Chen[1], Guo Li[1], Kristin A. Persson[1], John M. Gregoire[2], Jeff B. Neaton[1]
[1]Lawrence Berkeley National Laboratory; [2]California Institute of Technology

The discovery and design of new complex functional materials – and an understanding of their emergent phenomena and functional behavior in terms of their chemical composition and atomic-scale structure – is a grand challenge. In particular, the dearth of known low-band-gap photoelectrocatalytic materials poses roadblocks for the efficient generation of chemical fuels from sunlight. Here, we describe a new pipeline that integrates high-throughput ab initio density functional theory calculations with high-throughput experiments. Our pipeline has led to the rapid identification of 12 ternary vanadate oxide photoelectrocatalysts for water oxidation, nearly doubling the number of known photoanodes in the band gap range 1.2-2.8 eV, and establishing these vanadates as the most prolific class of photoanode materials for generation of chemical fuels from sunlight. Additionally, our calculations reveal new correlations between the VO_4 structure motif, d electron configuration, and electronic band edge character of these oxides. We will further describe how this work could be viewed as initiating a ‘genome’ for photoanode materials and future applications of our high-throughput theory-experiment pipeline for materials discovery. This work supported by JCAP and the Materials Project, and Molecular Foundry and NERSC.

2:30 PM

H-IV-4: MECHANISMS FOR CHARGE TRANSPORT AND PHOTOCONDUCTANCE IN MESOSCALE QUANTUM DOT ASSEMBLIES

[EFRC – CASP] Cherie R. Kagan[1], Daniel B. Straus[1], Eric Wong[1], Marton Voros[2], Nicholas P. Brawand[2], Matthew B. Goldey[2], Giulia Galli[2], Jason Tolentino[3], Kan Fu[3], Matt Law[3], Matthew C. Beard[4], Justin C. Johnson[4], Ashely R. Marshall[4], Joseph M. Luther[4], Andrew Shabaev[5], Alexander L. Efros[5], Hyeong-Jin Yun[6], Qianglu Lin[6], Istvan Robel[6], Victor I. Klimov[6]

[1]University of Pennsylvania; [2]University of Chicago; [3]University of California, Irvine; [4]National Renewable Energy Laboratory; [5]George Mason University; [6]Los Alamos National Laboratory

Colloidal semiconductor quantum dots (QDs) are an exciting materials class for next-generation thin-film solar photoconversion devices. In this talk, we describe the methods we use within CASP to engineer and probe electronically coupled, photoactive mesoscale assemblies of IV-VI, I-III-VI$_2$, and Group-IV QDs. Our specific focus is on processes that control charge carrier transport and recombination, and therefore the carrier diffusion lengths that govern photovoltaic performance. We tailor the energy, density, and occupancy of HOMO/LUMO and mid-gap electronic states from the QD core and surface by manipulating the QD synthesis and assembly conditions, as well as the matrix chemistry of QD thin films such as through use of ligands and infilling of materials by atomic layer deposition. To minimize sample variation, CASP has united experiment and theory to explore charge transport and recombination in a "standard" sample of IV-VI QDs, which yields high-performance photovoltaics. We employ a suite of optical measurements, highlighted by transient absorption spectroscopy, temperature dependent photoluminescence, THz spectroscopy, transient-microwave conductivity, and a newly developed method of ultrafast transient photocurrent spectroscopy, in combination with electrical transport measurements to probe carrier mobilities, lifetimes, and carrier multiplication yields and correlate these measurements with the electronic structure and carrier type/concentration of our engineered QD assemblies. We also combine density functional theory with thermal admittance spectroscopy and drive level capacitance profiling to map the energy, density, and occupancy of defect states in the dark and under illumination, and show that shallow states may be more detrimental to charge carrier transport than previously believed.

2:50 PM

H-IV-5: ORIGINS OF SINGLET FISSION IN SOLID PENTACENE FROM AN AB INITIO GREEN'S-FUNCTION APPROACH

[CMS – C2SEPEM] Sivan Refaely-Abramson[1], Felipe H. da Jornada[1,2], Steven G. Louie[1,2], Jeffrey B. Neaton[1,2]

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

Harnessing multiexciton generation processes, by which multiple charge carriers may ultimately result from a single photon, is of significant interest for achieving efficiencies beyond the Shockley-Queisser limit of conventional solar cell devices. One important multiexciton process is singlet fission, whereby a photo-generated singlet exciton decays into two spin-correlated triplet excitons. Here, we develop a new first-principles approach to predict and understand rates of singlet fission with an ab initio Green's-function formalism based on many-body perturbation theory. Starting with singlet and triplet excitons computed from a GW plus Bethe-Salpeter equation (GW-BSE) approach, we calculate the exciton-biexciton coupling to lowest order in the Coulomb interaction, assuming a final state consisting of two non-interacting spin-correlated triplets with finite center-of-mass momentum. For crystalline pentacene, symmetries dictate that the only purely Coulombic fission process involving a bright singlet exciton initial state requires a final state consisting of two inequivalent nearly degenerate triplets of nonzero, equal and

opposite, center-of-mass momenta. For such a process, we predict a singlet lifetime of the order of 40 to 150 fs, in very good agreement with experimental data, indicating that this process, neglected in prior studies, can dominate the rate of singlet fission in crystalline pentacene. Our approach is general and provides a framework for predicting and understanding multiexciton interactions in solids.

3:10 PM

H-IV-6: CARRIER MULTIPLICATION IN SEMICONDUCTOR QUANTUM DOTS: CURRENT STATUS AND FUTURE PROSPECTS

[EFRC – CASP] Matthew C. Beard[1], Daniel Kroupa[1], Yong Yan[1], Gregory Pach[1], Joseph M. Luther[1], Justin C. Johnson[1], Arthur J. Nozik[1], John Turner[1], Andrew Fidler[2], Istvan Robel[2], Victor I. Klimov[2], Marton Voros[3,4], Federico Giberti[3], Nicholas P. Brawand[3], Giulia Galli[3]

[1]National Renewable Energy Laboratory; [2]Los Alamos National Laboratory; [3]University of Chicago; [4]Argonne National Laboratory

This presentation discusses CASP's progress in studies of carrier multiplication, or multiple exciton generation (MEG), in semiconductor quantum dots (QDs), including the utility of MEG in solar-fuel generation. Specifically, we have developed PbS-QD-based photoanodes that can drive a hydrogen evolution reaction with quantum efficiency greater than 100%. These studies provide the first practical demonstration that excess carriers generated during the MEG process can be used to drive a photochemical reaction and not just extra photocurrent. Furthermore, using first-principle calculations coupled with experiments, we have developed design rules for QD films wherein the band edges of the QDs can be tuned over 2 eV, making them a highly flexible system for activating different types of photochemical transformations.

We will also discuss our progress in overcoming the limitations of MEG in spherical, single component nanocrystals through the engineering of asymmetric heterostructures. Recent work has focused on Janus-like nanocrystals of PbS/CdS, which are spherically shaped yet asymmetric in composition. We have observed that the MEG onset is reduced to near the energy conservation limit of twice the optical band gap. Our optical studies indicate that interfacial states play a key role in the enhanced MEG; we are using first-principle calculations to probe the interfacial electronic structure. Finally, we fabricate the first conductive films based on Janus, which we have incorporated into solar cells; optimization of the photoconductance of these films is being guided by ultrafast transient photocurrent spectroscopy studies.

I. SYNTHESIS SCIENCE

SESSION I: MONDAY, JULY 24, 2017; 3:00 – 5:00 PM; LINCOLN 2

3:00 PM

I-I-1: NOVEL CARBON MATERIALS SYNTHESIS IN EXTREME ENVIRONMENTS

[EFRC – EFree] Xiang Li[1], Maria Baldini[2], Tao Wang[1], Steve Juhl[1], Bo Chen[3], En-shi Xu[1,4], Brian Vermilyea[5], Vincent Crespi[1], Roald Hoffmann[3], Jamie Molaison[6], Chris Tulk[6], Malcolm Guthrie[2,7],Stanislav Sinogeikin[2], A.J. Ramirez-Cuesta[6], Chen Li[2,8], Klaus Schmidt-Rohr[9], Pu Duan[9], Nasim Alem[1], John Badding[1]

[1]Pennsylvania State University, [2]Carnegie Institution of Washington, [3]Cornell University, [4]George Washington University, [5]McGill University, [6]Spallation Neutron Source, Oak Ridge National Laboratory, [7]European Synchrotron Source, [8]University of California, Riverside, [9]Brandeis University

Synthesis of single crystals of carbon materials with extended bonding in one, two, or three dimensions remains a challenge. Relatively few single crystal organic monomers polymerize topochemically in the solid state with the minimal geometric changes that preserve single crystal order. Single crystals often exhibit a superior palette of properties and enable an improved understanding of structure-property relations. We have discovered a mechanochemical synthesis in which slow compression converts both polycrystalline as well as single crystal molecular benzene to single crystals of sp^3 bonded carbon nanothreads. Modeling suggests these “diamond” nanothreads could have the highest strength-to-weight ratio known and exhibit a unique combination of strength, flexibility, and resilience useful for applications from energy to medical to aerospace. The high pressure mechanochemical reaction produces single crystals despite a lack of reactant single crystal order and large geometric changes caused by the formation of three short, strong covalent bonds per monomer, and appears not to follow a topochemical pathway, but one guided by an imposed uniaxial stress. Low-dimensional crystals of stiff, aligned nanothreads with Van der Waals separations exfoliate into fibers, which may provide nanoscale building blocks with tunable strength and ductility that can be functionalized to control properties, processability, and assembly. We have characterized the nanothread reaction products by NMR, TEM, diffraction, and vibrational spectroscopy, coupled with extensive modeling. Our recent discovery that pyridine forms carbon-nitrogen nanothreads suggests that slow compression synthesis may allow many more molecular monomers to form single crystal polymers, carbon nanomaterials, and dense carbon networks that exhibit a new palette of properties.

3:20 PM

I-I-2: SOFT ROBOTICS

[EFRC – CBES] George M. Whitesides[1], Mohit Verma[1], Amit Nagarkar[1], Nicolar Fulleringer[1]

Harvard University[1]

"Robotics" is a field with broad scientific interest and practical importance: it combines mechanical engineering, information science, and animal physiology with manufacturing, workforce development, economics, and other areas. The most highly developed classes of robots have been build based on conceptual models provided by the body-plans of animals with skeletons (humans, horses), and have made it possible to carry out tasks that humans and animals could not (for a variety of reasons). We are interested in robots based a different, simpler class of organisms (invertebrates: starfish, worms, octopi)—so-called “soft” robots. Because these

organisms, and the robots having designs stimulated by them, have no skeletons, they provide enormous opportunities in materials and polymer science (particularly soft-matter science), rather than primarily in mechanical engineering. These robots (or actuators, or machines) are intrinsically "cooperative" (e.g., able to work safely with, or close to, humans). They dramatically simplify the complexity of the controllers required, by substituting the properties of materials for active controls. By using organic polymers for their structures (rather than metals and ceramics), they lower cost and weight, and often increase efficiency. By allowing the exploitation of large non-linearities in properties of soft materials and structures (especially buckling), they provide the basis for new types of actuation. The most highly developed of soft "robots" are actually actuators (especially grippers), and these systems are already transitioning to manufacturing.

3:40 PM

I-I-3: IN VITRO RECONSTITUTION OF PLANT CELLULOSE BIOSYNTHESIS

[EFRC – CLSF] Pallinti Purushotham[1], Sung Hyun Cho[2], Sara M. Díaz-Moreno[3], Manish Kumar[2], B. Tracy Nixon[2], Vincent Bulone[3,4], and Jochen Zimmer[1]

[1]University of Virginia School of Medicine, [2]The Pennsylvania State University; [3]Royal Institute of Technology; [4]Australian Research Council Centre of Excellence in Plant Cell Walls, University of Adelaide

Plant cell walls are a composite of polysaccharides, proteins, and other non-carbohydrate polymers. In the majority of plant tissues, the most abundant polysaccharide is cellulose, a linear polymer of glucose molecules. To form the load-bearing component of the cell wall, individual cellulose chains are often bundled into microfibrils and wrapped around the cell. The individual cellulose chains are synthesized by membrane-integrated processive glycosyltransferases, the cellulose synthase, and translocated across the plasma membrane by the same enzyme. Although plants express different cellulose synthase isoforms during primary and secondary cell wall formation, their specific functions are currently unknown. It is assumed that different subsets of cellulose synthase isoforms assemble into large membrane-embedded complexes and that these complexes are required to spin the individual cellulose chains into microfibrils. We show that heterologously expressed, purified, and membrane-reconstituted *Populus tremula x tremuloides* cellulose synthase-8 (PttCesA8) synthesizes cellulose in vitro. Using permethylation glycosyl linkage analysis, electron microscopy, and mutagenesis studies, we show that PttCesA8 is sufficient to not only synthesize cellulose but also to assemble the cellulose chains into microfibrils. PttCesA8's catalytic activity depends on the presence of a lipid bilayer environment and divalent manganese cations. Deletion of the enzyme's N-terminal RING-finger domain does not inhibit its function but almost completely abolishes microfibril formation. Our reconstituted cellulose biosynthesis system is an ideal platform to analyze the interactions of cellulose microfibrils with other plant cell wall components as well as protein-protein interactions underlying cellulose synthase complex formation.

4:00 PM

I-I-4: CLATHRATE COLLOIDAL CRYSTALS

[EFRC – CBES] Sharon C. Glotzer[1], Haixin Lin[2], Sangmin Lee[1], Matthew Spellings[1], Michael Engel[3], Chad A. Mirkin[2]
University of Michigan[1], Northwestern University[2], Friedrich-Alexander University Erlangen-Nürnberg[3]

DNA-programmable assembly has been used to deliberately synthesize hundreds of different colloidal crystals spanning dozens of symmetries, but the complexity of the achieved structures has so far been limited to small unit cells. We assembled DNA-modified triangular bipyramids (~250-nanometer long edge, 177-nanometer short edge) into clathrate architectures. Electron microscopy images revealed that at least three different structures form as large single-domain architectures or as multidomain materials. Ordered assemblies, isostructural to clathrates, were identified with the help of molecular simulations and geometric analysis. These structures are the most sophisticated architectures made via programmable assembly, and their formation can be understood based on the shape of the nanoparticle building blocks and mode of DNA functionalization.

4:20 PM

I-I-5: SILICON CLATHRATES AS NEW ENERGY MATERIALS

[EFRC – EFree] Tianshu Li[1], En-shi Xu[1], Yuanfei Bi[1], Timothy Strobel[2]
[1]*George Washington University,* [2]*Carnegie Institution of Washington*

Silicon possesses a rich free-energy landscape with many local minima, and a large number of metastable allotropes emerge when pressure and temperature are extended beyond ambient conditions. One type of such novel allotrope, Si clathrate, shows promising optoelectronic properties as a result of its quasi-direct electronic band gap. Although silicon clathrate can be synthesized through thermal decomposition of Zintl monosilicide followed by thermal degassing, a trace amount of remaining guests (alkali or alkaline earth metal) may already significantly deteriorate the desired electronic properties of the intrinsic clathrate framework.

Through high-throughput computer modeling, we discover that noble gas elements can help facilitate the formation of novel Si structures exhibiting desirable opto-electronic properties and thus promise as energy materials. Our results demonstrate that liquid Si can spontaneously transform into various novel crystalline phases when mixed with different noble gases under high pressure and high temperature. In particular, our study shows a medium or large size of noble gas, e.g., Ar, can trigger the nucleation and growth of inert gas Si clathrate, whereas a small noble gas such as He is able to induce the formation of an unconventional, inclusion-type compound Si_2He. Remarkably, electronic structure calculations at the GW level further show the the new compound possesses a direct electronic band gap of ~1.1 eV, a desirable property for energy applications. Guided by this theoretical prediction, experimental synthesis and characterization are currently being carried out to search for novel Si-noble gas structures.

4:40 PM

I-I-6: PATTERNING POLARIZED PHOTONIC NANOCOMPOSITES VIA DIRECT INK WRITING

[EFRC – LMI] Jennifer A. Lewis[1], Nanjia Zhou[1], Yehonadav Bekenstein[2], Carissa N. Eisler[2,3], Claas W. Visser[1], Dandan Zhang[2], Xiaoguang Wang[1], Joanna Aizenberg[1], Peidong Yang[2,3], Adam M. Schwartzberg[3], A. Paul Alivisatos[2,3], Jennifer A. Lewis[1]
[1]Harvard University; [2]University of California, Berkeley; [3]Lawrence Berkeley National Laboratory

The ability to precisely assemble one-dimensional (1D) nanorods with controlled spatial orientation is of interest for spectrum splitting, optical imaging, encryption, data storage, sensing, and full-color display. Using brightly emitting, cesium lead halide perovskite ($CsPbX_3$, X = Cl, Br, and I) nanowires as a model system, we developed novel inks composed of perovskite nanowires suspended in a block copolymer solution. We then created photonic nanocomposites via direct ink writing that exhibit highly polarized absorption and emission properties due to their programmed nanorod orientation. Several potential applications of these printed photonic nanocomposites will be highlighted.

SESSION II: TUESDAY, JULY 25, 2017; 8:30 – 10:10 AM; LINCOLN 2

8:30 AM

I-II-1: DISCOVERY AND SYNTHESIS OF NOVEL NITRIDES WITH TARGETED FUNCTIONALITY

[EFRC – CNGMD] Gerbrand Ceder[1], Andriy Zakutayev[2], Wenhao Sun[1], Bernardo Orvananos[1], Elisabetta Arca,[2] Aaron Holder[2], Yuki Iguchi[2], John Perkins[2], Stephan Lany[2], John Mangum[3], Brian Gorman[3], Laura Schelhas[4], Mike Toney[4], William Tumas[2]
[1]Lawrence Berkeley National Laboratory; [2]National Renewable Energy Laboratory; [3]Colorado School of Mines; [4]SLAC National Accelerator Laboratory

Depending on their nitrogen content, nitrides can exhibit electronic structures ranging from metallic to semiconducting, leading to materials relevant for superconductors, refractory ceramics, piezoelectrics, solid-state lighting, photovoltaics, and more. Furthermore, compared to oxides, the nitrides are relatively unexplored, making them a promising chemical space for novel materials discovery. We designed thermodynamic routes to metastable nitrogen-rich nitrides, which often possess useful semiconducting properties for electronic and optoelectronic applications. We implemented these thermodynamic strategies in a predictive computational search—exploring novel nitride materials across broad chemical spaces. Our search identified dozens of new metastable nitrogen-rich binary nitrides, and 87 previously unreported M_1-M_2-N chemical spaces with stable ternary nitrides. Using machine-learning algorithms, we cluster the resulting compounds across the ternary metal nitride space, categorizing the ternaries to guide deeper investigations. Using co-sputtering from metal targets in the presence of a nitrogen plasma, we synthesized several predicted binary and ternary nitride semiconductors and characterized their properties. In particular, scattering and spectroscopy measurements of a new group-II transition-metal (TM) nitride suggest that the metal composition ratio provides a handle to tune the TM valence state. These preliminary results hint at a broader new (II)-TM-N chemical space, with tuneable metal valence states and diverse optoelectronic properties. By formulating rational thermodynamic routes to metastable nitride compounds, we have expanded the search space for functional technological materials beyond equilibrium phases and compositions.

8:50 AM

I-II-2: COMPUTATIONAL SYNTHESIS OF LAYERED MATERIALS USING CHEMICAL VAPOR DECOMPOSITION AND LIQUID-PHASE EXFOLIATION

[CMS – MAGICS] Priya Vashishta[1], Malancha Gupta[1], Rajiv K. Kalia[1], Pulickel M. Ajayan[2], William A. Goddard, III[3]
[1]*University of Southern California*; [2]*Rice University*; [3]*California Institute of Technology*

Computational synthesis software is being developed for CVD synthesis and liquid-phase exfoliation of layered materials. We have used joint computational-experimental studies to synthesize new LMs. The salient accomplishments include: (1) growth of the first group-IV elemental monolayer (Te) using physical vapor deposition and identification of its structure using first-principles quantum molecular dynamics (QMD) simulations; (2) First-principles informed reactive molecular dynamics (RMD) simulations to understand mechanisms in CVD synthesis of LMs; (3) 100 million atom molecular dynamics (MD) simulation of liquid-phase exfoliation of LMs; and 4) dynamic fracture transformation toughening in $MoSe_2$ and WSe_2 layered materials.

9:10 AM – Team Science Finalist

I-II-3: EFFECTS OF ALLOY COMPLEXITY ON DEFECT PRODUCTION AND MICROSTRUCTURAL EVOLUTION IN CONCENTRATED ALLOYS

[EFRC – EDDE] Shijun Zhao[1], Taini Yang[2], Shi Shi[3], Chenyang Lu[2], Eva Zarkadoula[1], Hongbin Bei[1], Lumin Wang[2], Ian Robertson[3], Yanwen Zhang[1]
[1]Oak Ridge National Laboratory; [2]University of Michigan; [3]University of Wisconsin-Madison

How can we produce structural materials that are more durable in nuclear reactors? What are the keys to governing material degradation mechanisms under radiation? How can we design materials with better radiation tolerance for next-generation reactors? These are central topics in which our Energy Dissipation to Defect Evolution (EDDE) team are interested. Specifically, we are investigating a series of novel concentrated solid-solution alloys (CSAs) to reveal how energy dissipation and defect evolution mechanisms are affected by the random arrangement of mixed atoms with different alloy complexities. We aim to ultimately design alloys that are intrinsically resistant to damage production under different extreme conditions.

We present our findings about the influence of alloy complexity on defect production and microstructure evolution in CSAs based on theoretical models and experimental observations. Through density functional theory, low-energy recoil events in different CSAs are simulated and threshold energies required to knock atoms out of place are determined. We find that threshold energies in CSAs are only slightly influenced by alloy complexity. However, the energetics of interstitial and vacancy defects are strongly related to alloy compositions (specific elemental coupling), which can be interpreted by electronic properties of different constituent elements. Based on *ab initio* molecular dynamics, we show a preferential diffusion of point defects in CSAs, depending on alloy complexity,[1] validated by element segregation observed experimentally.[2] The diffusion of large defect clusters is further studied by classical molecular dynamics simulations and is directly observed in both *in-situ* and *ex-situ* transmission electron microscopy. We found that alloy complexity can effectively modify migration pathways of interstitial defect clusters: from a long-range one-dimensional mode in pure Ni and a simple binary NiCo alloy, to a short-range three-dimensional mode in more compositionally complex CSAs. Such modification leads to enhanced point defect recombination and improved swelling resistance, as shown in Figure 1.[3] Our results underline the importance of both constituent elements and composition in CSAs in determining defect behavior and microstructure evolution.

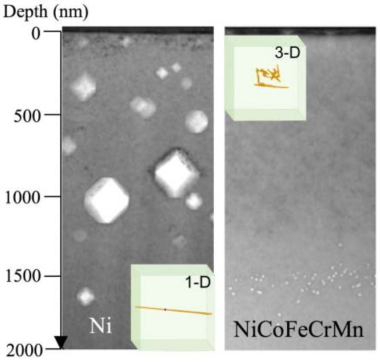


Figure 3 Transmission electron microscopy images showing different defect distributions and microstructure changes in Ni and NiCoFeCrMn CSA.[3]

[1] S. Zhao, Y. Osetsky, Y. Zhang, Acta Mater. 128 (2017) 391–399.
[2] M.-R. He, S. Wang, S. Shi, *et. al.*, Acta Mater., 126 (2017) 182-193 .
[3] C. Lu, L. Niu, N. Chen, *et. al.*, Nat. Commun. 7 (2016) 13564.

Contributions: S. Zhao conducted the theoretical simulations; T. Yang performed the *ex-situ* experiments and S. Shi carried out *in-situ* radiation experiments.

9:30 AM

I-II-4: SYNTHESIS OF FUNCTIONAL POLYMORPHIC MATERIALS

[EFRC – CNGMD] David Ginley[1], Kristin Persson[2], Lauren Garten[1], Praneetha Selvarasu[1], John Perkins[1], Wenhao Sun[2], Kirill Popov[2], Shyam Dwaraknath[2], Gerbrand Ceder[2], John Mangum[3], Brian Gorman[3], Laura Schelhas[4], Michael Toney[4], Zamyla Chan[5], Daniel Nocera[5], James Haggerty[6], Okan Agirseven[6], Janet Tate[6], Daniil Kitchaev[7], William Tumas[1]

[1]National Renewable Energy Laboratory; [2]Lawrence Berkeley National Laboratory; [3]Colorado School of Mines; [4]SLAC National Accelerator Laboratory; [5]Harvard University; [6]Oregon State University; [7]Massachusetts Institute of Technology

Polymorphic systems provide a wealth of opportunities for the development of new functional materials. A key goal is understanding how to realize specific polymorphs with the assistance of predictive computational models. We will report on recent efforts to use coupled theory and experiment to realize multi-functional polymorphs. We will discuss recent results on the prediction and synthetic realization of new piezoelectric and catalytic materials. We have surveyed Materials Project for potential piezoelectric materials and subsequently calculated the d_{33} piezoelectric coefficient for select candidates with the potential to be synthesized. Using the theory predictions, we have demonstrated novel non-centrosymmetric polymorphs with piezoelectric properties. In the case of strontium hafnium oxide (SHO), we have used pulsed laser deposition and substrate epitaxy to produce highly textured samples of a predicted, but previously unknown metastable P4mm polymorph which has both ferroelectric and piezoelectric properties. Additionally, recent work coupling theory with the synthesis of functional polymorphs of TiO_2 and MnO_x, which have focused on the synthesis of high-energy, potentially catalytic polymorphs. This has yielded new understanding of the mechanisms by which particular polymorphs can be synthetically targeted and yielded samples of nearly phase pure brookite TiO_2. Additionally, birnessite and todorokite MnO_x have been obtained. We will discuss how coupled theory and experiment provides an enhanced understanding of synthetic pathways of specific functional polymorphs.

9:50 AM

I-II-5: DIAMINE-APPENDED MG_2(DOBPDC) NANORODS AS FILLERS IN MIXED-MATRIX MEMBRANES FOR EFFICIENT CO_2/N_2 SEPARATIONS

[EFRC – CGS] Brett A. Helms[1], Lorenzo Maserati[1], Stephen M. Meckler[1,2], Jonathan E. Bachman[2], Jeffrey R. Long[1,2]

[1]Lawrence Berkeley National Laboratory (LBNL); [2]University of California, Berkeley

Gas separation membranes are well positioned to reduce the energy required for CO_2 capture compared to solid adsorbents or liquid absorbers. Here, we advance a new design strategy for gas separation membranes that incorporate the phase-change metal–organic framework (MOF) mmen-Mg_2(dobpdc) (mmen = *N*,*N*′-dimethylethylenediamine; dobpdc^{4-} = 4,4′-dioxidobiphenyl-3,3′-dicarboxylate). With this MOF dispersed into a conventional polymer matrix, the resulting mixed-matrix membrane significantly improves the CO_2 permeability while maintaining similarly high CO_2/N_2 selectivity, pushing the membrane performance toward the intrinsic permeability-selectivity performance limit of polymer membranes.

J. MATERIALS AND CHEMISTRY BY DESIGN

SESSION I: MONDAY, JULY 24, 2017; 3:00 – 5:00 PM; THURGOOD MARSHALL WEST

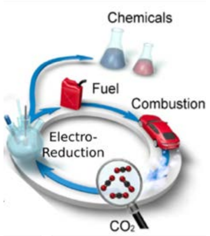
3:00 PM – Team Science Finalist

J-I-1: MATERIALS DISCOVERY, THEORY, AND CHARACTERIZATION OF INTERMETALLICS FOR ELECTROCHEMICAL CO_2 REDUCTION

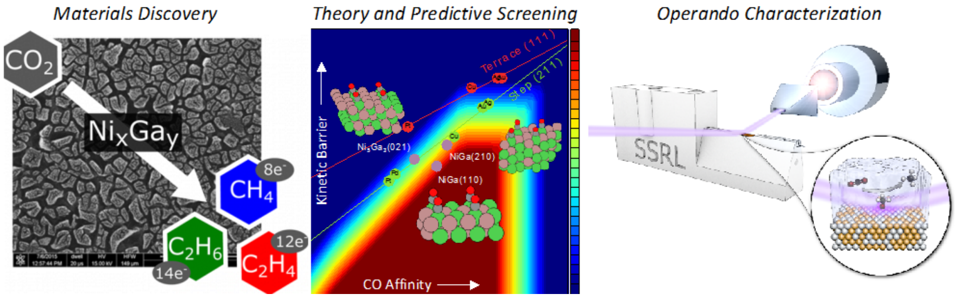
[Hub – JCAP] Jeremy T. Feaster[1,4], Daniel A. Torelli[2,4], Zachary W. Ulissi[1,4], Maryam Farmand[3,4], Sean W. Fackler[3,4], Jeffrey W. Beeman[3], Apurva Mehta[1], Ryan Davis[1], Alan T. Landers[1,4], John C. Lin[1,4], Drew C. Higgins[1,4], Sonja A. Francis[2,4], J. Chance Crompton[2,4], Alnald Javier[2,4], Jonathan R. Thompson[2], Michael T. Tang[1,4], Jianping Xiao[1,4], Xinyan Liu[1,4], Mohammadreza Karamad[1], Robert Sandberg[1,4], Karen Chan[1,4], Christopher Hahn[1,4], Bruce S. Brunschwig[2,4], Manuel P. Soriaga[2,4], Walter S. Drisdell[3,4], Junko Yano[3,4], Thomas F. Jaramillo[1,4], Nathan S. Lewis[2,4], Jens K. Nørskov[1,4]

[1]Stanford Univ./Stanford Linear Accel., [2]Cal. Inst. of Tech., [3]Lawrence Berkeley National Laboratory, [4]JCAP

Despite the explosive growth of renewable sources of electricity, making hydrocarbon building blocks and high energy density fuel sources in a renewable fashion is a major challenge. The challenge lies in designing catalysts to perform this hydrogenation selectively in solution. This joint experimental-theoretical work presents the first material with better performance for this reaction than copper, and has required contributions from materials discovery, first-principles theory, and *operando* characterization at the Joint Center for Artificial Photosynthesis.



Our team started with a nickel-gallium intermetallic catalyst known to be active for thermal CO hydrogenation. Nickel-gallium thin films of various stoichiometries were found to reduce CO_2 to methane, ethane, and ethylene, at overpotentials lower than the best polycrystalline catalyst, copper. *Ex-situ* characterization was carried out before and after catalysis to demonstrate the stability of the catalysts. It was found that even after long-term polarizations both Ni and Ga are present on the surface and contribute to the observed activity. These experiments raised two questions: what was the active site of these new catalysts, and why did existing theoretical screens not capture their activity for electrochemical CO_2 reduction? Answering these questions required modeling the many diverse active sites on these polycrystalline bimetallic samples. Adsorption sites for every stable facet were cataloged. Using machine learning methods, we inferred that most of these facets had similar activity to Ni surfaces but that a few exposed Ni sites surrounded by Ga atoms had a favorable on-top CO configuration with improved kinetics. This motif emerged from the predictive modeling and suggested that these surfaces represent a new class of intermetallic CO_2 reduction catalysts. Finally, we used *operando* grazing incidence x-ray absorption and diffraction characterization at the Stanford Synchrotron Radiation Lightsource to compare theoretical and measured reaction rates. These techniques show that kinetically trapped surface oxide species exist at reducing potentials and confirm that the surface structure changes at different reaction conditions. These results provide the foundation for our team at JCAP to screen, characterize, and deploy new catalysts for the most challenging electrochemical reactions.



Contributions: DAT, SAF, JCC, AJ, and JRT performed expt. measurements. JTF, MF, SWF, JWB, AM, RD, AM, RD, ATL, JCL, DCH and CH did the *operando* characterization. ZWU, MTT, JX, XL, MK, RS, and KC did the theory. All authors contributed to the interpretation and presentation. BSB, MPS, WSD, JY, TFJ, NSL, and JKN conceived the problems and approaches.

3:20 PM

J-I-2: Materials Genomics Design and Electrochemical Realization of Improved Electrodes and Electrolytes for Future Multivalent Energy Storage

[Hub – JCESR] Kristin A. Persson[1], Gerbrand Ceder[1], Miao Liu[1], Donny Winston[1], Nav Nidhi Rajput[1], Trevor Seguin[1], Xiaohui Qu[1], Pieromanuele Canepa[1], Sai Gopalakrishnan[1], Ziqin Rong[1], Daniel Hannah[1], Patrick Bonnick[2], Xiaoqi Sun[2], Victor Duffort[2], Linda Nazar[2], Christopher Johnson[3], Ka-Cheong Lau[3], Chen Liao[3], Brian Ingram[3], Kevin Zavadil[4], Nathan T. Hahn[4], Tylan Watkins[4], Vijayakumar Murugasen[5], Jian Zhi Hu[5], John T. Vaughey[3], Premkumar Senguttuvan[3], Niya Sa[3], Sang-Don Han[3], and Anthony Burrell[3]
[1]Lawrence Berkeley National Laboratory; [2]University of Waterloo; [3]Argonne National Laboratory; [4]Sandia National Laboratories; [5]Pacific Northwest National Laboratory

The Joint Center for Energy Storage Research (JCESR) is committed to advancing novel systems and solutions to meet the future demands for sustainable energy storage. Because the materials challenges span both solid as well as liquid bulk and interfaces, a comprehensive approach is required to elucidate and address the limitations at the relevant length scales in these complex interactive systems. In this talk we highlight our work leveraging a combined computational and experimental strategy to uncover novel, rationally designed multivalent (Mg, Ca, and Zn) cathodes and liquid electrolytes. We employ materials genomic high-throughput density-functional-theory calculations to both bulk, interface, and electrolytes in order to understand the stability and transport bottlenecks for each case. Novel solid phases and liquid systems were synthesized, and then structurally and electrochemically characterized to investigate phase purity, stability, solvation structure, speciation, and ionic transport, where applicable. The joint experimental-theory teams work in tandem towards delivering novel solid materials and liquids with rationally-designed enhanced stability and facile transport for future-looking MV energy storage.

3:40 PM

J-I-3: CRITICAL-CURRENT-BY-DESIGN

[EFRC – CES] W. –K. Kwok[1], U. Welp[1], A. E. Koshelev[1], D. J. Miller[1], H. P. Sheng[1], A. Glatz[12], I. A. Sadovskyy[1,3], Y. Zhang[3], M. W. Rupich[5], S. Sathyamurthy[5], S. Fleshler[5], S. Eley[6], L. Civale[6], A. Kayan7, P. M. Niraula[7], J.H. Kwon[8], J. M. Zuo[8]
[1]Argonne National Laboratory, [2]Northern Illinois University, [3]University of Chicago, [4]SuperPower Corp., [5]American Superconductor Corp., [6]Los Alamos National Laboratory, [7]Western Michigan University, [8]University of Illinois-Urbana Champaign

We present a new paradigm, critical-current-by-design, that aims at predicting the optimal pinning landscape for maximum critical current in high temperautre superconducting (HTS) applications. This approach uses large scale time dependent Ginzburg-Landau simulations is to elucidate the vortex dynamics in complex pinning landscapes. On the experimental side, we use controlled particle irradiation to create defects of various morphologies in HTS coated conductors to enhance their critical current. We illustrate this new paradigm by predicting the critical current (J_c) and the non-additive pinning action of different defects in irradiated samples. An example of the latter is the recently discovered *reduction* of J_c at low fields in oxygen and copper irradiated HTS coated conductors which contain self-assembled BaZrO nanorods. In a new development, we discovered that off-angle irradiation can mitigate this issue. Furthermore, vortex creep studies in HTS coated conductors indicate that the J_c reduction could also be a consequence of faster creep in the presence of different vortex pinning sites. Another development is the discovery of double chain layer defects in HTS coated conductors, induced by high-energy, heavy-ion irradiation. These defects intersect the ion irradiation induced tracks and show a decrease in the oxygen and copper content at the interface, resulting in interfacial strain. These revelations directly demonstrate the extension of the electronic inhomogeneity following irradiation and the potential of strain-induced vortex pinning. We show that the combination of large scale TDGL simulations with bulk critical current and microstructural characterization provides the necessary ingredients for realizing the critical-current-by-design paradigm.

4:00 PM

J-I-4: MODELING STRUCTURE AND ACTIVITY FOR CATALYSTS SUPPORTED ON METAL-ORGANIC FRAMEWORKS

[EFRC – ICDC] Donald G. Truhlar
University of Minnesota

The ideal partnership of theory and experiment finds them employed concomitantly, with available experimental results serving to validate a theoretical model, theory being used to rationalize variations in experimental observables as a function of alternative conditions or variables, and theory ultimately being employed a priori to streamline the design of improved, next-generation systems having improved properties or characteristics. In the case of catalysis, especially relevant properties tend to be structure, activity, and selectivity.

In collaboration with experimental groups in the Inorganometallic Catalyst Design Center, theoretical groups have been focusing on a wide variety of catalytic processes, including especially reactions relevant to the exploitation of shale-gas products employing metal-organic-framework (MOF) nodes as catalytic supports for isolated transition-metal catalysts. I will describe some of the Center's recent progress in this area, paying special attention to the critical interplay of theory and experiment as it has fostered progress. Remaining challenges and opportunities for theory in particular will be highlighted.

4:20 PM

J-I-5: COMPUTATIONAL SCREENING OF NANOPOROUS MATERIALS FOR GAS SEPARATIONS

[EFRC – CGS] Matthew Wittman[1], Efrem Braun[1], Michelle Liu[1], Sudi Jawahery[1], Rocio Mercado[1], Johanna Huck[1], Katie Deeg[1], Berend Smit[1,2]

[1]University of California, Berkeley; [2]École Polytechnique Fédérale de Lausanne (EPFL), Switzerland

One of the most attractive features of metal organic frameworks and related materials is their chemical tunability. By changing the metal and/or linkers millions of possible materials can be synthesized. However, synthesizing and fully characterizing a novel material is relatively time consuming and therefore in practice we will only synthesize small fraction of all possible materials. In this presentation, we show how computational techniques can help us finding the most promising candidates for energy efficient gas separations. We discuss different strategies to generate libraries of nanoporous materials and how big-data techniques can be used to efficiently screen these libraries.

4:40 PM

J-I-6: TUNING THE CATALYTIC ACTIVITY OF FEW-ATOM CLUSTERS DEPOSITED IN METAL-ORGANIC FRAMEWORKS

[EFRC – ICDC] Zhanyong Li[1], Aaron W. Peters[1], Manuel A. Ortuño[2], Varinia Bernales[2], Jian Liu[1], Ana E. Platero-Prats[3], Neil M. Schweitzer[1], Wei-Guang Liu[2], Karena W. Chapman[3], Donald G. Truhlar[2], Christopher J. Cramer[2], Laura Gagliardi[2], Joseph T. Hupp[1], Omar K. Farha[1,4]

[1]Northwestern University; [2]University of Minnesota; [3]Argonne National Laboratory; [4]King Abdulaziz University

Given the exceptional stability of Zr-based metal–organic frameworks (MOFs), in conjunction with their isolated and well-defined grafting sites in the form of –OH and $–OH_2$ ligands on the zirconium nodes, these high surface area materials afford an ideal scaffold for the deposition of structurally uniform few-atom metal oxide/sulfide clusters. Herein, complimentary deposition methods (solvothermal deposition in MOFs = SIM, and atomic layer deposition in MOFs = AIM) are used to synthesize a variety of MOF-supported metal oxide/sulfide materials. A host of in-situ and ex-situ characterization techniques were used to probe the structural information of these materials and their potential in catalysis was also evaluated using continuous flow gas-phase reactions. Furthermore, the mechanisms for the catalysis were investigated using DFT calculations. Guided by the theoretical prediction, we took full advantage of the high modular nature of MOFs, e.g. the size, elemental composition, electronic structure, and location of the deposited clusters, to tune the catalytic activity of these MOF-supported materials for the selected probe reactions.

SESSION III: TUESDAY, JULY 25, 2017; 10:40 AM – 12:00PM; THURGOOD MARSHALL WEST

10:40 AM

J-III-1: EFFECTIVELY DEVELOPING AND DISTRIBUTING OPEN SOURCE CODE AND DATA: EXPERIENCES FROM QMCPACK

[CMS – CPSFM] Paul Kent[1], Jaron Krogel[1], Luke Shulenburger[2], Olle Heinonen[3], Ben Blaisik[3]
[1]Oak Ridge National Laboratory; [2]Sandia National Laboratories; [3]Argonne National Laboratory

Developing and distributing open source codes and scientific data is a key activity of the Center for Predictive Simulation of Functional Materials, as well as the other 4 Computational Materials Sciences Centers, and an increasing component of mainstream science. In this talk I will first outline how we have approached this task in our Center, including our adoption of open code and data repositories such as GitHub and the Materials Data Facility. We have transitioned from informal development practices to modern practices with strong testing and validation. This has yielded significant benefits in reproducibility, productivity, and in our ability to collaborate with scientists as well as computational specialists. A second challenge has been to increase the reproducibility of our research calculations and tackle the increasing complexity of research calculations. We have done so by developing and adopting the workflow software NEXUS, specifically developed for electronic structure calculations and use on supercomputers such as those at the Leadership Computing Facilities. We hope that other projects will be encouraged to adopt these or similar practices.

11:00 AM

J-III-2: DEVELOPMENT AND INTEROPERABILITY OF THE QBOX FIRST-PRINCIPLES MOLECULAR DYNAMICS CODE

[CMS – MICCoM] Francois Gygi[1], Marco Govoni[2], Giulia Galli[2,3], Ma He[3], Huihuo Zheng[2]
[1]University of California Davis; [2]Argonne National Laboratory; [3]University of Chicago

We present the development activity of Qbox (http://qboxcode.org/) with focus on interoperability with other codes developed within MICCoM. A client-server interface was used to couple Qbox to the SSAGES framework, enabling simulations in which both SSAGES and Qbox run concurrently while exchanging messages. This coupling enables simulations in which the advanced sampling algorithms of the SSAGES suite can use DFT energies and forces. An application to the computation of the free energy of a dipeptide was demonstrated. The protocol adopted for information exchange between Qbox and SSAGES, minimizes software dependencies between the two codes. Qbox was also modified for coupling with the WEST code. In that scenario, Qbox generates DFT linear response data that is used by WEST in GW calculations. Additional functionality was implemented in Qbox to compute the density response to arbitrary external potentials, using a finite difference approach. Similarly to the coupling with SSAGES, the coupled calculation involves copies of WEST and Qbox running concurrently on a parallel platform, and exchanging information describing perturbations and density response respectively. Qbox was ported to the new ANL Theta platform. Optimization work was initiated in order to make efficient use of the Xeon Phi architecture.

We conclude with a discussion of improvements in the Qbox software engineering infrastructure. A github organization was created (qboxcode) to provide a mirror of the current repository. A Gitlab web site was created to provide a git-friendly environment for developers within the project, in addition to the original SVN repository and bug tracking system.

11:20 AM

J-III-3: LARGE-SCALE GW CALCULATIONS ON PRE-EXASCALE HPC SYSTEMS

[CMS – C2SEPEM] Jack Deslippe[1], Mauro Del Ben[1], Felipe H. da Jornada[1,2] Chao Yang[1], Steven G. Louie[1,2]
[1]Lawrence Berkeley National Laboratory; [2]University of California, Berkeley

Many-body perturbation-theory methods, and the *ab initio* GW and GW plus Bethe-Salpeter Equation (GW-BSE) approaches in particular, have emerged over the last decades as the gold standard for computing excitation spectra of real materials. However, conventional *ab initio* GW-based methodology in the past was often limited to systems of ~100 atoms due to its computational complexity. We present large-scale GW calculations with nearly 2,000 atoms on pre-exascale HPC systems (notably the Cori system at NERSC) utilizing over 500,000 cores. We discuss the optimization of the GW approach for such systems and show that the GW method is particularly well suited for exascale. Our implementation, which uses a combination of new algorithms and optimizations, scales well to the entire Cori system and obtains a significant fraction of theoretical peak performance of the machine.

11:40 AM

J-III-4: SCALABLE SIMULATION SOFTWARE AND DATA ANALYTICS FOR LAYERED MATERIALS

[CMS – MAGICS] Aiichiro Nakano[1], Rajiv K. Kalia[1], Oleg Prezhdo[1], Priya Vashishta[1], William A. Goddard, III[2], Kristin A. Persson[3], David J. Singh[4]
[1]*University of Southern California*; [2]*California Institute of Technology*; [3]*Lawrence Berkeley National Laboratory, University of California Berkeley*; [4]*University of Missouri*

We have developed a multipurpose computational synthesis and characterization software to guide the synthesis of a large family of LMs by CVD and liquid-phase exfoliation. The MAGICS software plays an important role in the analysis of ultrafast X-ray laser and electron-diffraction experiments at SLAC at exactly the same space and time scales. The MAGICS software stack comprises NAQMD and RMD simulation engines that continue to scale on current and future computing platforms, along with core libraries and extensible plug-ins to study structural, dynamical, mechanical, electrical, optical, magnetic and chemical properties of stacked LMs over a wide range of length and time scales. We have developed infrastructure to and disseminate our software and computational and experimental data via the Materials Project framework.

SESSION IV: TUESDAY, JULY 25, 2017; 1:30 – 3:30PM; THURGOOD MARSHALL WEST

1:30 PM

J-IV-1: SSAGES AND COPSS – MODERN SOFTWARE FOR ADVANCED MATERIALS MODELING

[CMS – MICCoM] Juan J. de Pablo [1,2], Jonathan Whitmer [3]
[1]University of Chicago; [2]Argonne National Laboratory; [3]University of Notre Dame

This presentation will describe the SSAGES and COPSS software suites, which have been developed to enable and accelerate simulations of advanced materials. The Simulation Suite for Advanced Generalized Ensemble Sampling (SSAGES) couples to publicly available molecular dynamics (MD) or Monte Carlo (MC) "engines" to facilitate sampling of rugged free energy landscapes. SSAGES is designed to drive an underlying engine along directions that a naïve molecular dynamics simulation would not necessarily follow, but that are important contributors to the structure and free energy of a system of interest. By doing so, conformational sampling is improved, and thermodynamic and dynamic properties that are not directly accessible in conventional MD or MC approaches become available as byproducts of the simulation. Numerous algorithms, developed by MICCoM investigators and by the simulation community in general, are now available in SSAGES; users can choose from a variety of different options, and compare the efficiency of distinct simulation approaches for a particular system or materials research problem. The Continuum-Particle Simulation Suite (COPSS) was created for simulation of nanoscale or mesoscale particles in a dielectric or hydrodynamic continuum. The particles can be charged, magnetic, polarizable, and have arbitrary shape. Polarization or magnetization is determined with algorithms that scale linearly with the number of particles and processors. For hydrodynamic-particle coupling, COPSS relies on efficient implementations of far-field and near-field hydrodynamic forces, also giving rise to linear scaling. The use and capabilities of SSAGES and COPSS will be illustrated by presenting results for a variety of examples.

1:50 PM

J-IV-2: LOW-RANK APPROXIMATION FOR SOLVING THE BETHE-SALPETER EQUATION

[CMS – C2SEPEM] Wei Hu[1], Meiyue Shao[1], Lin Lin[1], Felipe H. da Jornada[1, 2], Chao Yang[1], Jack Deslippe[1], Steven G. Louie[1, 2]

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

We present a density fitting algorithm for constructing a low rank approximation to the direct and exchange electron-hole interaction kernel within the GW-BSE approach. The algorithm uses a randomized rank-revealing QR factorization scheme to select a number of interpolating points on which the fitting coefficients are defined. A least squares procedure is then used to obtain a set of auxiliary basis. The number of these auxiliary basis functions (rank) is typically on the order of O(n) instead of O(n^2), where n is proportional to the number of electrons. By taking advantage of the separable nature of the basis functions to be fitted, we can solve the least squares problem in O(n^3) operations. We show by numerical examples that the use of density-fitting based low-rank approximation to the direct and exchange kernel can significantly reduce the cost of iterative solution to the Bethe-Salpeter eigenvalue problem without losing accuracy.

2:10 PM

J-IV-3: DEVELOPMENT OF THE WEST CODE FOR LARGE SCALE GW CODE AND OF DATA INFRASTRUCTURE

[CMS – MICCoM] Marco Govoni[1,2], Ryan McAvoy[2], Huihuo Zheng[1], He Ma[2], Peter Scherpelz[2], Han Yang[2], Aditya Tanikanti[2], Giulia Galli[1,2]

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

We present the development and applications of the WEST code (http://www.west-code.org/), ongoing within the MICCoM CMS. WEST enables the calculation of accurate electronic structure properties of large, heterogeneous systems, encompassing solids and molecules, using many-body perturbation theory. In particular, we discuss recent methodological developments including efficient calculations of electron-phonon interaction, spin-orbit interaction and electronic lifetimes. The algorithms implemented in WEST do not require the explicit calculation of virtual states, nor the storage and inversion of large dielectric matrices. We present results for nanostructured materials and solid/liquid interfaces with hundreds of electrons and illustrate molecular data collections, which have been made available to the public (http://www.west-code.org/database/index.php). In addition WEST has been ported to the ALCF Theta platform at ANL, and parallelization and optimization strategies for the Intel Xeon Phi architecture will be briefly summarized.

We conclude with a discussion of the MICCoM digital data infrastructure, based on collections of notebooks associated with papers, which in line with the DOE data management requirements, yields long-term preservation and reproducibility of data while enabling to share and search the results of simulations and experiments.

2:30 PM

J-IV-4: NOVEL PHASE DIAGRAM BEHAVIOR AND MATERIALS DESIGN IN HETEROSTRUCTURAL SEMICONDUCTOR ALLOYS

[EFRC – CNGMD] Stephan Lany[1], Janet Tate[2], Aaron Holder[1], Sebastian Siol[1], Paul Ndione[1], Haowei Peng[1], Lauren Garten[1], John Perkins[1], David Ginley[1], Andriy Zakutayev[1], Bethany Matthews[2], Ann Deml[3], Brian Gorman[3], Laura Schelhas[4], Kevin Stone[4], Michael Toney[4], Roy Gordon[5], William Tumas[1]
[1]National Renewable Energy Laboratory; [2]Oregon State University; [3]Colorado School of Mines, [4]SLAC National Accelerator Laboratory; [5]Harvard University

Structure and composition control the behavior of materials. The development of alloys, despite their enormous technological importance, has conventionally exploited compositional control over materials and properties. In this talk, we report the discovery and confirmation of a remarkable new materials metastability that arises from simultaneous control over both composition and structure through heterostructural alloying. The newly accessible phase space and additional structural degree of freedom we have identified enables novel Materials by Design strategies to tailor properties in a non-linear or even discontinuous fashion, providing a mechanism for materials design that does not exist in conventional alloys. Using first principle calculations and thin-film synthesis of $Sn_{1-x}Ca_xS$, $Mn_{1-x}Zn_xO$, and $MnSe_{1-x}Te_x$ alloys, we realize metastable polymorphs with targeted functional materials properties strikingly different from those of the parent materials. Our work demonstrates the first predictive design of metastable heterostructural alloys and establishes a broadly applicable approach for developing new non-equilibrium solid-solutions with controlled composition, structure and functionality.

2:50 PM

J-IV-5: DIFFUSION AND MASS TRANSPORT IN CONCENTRATED SOLID SOLUTION ALLOYS: FEATURES AND EFFECTS TO RADIATION DAMAGE

[EFRC – EDDE] Yuri N. Osetskiy[1], Shijun Zhao[1], Yanwen Zhang[1], Lumin Wang[2], Ian Robertson[3]
[1]Oak Ridge National Laboratory; [2]University of Michigan-Ann Arbor; [3]University of Wisconsin-Madison

Alloy stability and degradation under thermal and radiation treatments depend mainly on the mobility of dominating defects under certain conditions. Defect diffusion and mass transport in concentrated solid solution alloys (CSAs) have significant features that are not treatable within the existing theories developed for dilute alloys. We have used a multiscale approach to study point defects and their transport properties in CSAs. Two new effects are revealed; 1) chemically biased diffusion – when different defects migrate via preferable chemical configurations, and 2) percolation effects – when defect diffusion paths are significantly modified near the percolation threshold. Consequently, suppressed three dimensional and one dimensional cluster motion and sluggish diffusion are observed, leading to increased radiation tolerance, elemental segregation at dislocation loops and voids, and various volume swelling responses. This new understanding based on the multiscale approach will allow preselection of the composition of multicomponent CSAs with desirable stability and diffusion properties prior to their fabrication, experimental validation, and application.

3:10 PM

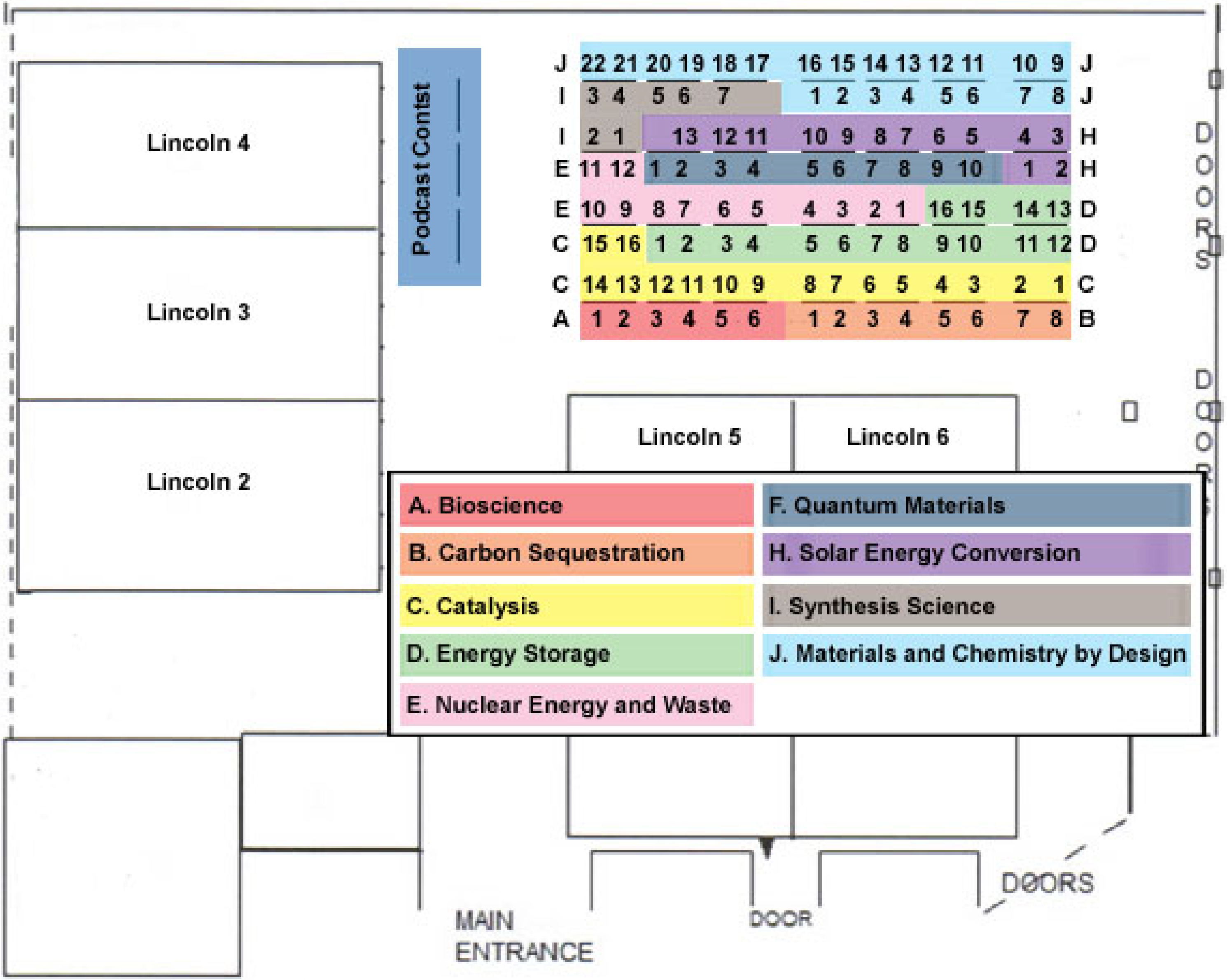
J-IV-6: DEVELOPING A MULTISCALE UNDERSTANDING OF ALUMINUM TRANSFORMATIONS WITH INTEGRATED SIMULATION AND SPECTROSCOPY

[EFRC – IDREAM] Aurora E. Clark[2], Xiaosong Li[3], Greg Schenter[1], Carolyn Pearce[1], Sebastien Kerisit[1], Kate Page[4], Jianzhi Hu[1], David Semrouni[2], Kevin Rosso[1], Zhizhang Shen[1], Ernesto Martinez-Baez[2], Torin Stetina[3], Andrew Wildman[3], Tiecheng Zhou[2], Sue B. Clark[1]

[1]Pacific Northwest National Laboratory, [2]Washington State University, [3]University of Washington, [4]Oak Ridge National Laboratory

Removal of high level radioactive wastes from their storage tanks will require dissolution of the bulk matrix, which is largely aluminum hydroxide and oxyhydroxide solids, such as gibbsite ($Al(OH)_3$) and boehmite ($AlO(OH)$). Dissolution requires a change in aluminum coordination from octahedral (Oh) in the solid phase to tetrahedral (Td) in the solution phase. Understanding this molecular transformation requires an integrated simulation and experimental effort that firmly links the local (and even extended) structure to spectroscopic observables. Herein we illustrate a series of condensed and solid state simulations of aqueous aluminum, highly concentrated electrolyte solutions, and solid aluminum oxyhydroxide surfaces, alongside the essential spectroscopic observables that can help identify molecular and extended structure. The focus is upon NMR, IR/Raman, X-ray absorption spectroscopy (XAS), and scattering experiments, alongside their theoretically predicted features. As an example, distinct spectral features are observed within the XAS of highly structured water present in concentrated electrolyte solutions, aqueous $Al(OH)_4^-$ in the presence of monovalent cations, and the surfaces of boehmite and gibbsite minerals. This work highlights the progress toward developing a one-to-one mapping of local and structure with characteristic spectral features.

Map of Poster Sessions, *Exhibition Hall C*



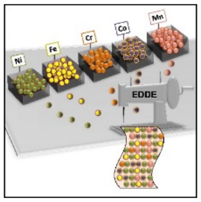
INTERSECTION OF SOUND AND SCIENCE PODCAST CONTEST ENTRIES, *EXHIBITION HALL C*

As part of the 2017 EFRC-Hub-CMS Principal Investigators' Meeting, the Department of Energy's Office of Basic Energy Sciences (BES) sponsored a *Sound ∩ Science Podcast Contest*. Following the EFRC tradition, during each meeting there is an optional contest designed to educate, inspire and entertain an intelligent, but not expert, audience with the extraordinary science, innovation, and people in the EFRCs, Hubs, and CMSs. The Intersection of Sound and Science Podcast Contest is an opportunity to share the excitement and mystery of science using sounds. To listen to all the podcasts, visit http://www.energyfrontier.us/podcast-contest.

Overall Winner

Sound to Analyze, Interpret, and Understand Data from Experiment and Theory

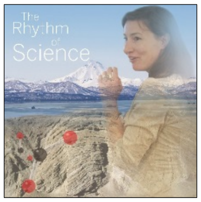
Interfacial Dynamics in Radioactive Environments and Materials (IDREAM)



Best Team Effort

Tailoring Alloys to be Radiation-tolerant for Clean and Safe Energy Production

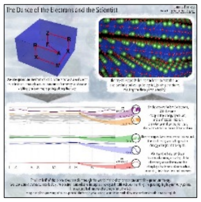
Energy Dissipation to Defect Evolution (EDDE)



Best Narrative

The Rhythm of Science

Center for Frontiers of Subsurface Energy Security (CFSES)



Best Science Music Composition

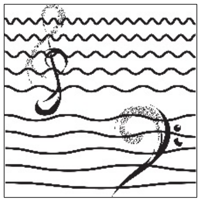
The Dance of the Electrons and the Scientist

Center for the Computational Design of Functional Layered Materials (CCDM)

Best Explanation of a Scientific Concept

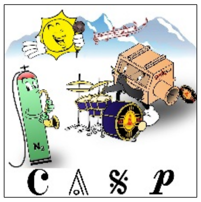
Plant Cell Walls, a Symphony of Solid Sunlight

Center for Lignocellulose Structure and Formation (CLSF)



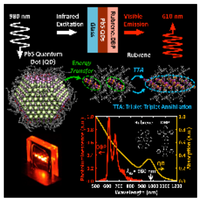
The Musicality of Electrons

Biological Electron Transfer and Catalysis Center (BETCy)



The Sounds of Science

Center for Advanced Solar Photophysics (CASP)



Hacking the Sun: Infrared-to-Visible Photon Upconversion for Next-Generation Solar Energy Harvesting

Center for Excitonics (CE)

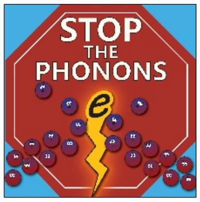
The Kitchen and the Lab: Two Parallel Universes for Making Things by Design

Center for Next Generation of Materials by Design (CNGMD)

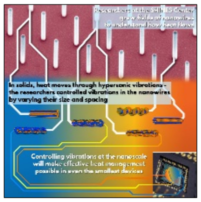
[This Side of Perfect](#)
Light Material Interactions in Energy Conversion (LMI)

[Listening to Batteries](#)
NorthEast Center for Chemical Energy Storage (NECCES)

[Big Things, Small Packages](#)
Nanostructures for Electrical Energy Storage (NEES)



[Stop the Phonons](#)
Solid-State Solar-Thermal Energy Conversion Center (S3TEC)



[How to Control Heat with Hypersound](#)
Spins and Heat in Nanoscale Electronic Systems (SHINES)

POSTER SESSION I: MONDAY, JULY 24, 2017; 5:00 – 6:30 PM, *EXHIBITION HALL C*

A. BIOSCIENCE

PI-A-1: CELLULOSE ASSEMBLY IN PLANT CELL WALLS IN THEIR NATIVE STATES – NEW INSIGHTS AND NEW QUESTIONS FROM SUM-FREQUENCY-GENERATION VIBRATIONAL SPECTROSCOPY STUDY

[EFRC – CLSF] Seong H. Kim, Shixin Huang, Mohamadamin Makarem, Sarah Kiemle, Daniel J. Cosgrove, Chaowen Xiao, Charlie T. Anderson, Xiaoran Xin, Ying Gu
The Pennsylvania State University

PI-A-2: PHOTOSYNTHETIC ANTENNA RESEARCH CENTER (PARC) OVERVIEW

[EFRC – PARC] Robert Blankenship[1]
[1]*Washington University in St. Louis*

PI-A-3: PROBING LIGNIN EFFECTS ON THE PLANT CELL WALL ULTRASTRUCTURE AND MECHANICAL PROPERTIES

[EFRC – CLSF] Sarah N. Kiemle[1], Chang-Jun Liu[2], Liza A. Wilson[1], Daniel J. Cosgrove[1]
[1]*The Pennsylvania State University;* [2] *Brookhaven National Laboratory*

PI-A-4: PHYSICAL AND THERMODYNAMIC DETERMINANTS OF FLAVIN-BASED ELECTRON BIFURCATION

[EFRC – BETCy] Carolyn E. Lubner[1], Diep M.N. Nguyen[2], David N. Beratan[3], Rhesa Leadbetter[4], Gerrit J. Schut[2], Oleg A. Zadvornyy[5,6], John Hoben[7], Peng Zhang[3], Monika Tokmina-Lukaszewska[5], Luke M. Berry[5], Gina L. Lipscomb[2], Brian Bothner[5], Anne K. Jones[8], Anne-Frances Miller[7], Lance C. Seefeldt[4], Michael W.W. Adams[2], John W. Peters[5,6], Paul W. King[1]
[1]*National Renewable Energy Laboratory;* [2]*University of Georgia;* [3]*Duke University;* [4]*Utah State University;* [5]*Montana State University;* [6]*Washington State University;* [7]*University of Kentucky;* [8]*Arizona State University*

PI-A-5: PARC'S MODEL OUTREACH PROGRAM INTERESTS AND INFORMS

[EFRC – PARC] Dewey Holten[1]; Kaslina Love Mosley[1]
[1]*Washington University in St. Louis*

PI-A-6: THE STRUCTURAL ROLE OF PECTINS IN CELL WALL LOOSENING FROM SOLID-STATE NMR SPECTROSCOPY

[EFRC – CLSF] Pyae Phyo[1], Tuo Wang[1], Sarah Kiemle[2], Chaowen Xiao[2], Charles T. Anderson[2], Daniel J. Cosgrove[2], Mei Hong[1]
[1]*Massachusetts Institute of Technology;* [2]*The Pennsylvania State University*

B. CARBON SEQUESTRATION

PI-B-1: BURIED METEORITE IMPACT STRUCTURES AND THEIR IMPLICATIONS FOR INDUCED SEISMICITY

[EFRC – GSCO2] Charles C. Monson[1,2], James L. Best[2], Scott Frailey[1,2], Nathan Grigsby[1], Susan W. Kieffer[2], Christopher P. Korose[1], Roman Makhnenko[2], Volker Oye[3], Ali Tarokh[2]
[1]Illinois State Geological Survey, [2]University of Illinois at Urbana-Champaign, [3]NORSAR

PI-B-2: THE EFFECTS OF HYDROUS SUPERCRITICAL CO_2 ON RESERVOIR ROCK INTEGRITY OVER VARIOUS TIME SCALES

[EFRC – CFSES] Charles Choens[1], Thomas Dewers[1], Anastasia Ilgen[1], Nicholas Espinoza[2], Michael Aman[2], Pania Newell[3], Rich Regueiro[4]
[1]Sandia National Laboratories, [2]The University of Texas at Austin, [3]The University of Utah, [4]The University of Colorado at Boulder

PI-B-3: WETTING AND TRANSPORT PROPERTIES OF CO_2 FROM OPTICAL AND X-RAY SPECTROSCOPY

[EFRC – NCGC] Pradeep Perera[1], Hang Deng[1], Dimosthenis Sokaras[2], Ian Bourg[3], Tetsu Tokunaga[1], P. Jim Schuck[1], Benjamin Gilbert[1]
[1]Lawrence Berkeley National Laboratory; [2]Stanford University; [3]Princeton University

PI-B-4: COMPARISON OF LATTICE BOLTZMANN SIMULATION AND EXPERIMENT OF PORE-SCALE PHENOMENA IN 2D POROUS MICROMODELS: MULTIPHASE FLOW TOWARDS COUPLED SOLID-LIQUID INTERACTIONS

[EFRC – GSCO2] Yu Chen[2], Yaofa Li[1,3], Gianluca Blois[1,3], Albert J. Valocchi[2], Kenneth T. Christensen[1,3]
[1]University of Notre Dame, [2]University of Illinois at Urbana-Champaign, [3]International Institute for Carbon-Neutral Energy Research (I^{2}CNER), Kyushu University, Japan

PI-B-5: ENGINEERED HETEROGENEITY IN SAND PACKS FOR EVALUATING CO_2 SATURATION DURING BUOYANCY-DRIVEN FLOW

[EFRC – CFSES] Prasanna G. Krishnamurthy[1], Luca Trevisan[1], Tip Meckel[1]
[1]The University of Texas at Austin

PI-B-6: GRAVITY-DRIVEN CHEMICAL CONTROLS ON $CaCO_3$ PRECIPITATION IN A FRACTURE

[EFRC – NCGC] Zhenyu Xu[1], Julie Sheets[2], Lijie Zhang[3], Doyoon Kim[3], Timothy J. Kneafsey[4], David Cole[2], Young-Shin Jun[3], Laura J. Pyrak-Nolte[1]
[1]Purdue University, [2]Ohio State University, [3]Washington University in St. Louis, [4]Lawrence Berkeley National Laboratory

PI-B-7: COUPLED FLUID FLOW AND DEFORMATION SIMULATION OF TWO-PHASE SUPERCRITICAL CO_2-BRINE FLOW THROUGH MICRO-CT IMAGES OF SANDSTONE

[EFRC – GSCO2] Mahsa Rahromostaqim[1], Muhammad Sahimi[1], Al Valocchi[2], Ahmed Elbanna[2], Pejman Tahmasebi[3]
[1]University of Southern California, [2]University of Illinois at Urbana-Champaign, [3]University of Wyoming

PI-B-8: FLUID DYNAMICS MODEL FOR PORE-SCALE WETTING PHENOMENA

[EFRC – CFSES] Alec Kucala[1], Mario J. Martinez[1], David R. Noble[1]
[1]Sandia National Laboratories Engineering Sciences Center

C. CATALYSIS

PI-C-1: PRODUCTION AND UTILIZATION OF LEVOGLUCOSAN (LGA) AND GLYCOLALDEHYDE (GA) FROM CELLULOSE FAST PYROLYSIS VAPORS: THEORY AND EXPERIMENT

[EFRC – C3Bio] Richard Caulkins, Taufik Ridha, Mckay Easton, Priya Murria, Abhijit Talpade, Zaikuan Yu, Hilkka I. Kenttämaa, Rakesh Agrawal, Fabio H. Ribeiro, W. Nicholas Delgass
Purdue University

PI-C-2: NITROGENASE FE PROTEIN CYCLE

[EFRC – BETCy] Monika Tokmina-Lukaszewska[1], John W. Peters[1,2], Natasha K. Pence[1,2], Zhi-Yong Yang[3], Rhesa N. Ledbetter[3], Lance C. Seefeldt[3], Brian Bothner[1]
[1]Montana State University; [2]Washington State University; [3]Utah State University

PI-C-3: MoS_2 AS A BETTER AND CHEAPER HYDROGEN EVOLUTION CATALYST THAN PT

[EFRC – CCDM] L. Cao[1], G. Li[1], Q. Qiao[2], W. Yang[3], D. Zhang[3], Y. Zhu[2]
[1]*North Carolina State University,* [2]*Brookhaven National Laboratory,* [3]*Duke University*

PI-C-4: ELECTROCATALYTIC OXIDATION AND PRODUCTION OF HYDROGEN: STRATEGIES FOR LOWERING THE OVERPOTENTIAL

[EFRC – CME] Eric. S. Wiedner[1], Geoffrey M. Chambers[1], Christina M. Klug[1], Aaron M. Appel[1], Molly O'Hagan[1], R. Morris Bullock[1]
[1]Pacific Northwest National Laboratory

PI-C-5: UNDERSTANDING REACTIVE SURFACE REORGANIZATION ON AU SURFACES

[EFRC – IMASC] Christopher O'Connor,[1] Fang Xu,[1] Ioanna Fampiou,[1] Stavros Karakalos,[1] Fanny Hiebel,[1] Efthimios Kaxiras,[1] Robert J. Madix,[1] Cynthia M. Friend[1]
[1]Harvard University

PI-C-6: INSIGHTS INTO THE MECHANISMS AND KINETICS THAT CONTROL ELECTROCATALYSIS AT FLUID-SOLID INTERFACES

[EFRC – FIRST] Matthew Neurock[1], Stuart Winikoff[1], Wenjie Tang[1], Peng Bai[1], John DiMeglio[2], Stephanie Velardo[2], Joel Rosenthal[2], Jonnathan Medina-Ramos[3], Paul Fenter[3], Daniel Lutterman[4], David Mullins[4], Robert Sacci[4], Huiyuan Zhu[4], Zhiyong Zhang[4], Steven Overbury[4], Matthew Thompson[5], Peter Cummings[5]
[1]University of Minnesota; [2]University of Delaware; [3]Penn State University; [4]Oak Ridge National Laboratory; [5]Vanderbilt University

PI-C-7: OVERVIEW OF THE INORGANIC CATALYSIS DESIGN CENTER

[EFRC – ICDC] Manuel A. Ortuño[1], Joseph T. Hupp[2], Laura Gagliardi[1]
[1]University of Minnesota; [2]Northwestern University

PI-C-8: A COMPARATIVE STUDY OF ANHYDROUS DEHYDROGENATION OF LINEAR-CHAIN ALCOHOLS ON CU SINGLE CRYSTALS

[EFRC – IMASC] Wei Chen[1], Robert Hoyt[1], Matthew M. Montemore[1], Zhitao Wang[2], E. Charles H. Sykes[2], Robert J. Madix[1], Cynthia M. Friend[1], Efthimios Kaxiras[1]
[1]Harvard University; [2]Tufts University

PI-C-9: ACID-CATALYZED FORMALDEHYDE CONDENSATION WITH PROPYLENE: A ROUTE TO FORM 1,3-BUTADIENE PRECURSORS

[EFRC – CCEI] Efterpi S Vasiliadou[1], Raul F. Lobo[1]
[1]University of Delaware

PI-C-10: FE-NITROGENASE: C-H AND N-H BOND FORMATION

[EFRC – BETCy] Yanning Zheng[1], Rhesa N. Ledbetter[2], Lance C. Seefeldt[2], Derek F. Harris[2], Saroj Poudel[3], Kathryn R. Fixen[1], Zhi-Yong Yang[2], Paul W. King[4], Eric S. Boyd[3], Caroline S. Harwood[1]
[1]University of Washington; [2]Utah State University; [3]Montana State University; [4]National Renewable Energy Laboratory

PI-C-11: DEACTIVATION MECHANISMS FOR CO AND CU CATALYZED OXIDATION OF LIGNIN MODELS

[EFRC – C3Bio] Rebecca Key[1], Ernesto Zuleta[1], Thomas Elder[2], Joseph J. Bozell[1]
[1]Center for Renewable Carbon, University of Tennessee, [2]US Forest Service

PI-C-12: ELECTROCHEMICAL CO_2 REDUCTION OVER CUAG BIMETALLIC ELECTRODES AND SURFACE ALLOYS

[Hub – JCAP] Ezra L. Clark[1], Christopher Hahn[2], Thomas F. Jaramillo[2], Alexis T. Bell[1]
[1]Lawrence Berkeley National Laboratory; [2]SLAC National Accelerator Laboratory

PI-C-13: TUNING ELECTRON-PROTON TRANSFER MEDIATORS FOR MOLECULAR ELECTROCATALYSIS

[EFRC – CME] Mioy T. Huynh[1], Colin W. Anson[2], Shannon S. Stahl[2], Thomas A. Moore[3], Ana L. Moore[3], Sharon Hammes-Schiffer[1]
[1]University of Illinois at Urbana-Champaign; [2]University of Wisconsin-Madison; [3]Arizona State University

PI-C-14: STRUCTURAL ANALYSIS OF HUMINS FORMED IN THE BRØNSTED CATALYZED DEHYDRATION OF FRUCTOSE

[EFRC – CCEI] (Lily) Ziwei Cheng[1], Jeffrey L. Everhart[1], George Tsilomelekis[2], Vladimiros Nikolakis[1], Basudeb Saha[1], Dionisios G. Vlachos[1]
[1]University of Delaware; [2]Rutgers University

PI-C-15: PDAU SINGLE-ATOM ALLOY CATALYSTS FOR LIQUID PHASE SELECTIVE HYDROGENATION OF 1-HEXYNE TO 1-HEXENE

[EFRC – IMASC] Jilei Liu[1], Junjun Shan[1], Matthew B. Uhlman[1], E. Charles H. Sykes[1], Maria Flytzani-Stephanopoulos[1]
[1]Tufts University

PI-C-16: METHODOLOGY FOR THE DISCOVERY OF NEW AND IMPROVED CO_2 REDUCTION ELECTROCATALYSTS

[Hub – JCAP] Daniel A. Torelli[1], Christopher Hahn[2], Zachary W. Ulissi[2], Jeremey T. Feaster[2], Kyle Cummins[1], Walter Drisdell[3], Jack H. Baricuatro[1], Alnald Javier[1], Carlos G. Read[1], Manuel P. Soriaga[1], Jens K. Norskov[2], Thomas F. Jaramillo[2], Nathan S. Lewis[1]
[1]California Institute of Technology; [2]SLAC National Accelerator Laboratory; [3]Lawrence Berkeley National Laboratory

D. ENERGY STORAGE

PI-D-1: UNDERSTANDING AND CONTROLLING THE REACTIVITY OF LIMn$_2$O$_4$-ELECTROLYTE INTERFACES

[EFRC – CEES] Robert Warburton[1], Bruno Nicolau[2], Kendra Letchworth-Weaver[3], Kan-Sheng Chen[4], Aaron Petronico[2], Laila Jaber-Ansari[4], Xiao Chen[3], Yasaman Ghadar[3], Maria Chan[3], Ralph Nuzzo[2], Andrew Gewirth[2], Jeffrey P. Greeley[1], Mark Hersam[3], Paul Fenter[3]

[1]Purdue University, [2]University of Illinois, [3]Argonne National Laboratory, [4]Northwestern University

PI-D-2: PHYSICAL ORGANIC APPROACHES TO DESIGNING REDOX-ACTIVE ORGANICS AND UNDERSTANDING ELECTROLYTE EFFECTS FOR FLOW BATTERY APPLICATIONS

[Hub – JCESR] Christo S. Sevov[1], David P. Hickey[2], Emily V. Carino[3], Monique E. Cook[1], Sophia G. Robinson[2], Koen H. Hendriks[2], Shoshanna Barnett[1], Rajeev S. Assary[3], Larry A. Curtiss[3], Fikile R. Brushett[4], Nenad M. Markovic[3], Shelley D. Minteer[2], Matthew S. Sigman[2], Melanie S. Sanford[1]

[1]University of Michigan; [2]University of Utah; [3]Argonne National Laboratory; [4]Massachusetts Institute of Technology

PI-D-3: IDENTIFYING THE CHEMICAL AND STRUCTURAL IRREVERSIBILITY IN LINI0.8CO0.15AL0.05O2 - A MODEL SYSTEM FOR CLASSICAL LAYERED INTERCALATION

[EFRC – NECCES] Haodong Liu[1], Hao Liu[2], Ieuan Seymour[3], Natasha A. Chernova[4], Max Radin[5], Julija Vinckeviciute[5], Kamila M. Wiaderek[2], Antonin Grenier[2], Peter J. Chupas[2], M. Stanley Whittingham[4], Clare Grey[3], Karena W. Chapman[2], Anton Ven der Ven[5], Ying Shirley Meng[1].

[1]University of California, San Diego; [2]Argonne National Laboratory; [3]University of Cambridge; [4]Binghamton University; [5]University of California, Santa Barbara

PI-D-4: LOCAL STRUCTURAL FINGERPRINT FOR TRACKING LI INTERCALATION IN ZERO-STRAIN LITHIUM TITANATE

[EFRC – m2M] Wei Zhang[1], Mehmet Topsakal[1], Christina Cama[2], Christopher Pelliccione[1], Hu Zhao[1], Lijun Wu[1], Yimei Zhu[1], Anatoly Frenkel[1,2], Amy Marschilok[2], Kenneth Takeuchi[2], Esther Takeuchi[2], Deyu Lu[1], Feng Wang[1]

[1]Brookhaven National Laboratory, [2]Stony Brook University

PI-D-5: SOLID STATE BATTERIES AT THE NANO- & MICRO- SCALES

[EFRC – NEES] Jonathan Larson[1], A. Alec Talin[2], Eleanor Gillette[3], Alex Pearse[1], Sang Bok Lee[1], Gary Rubloff[1], Janice Reutt-Robey[1]

[1]Univeristy of Maryland; [2]Sandia National Laboratories; [3]NIST

PI-D-6: OXYGEN REDOX ACTIVITY IN LITHIUM-RICH CATHODE MATERIALS

[EFRC – CEES] Liang Li[1], Fernando C. Castro[2], Joong Sun Park[1], Eungje Lee[1], John Freeland[1], Zhenpeng Yao[2], Tim Fister[1], John Vinson[3], Eric L. Shirley[3], Christopher Wolverton[2], Vinayak Dravid[2], Michael Thackeray[1], Maria K. Y. Chan[1]

[1]Argonne National Laboratory; [2]Northwestern University; [3]National Institute of Standards and Technology

PI-D-7: ELECTROCHEMICALLY INITIATED SURFACE CHEMISTRIES INHIBITING THE REALIZATION OF THEORETICAL CAPACITY OF LINI0.8CO0.15AL0.05O2

[EFRC – NECCES] Nicholas V. Faenza[1], Zachary W. Lebens-Higgins[2], Pinaki Mukherjee[1], Shawn Sallis[2] , Nathalie Pereira[1], Fadwa Badway[1], Anna Halajko[1], Hena Das[3], Penghao Xiao[3], Gerbrand Ceder[3], Frederic Cosandey [1], Louis. F. J. Piper[2], Glenn G. Amatucci[1].

[1]Rutgers, The State University of New Jersey; [2]Binghamton University; [3]University of California, Berkeley

PI-D-8: Development of Thermo-Electrochemical System for Harvesting Low Grade Heat

[EFRC – S^3TEC] Botao Huang[1], Sokseiha Muy[1], Shuting Feng[1], Yuan Yang[1], Gang Chen[1], Yang Shao-Horn[1]
[1]Massachusetts Institute of Technology

PI-D-9: Insights into the Interaction between 2D Transition Metal Carbide and Nitride (Mxenes), Ions, and Water

[EFRC – FIRST] Michael Naguib[1] Hsiu-Wen Wang[1], Naresh C. Osti[1], Lukas Vlcek[1], Geetu Sharma[2], Alireza Ostadhossein[3,] Yu Xie[1], Eric S. Muckley[1], Ilia N. Ivanov[1], Robert L. Sacci[1], Paul R.C. Kent[1], Elayaraja Muthuswamy[2], Di Wu[2], Madhusudan Tyagi[4], Boris Dyatkin[5], Gernot Rother[1], William T. Heller[1], Eugene Mamontov[1], Katharine Page[1], Adri C.T. van Duin[3], Alexandra Navrotsky[2], Yury Gogotsi[6], David J. Wesolowski[1]
[1]Oak Ridge National Laboratory; [2]University of California at Davis; [3]Penn State University; [4]National Institute of Standards and Technology; [5]Naval Research Laboratory; [6]Drexel University

PI-D-10: Directing battery development path by techno-economic modeling

[Hub – JCESR] Lei Cheng[1], Kyle C. Smith[2], Kevin G. Gallagher[1], Fikile R. Brushett[3], Robert M. Darling[4], Damla Erogula[1], Seungbum Ha[1], Rylan Dmello[2], Vinay Iyer[2], Jarrod Milshtein[3], Pavan Nemani[2]
[1]Argonne National Laboratory; [2]University of Illinois at Urbana-Champaign; [3]Massachusetts Institute of Technology; [4]United Technologies Research Center

PI-D-11: The role of interfaces in lithium battery conversion reactions

[EFRC – CEES] Jae Jin Kim[1], Guennadi Evmenenko[2], Fernando Castro[2], Robert Warburton[3], Zhenpeng Yao[2], Kimberly Lundberg[4], Hyo Seon Suh, Handan Yildrim[3], Anil U. Mane[1], Jinsong Wu[2], Vinayak Dravid[2], Jeffrey Greeley[3], Chris Wolverton[2], Andrew Gewirth[4], Paul F. Nealey[5], Jeffrey W. Elam[1], Paul Fenter[1], Michael Bedzyk[2], Timothy T. Fister[1]
[1]Argonne National Laboratory, [2]Northwestern University, [3]Purdue University, [4]University of Illinois, [5]University of Chicago.

PI-D-12: Synchrotron Radiation Techniques for Determination of Electrochemically Induced Spatial and Time-Resolved Phase Evolution

[EFRC – m2M] Andrea Bruck[1], Matthew Huie[1], Alexander Brady[1], David Bock[2], Christopher Pelliccione[2], Qing Zhang[1], Yiman Zhang[1], Jiefu Yin[1], Zhong Zhong[2], Kenneth Takeuchi[1], Esther Takeuchi[1], Amy Marschilok[1].
[1]Stony Brook University, [2]Brookhaven National Laboratory

PI-D-13: Pathways to Multifunctional Solid Electrolytes

[EFRC – NEES] David Ashby[1], Alexander Pearse[2], Keith Gregorczyk[2], Kim McKelvey[3], A. Alec Talin[4], Henry White[3], Gary Rubloff[2], Bruce Dunn[1]
[1]University of California, Los Angeles; [2]University of Maryland; [3]University of Utah; [4]Sandia National Laboratories

PI-D-14: High Capacity Hydrogen Storage On Surfaces and In Metals

[EFRC – EFree] Nicholas Weadock[1], Heng Yang[1], Maxwell Murialdo[1], Yiqun Liu[2], Hongjin Tan[1.3], Kai Landskron[2], Brent Fultz[1]
[1]California Institute of Technology, [2]Lehigh University, [3]Liox Power, Inc.

PI-D-15: Next Generation of Vanadium-based Multi-electron Cathode Materials

[EFRC – NECCES] Jia Ding[1], Xiaoya Wang[1], Fredrick Omenya[1], Hui Zhou[1], Natasha A. Chernova[1], Yuh-Chieh Lin[2], Lek-Heng Chu[2], Shawn Sallis[1], Jatinkumar Rana[1], Kamila M. Wiaderek[3], Karena W. Chapman[3], Jue Liu[4], Louis F. J. Piper[1], Shyue Ping Ong[2], M. Stanley Whittingham[1]

[1]Binghamton University; [2] University of California San Diego; [3]Argonne National Laboratory; [4]Oak Ridge National Laboratory

PI-D-16: Experimental evaluation of the intercalation of multivalent cations in oxide hosts

[Hub – JCESR] Ryan D. Bayliss[1], Patrick J. Bonnick[2], Jordi Cabana[1], Pieremanuele Canepa[3], Gerbrand Ceder[3], Fulya Dogan[4], Gopalakrishnan Sai Gautam[3], Justin C. Hancock[5], Linhua Hu[1], Brian J. Ingram[4], Baris Key[4], Ka-Cheong Lau[4], Chen Liao[4], Linda F. Nazar[2], Gene M. Nolis[1], Kenneth R. Poeppelmeier[5], Xiaoqi Sun[2], John T. Vaughey[4], Allison Wustrow[5], Hyun Deog Yoo[1]

[1]University of Illinois at Chicago; [2]University of Waterloo; [3]Lawrence Berkeley National Laboratory; [4]Argonne National Laboratory; [5]Northwestern University

E. Nuclear Energy and Waste

PI-E-1: Molten Flux Synthesis and Ion-exchange of Uranyl Silicate Salt Inclusion Materials

[EFRC – CHWM] Gregory Morrison[1], Rob Koch[2], Mark J. Noordhoek[1], Simerjeet Gill[3], Scott Misture[2], Theodore M. Besmann[1], Hans-Conrad zur Loye[1]

[1]University of South Carolina (lead institution); [2]Alfred University; [3]Brookhaven National laboratory

PI-E-2: Solvation shells and chemical dynamics in radiation environments

[EFRC – IDREAM] Xiaosong Li[3], Larry Anovitz[4], Jaehun Chun[1], Aurora Clark[2], Lance Edens[2], Joseph Kasper[3], Sebastien Kerisit[1], Ernesto Martinez-Baez[2], Daniel Pope[2], Maxime Pouvreau[2], Micah Prange[1], Gregory Schenter[1], David Semrouni[2], Zhizhang, Shen[1], Andrew Stack[4], Torin Stetina[3], Shichao Sun[3], Tiecheng Zhou[2]

[1]Pacific Northwest National Laboratory, [2]Washington State University, [3]University of Washington, [4]Oak Ridge National Laboratory

PI-E-3: Iodine Incorporation and Confinement in Apatite Waste Forms - Mechanistic Understanding and Long Term Performance

[EFRC – WastePD] Zelong Zhang,[1] Tiankai Yao,[2] Jianwei Wang,[1] Joseph V. Ryan,[3] John D. Vienna,[3] Jie Lian[1]

[1]Louisiana State University; [2]Rensselaer Polytechnic Institute; [3]Pacific Northwest National Laboratory

PI-E-4: Synthesis, Characterization, and Thermodynamic Studies of Neptunyl Peroxide Compounds

[EFRC – MSA] Sarah Hickam[1], Lei Zhang[1], Jennifer E.S. Szymanowski[1], Mateusz Dembowski[1], Ginger E. Sigmon[1], Peter C. Burns[1]

[1] University of Notre Dame

PI-E-5: Mesoscale Phase Field Modeling of Radioactive Species Extraction in Hierarchical Waste Form Materials: Ion Exchange in LTA Zeolite

[EFRC – CHWM] Shenyang Hu[2], Yulan Li[2], Benjamin Zeidman[2], Charles Henager, Jr.[2], Theodore M. Besmann[1], Agnes Grandjean[3]

[1]University of South Carolina (lead institution); [2]Pacific Northwest National Laboratory; [3]Commissariat à l'Energie Atomique

PI-E-6: QUANTIFYING THE ROLE OF β AND γ RADIATION IN DRIVING MOLECULAR SPECIATION AND INTERFACIAL REACTIVITY FAR FROM EQUILIBRIUM
[EFRC – IDREAM] Thom Orlando[4], Greg Kimmel[1], Alex Alexandrov[4], Patricia Huestis[5], AJ Krzysko[2], Jay La Verne[5], Xiaosong, Li[3], Nik Petrik[1], Shichao Sun[3], Sue Clark[2]
[1]Pacific Northwest National Laboratory, [2]Washington State University, [3]University of Washington, [4]Georgia Institute of Technology, [5]University of Notre Dame

PI-E-7: RECENT DEVELOPMENT OF CALORIMETRIC STUDIES ON TRANSURANIC MATERIALS
[EFRC – MSA] Lei Zhang[1], Ewa Dzik[1], Hrafn Traustason[1], Jennifer E.S. Szymanowski[1], Ginger E. Sigmon[1], Alexandra Navrotsky[2], Peter C. Burns[1]
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PI-E-8: TRANSFORMATION OF THE RAMPAGE POTENTIAL FITTING PROGRAM INTO A QUANTIFIED HIGH-PERFORMANCE CODE: A WASTEPD - SCIDAC COLLABORATION
[EFRC – WastePD] Wolfgang Windl,[1] David Riegner,[1] Nikolas Antolin,[1] Christian Oberdorfer,[1] Christopher Taylor,[1] Adib Samin,[1] Jianwei Wang,[2] Zelong Zhang,[2] Jincheng Du,[3] Philip C. Roth,[4] Sarat Sreepathi,[4] Shirley Moore,[4] Hongzhang Shan,[5] Leonid Oliker[5]
[1]Ohio State University; [2]Louisiana State University; [3]University of North Texas; [4]Oak Ridge National Laboratory; [5]Lawrence Berkeley National Laboratory

PI-E-9: SYNCHROTRON BASED X-RAY DIFFRACTION METHODS FOR REAL TIME EVALUATION OF HIERARCHICAL WASTE FORMS
[EFRC – CHWM] Simerjeet Gill[2], Mohamed Elbakshwan[2], Rob Koch[3], Gregory Morrison[1], Lynne Ecker[2], Jianming Bai[2], Eric Dooryhee[2], Scott Misture[3], Hans-Conrad zur Loye[1]
[1]University of South Carolina; [2]Brookhaven National Laboratory; [3]Alfred University

PI-E-10: THE STRUCTURE AND DIFFUSION OF ISG NUCLEAR WASTE GLASSES AND THEIR ALTERATION LAYERS DURING DISSOLUTION: AN INTEGRATED SIMULATION AND EXPERIMENTAL STUDY
[EFRC – WastePD] Xiaonan Lu,[1] Lu Deng,[1] Mengguo Ren,[1] Thiruvil S. Mahadevan,[1] Hongshen Liu,[2] Marie Collin,[3] Joseph V. Ryan,[4] John D. Vienna,[4] Seong H. Kim,[2] Stephane Gin,[3] Jincheng Du[1]
[1]University of North Texas; [2]Pennsylvania State University; [3]Commissariat à l'énergie atomique et aux énergies alternatives (CEA), France; [4]Pacific Northwest National Laboratory;

PI-E-11: LINKING FLUID PHASE DYNAMICS TO NUCLEATION, PARTICLE GROWTH, AND INTERFACIAL REACTIVITY IN HIGHLY ALKALINE SYSTEMS OF CONCENTRATED ELECTROLYTES
[EFRC – IDREAM] Andrew Stack[4], Kevin Rosso[1], Trent Graham[2], Jianzhi Hu[1], Sebastien Kerisit[1], Xiaosong Li[3], Katharine Page[4], Carolyn Pearce[1], Maxime Pouvreau[2], Micah Prange[1], Zhizhang Shen[1], Torin Stetina[3], Hsui-Wen Wang[4], Zheming Wang[1], Xin Zhang[1]
[1]Pacific Northwest National Laboratory, [2]Washington State University, [3]University of Washington, [4]Oak Ridge National Laboratory

PI-E-12: INVESTIGATIONS OF BI-TRIAZYNOL PYRIDINES FOR POTENTIAL NUCLEAR WASTE SEPARATIONS
[EFRC – CAST] David Dan
Florida State University

F. QUANTUM MATERIALS

PI-F-1: GROUND STATE PROPERTIES OF 3D METALS FROM AB-INITIO DIAGRAMMATIC APPROACHES
[CMS – CDMFTS] Andrey Kutepov[1]
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PI-F-2: ELECTRONIC AND STRUCTURAL PROPERTIES OF BULK AND K-DOPED NICKEL OXIDES FROM QUANTUM MONTE CARLO
[CMS – CPSFM] Hyeondeok Shin[1], Ye Luo[1], Anouar Benali[1], Jaron Krogel[2], Panchapakesan Ganesh[2], Janakiraman Balachandran[2], Paul Kent[2], Olle Heinonen[1]
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PI-F-3: DISCOVERY OF ORBITAL-SELECTIVE COOPER PAIRING IN THE ORBITAL-SELECTIVE MOTT PHASE OF IRON-BASED SUPERCONDUCTORS
[EFRC – CES] A. Kostin[1,2], P.O. Sprau[1,2], A. Kreisel[3*], Yi Xue Chong[1,2], A. Boehmer[4], P.C. Canfield[4,5], P.J. Hirschfeld[6], B.M. Andersen[7], J.C. Séamus Davis[1,2]
[1]Brookhaven National Laboratory, [2]Cornell University, [3]Universit¨at Leipzig, [4]Ames Laboratory, [5] Iowa State University, [6]University of Florida, [7] University of Copenhagen

PI-F-4: THERMAL EQUILIBRATION IN ELECTRON-PHONON COUPLED MOLECULAR DYNAMICS
[EFRC – EDDE] Artur Tamm[1], Magdalena Caro[2], Alfredo Caro[3], Alfredo A. Correa[1]
[1]Lawrence Livermore National Laboratory; [2]Virginia Tech; [3]Los Alamos National Laboratory

PI-F-5: ANTIFERROMAGNETIC SPINTRONICS
[EFRC – SHINES] Weiwei Lin[1], Zhong Shi[2], Bochao Li[3], Xin Ma[4], C. L. Chien[1], Jing Shi[2], Tingyong Chen[3], Xiaoqin Li[4]
[1]Johns Hopkins University; [2]University of California, Riverside; [3]Arizona State University; [4]University of Texas at Austin

PI-F-6: ELECTRONIC AND STRUCTURAL PROPERTIES OF 2D MATERIALS
[EFRC – CCDM] M. Iavarone[1] and E. Borguet[1], A. Bansil[2], I. Cone[1], G. Karapetrov[3], C. Lane[2], T. Polakovic[3], M. Precner[3], A. Putilov[1], Q. Qiao[4], D. Trainer[1], B. Wang[2], X. X. Xi[1], A. Yaroslav[1], Y. Zhu[4]
[1]Temple University, [2]Northeastern University, [3]Drexel University, [4]Brookhaven National Laboratory

PI-F-7: ELECTROCHEMICAL AND MECHANICAL CONTROL OF METAL-INSULATOR TRANSITIONS IN EPITAXIAL VANADIUM DIOXIDES
[CMS – CPSFM] Yogesh Sharma[1], Janakiraman Balachandran[2], Changhee Sohn[1], Liam Collins[2], Nina Balke[2], Jaron Krogel[1], Panchapakesan Ganesh[2], Olle Heinonen[3], Ho Nyung Lee[1]
[1]Oak Ridge National Laboratory; [2]Argonne National Laboratory

PI-F-8: SPIN - PHONON COUPLING IN NIO: UV AND VISIBLE RAMAN SPECTROSCOPY INVESTIGATION
[EFRC – SHINES] Ece Aytan[1], Monica Lacerda[1,2], Fariborz Kargar[1], Junxue Li[1], Bishwajit Debnath[1], Roger Lake[1], Jing Shi[1], Alexander A. Balandin[1]
[1]University of California, Riverside; [2]Universidade Federal do Rio de Janeiro, Brazil

PI-F-9: LARGE THERMOPOWER IN COSBS
[CMS – CDMFTS] Qianheng Du[1,2], Yu Liu[1], C. Petrovic[1,2]
[1]Brookhaven National Lab; [2]Stony Brook University

PI-F-10: NEUTRON AND X-RAY SCATTERING STUDIES OF PHONONS IN THERMOELECTRIC MATERIALS
[EFRC – S^{3}TEC] Jennifer L. Niedziela[1], Dipanshu Bansal[1], Andrew F. May[1], Jeff Snyder[2], Riley Hannus[2], Ian Witting[2], Thomas Chasapis[2], Jun Mao[3], Zhifeng Ren[3], Olivier Delaire[1,4]
[1]Oak Ridge National Laboratory, [2]Northwestern University, [3]University of Houston, [4]Duke University

H. SOLAR ENERGY CONVERSION

PI-H-1: TOWARDS SOLAR-FUEL PRODUCTION VIA PHOTOCATALYTIC WATER OXIDATION
[EFRC – ANSER] Gary W. Brudvig[3], Victor S. Batista[3], Robert H. Crabtree[1], Lin X. Chen[1,2], Joseph T. Hupp[1], James M. Mayer[3], David M. Tiede[2], Michael R. Wasielewski[1], Omar K. Farha[1], Katherine J. Fisher[3], William L. Hoffeditz[1], Jiyun Hong[3], Rebecca J. Kamire[1], Gihan Kwon[1,2], Kelly L. Materna[3], Adam J. Matula[3], Brian T. Phelan[1], Jennifer L. Peper[3], Liam S. Sharninghausen[3], Stafford W. Sheehan[3], Dimitar Y. Shopov[3], Shashi B. Sinha[3], Julianne M. Thomsen[3], Ke R. Yang[3]
[1]Northwestern University; [2]Argonne National Laboratory; [3]Yale University

PI-H-2: SOLID-STATE PHOTON UPCONVERSION AND DOWNCONVERSION IN HYBRID ORGANIC-INORGANIC SYSTEMS
[EFRC – CE] Mengfei Wu[1], Markus Einzinger[1], Tony Wu[1], Lea Nienhaus[1], Joel Jean[1], Cole Perkinson[1], Moungi Bawendi[1], Vladimir Bulovic[1], Marc Baldo[1]
[1]Massachusetts Institute of Technology

PI-H-3: SOLAR-DRIVEN CO_2 REDUCTION TO HYDROCARBONS AND OXYGENATES
[Hub – JCAP] Joel W. Ager[1], Yanwei Lum[1], Gurudayal[1]
[1]Lawrence Berkeley National Laboratory

PI-H-4: BIOHYBRID MOLECULAR ARCHITECTURES FOR PANCHROMATIC SOLAR LIGHT-HARVESTING
[EFRC – PARC] Rui Liu[1], Yunlong Zhang[1], Jianbing Jiang[1], Tuba Sahin[1], Paul A. Loach[2], David F. Bocian[3], Dewey Holten[4], Jonathan S. Lindsey[1]
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PI-H-5: CHROMOPHORE-CATALYST ASSEMBLIES FOR SOLAR FUELS PRODUCTION
[EFRC – UNC] Gyu Leem[1], Ludovic Troian-Gautier[2], Animesh Nayak[2], Linda Nhon[3], Michael S. Eberhart[2], Benjamin D. Sherman[2], Zachary A. Morseth[2], Leila Alibabaei[2], Yan Zhao[1], Yukyung Eom[1], Gerald J. Meyer[2], Thomas J. Meyer[2], John M. Papanikolas[2], John R. Reynolds[3], Kirk S. Schanze[1]
[1]University of Texas at San Antonio; [2]University of North Carolina at Chapel Hill; [3]Georgia Institute of Technology

PI-H-6: RESOLVING STRUCTURES FOR SOLAR-DRIVEN CATALYSIS IN AMORPHOUS OXIDE AND MOLECULAR WATER-OXIDATION CATALYSTS USING *IN-SITU* X-RAY TECHNIQUES

[EFRC – ANSER] Gihan Kwon[1,2], In Soo Kim[2], Jiyun Hong[1], Ke R. Yang[3], Adam J. Matula[3], Hoyoung Jang[4], Jun-Sik Lee[4], Victor S. Batista[3], Gary W. Brudvig[3], Robert H. Crabtree[3], Lin X. Chen[1,2], Alex B. F. Martinson[2], David M. Tiede[2]

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PI-H-7: SYNTHESIS AND CHARACTERIZATION OF FUNCTIONAL GROUP 14 MATERIALS AT THE SPALLATION NEUTRON SOURCE

[EFRC – EFree] Bianca Haberl[1], Chen Li[2,3], Jamie Molaison[1], Abhisek Basu[3], Luke Daemen[1], A.J. Ramirez-Cuesta[1], Timothy Strobel[3], Reinhard Boheler[1,3]

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PI-H-8: DAYTIME RADIATIVE COOLING USING NEAR-BLACK INFRARED EMITTERS

[EFRC – LMI] Jun-long Kou[1], Zoila Jurado[1], Zhen Chen[2], Shanhui Fan[2], Austin J. Minnich[1]

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PI-H-9: THE ROAD TO DISCOVERY: RECENT PROGRESS IN QUANTUM DOT SOLAR CELLS

[EFRC – CASP] Joseph M. Luther[1], Matthew C. Beard[1], Matt Law[2], Jeffrey M. Pietryga[3], Victor I. Klimov[3], Arthur Nozik[1], Jianbo Gao[1,3], Ashley R. Marshall[1], Erin M. Sanehira[1], Ryan W. Crisp[1], Gregory Pach[1], Hunter McDaniel[3], Jianbing Zhang[1], Sungwoo Kim[1], Boris Chernomordik[1]

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PI-H-10: TEACHING PEROVSKITES TO SWIM

[EFRC – ANSER] In Soo Kim[2], Duyen H. Cao[1,2], D. Bruce Buchholz[1], Jonathan D. Emery[1], Omar K. Farha[1], Joseph T. Hupp[1], Mercouri G. Kanatzidis[1], Alex B. F. Martinson[2]

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PI-H-11: INTERFACIAL ELECTRON AND HOLE TRANSFER DYNAMICS OF DYE-SENSITIZED METAL OXIDE ARCHITECTURES

[EFRC – UNC] Melissa K. Gish, Lenzi J. Williams, M. Kyle Brennaman, Robert J. Dillon, Alexander M. Lapides, Aaron D. Taggart, Leila Alibabaei, Taylor H. Moot, Bing Shan, Ludovic Troian-Gautier, Joseph L. Templeton, James F. Cahoon, Thomas J. Meyer, John M. Papanikolas

University of North Carolina at Chapel Hill

PI-H-12: EXCITON DYNAMICS AND TRANSPORT IN ACID-TREATED MoS_2

[EFRC – CE] Aaron J. Goodman[1], Mark C. Weidman[1], Adam P. Willard[1], William A. Tisdale[1]

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I. SYNTHESIS SCIENCE

PI-I-1: STRUCTURAL CHARACTERIZATION OF FRAMEWORK–GUEST INTERACTIONS IN METAL–ORGANIC FRAMEWORKS

[EFRC – CGS] Rebecca L. Siegelman[1], Miguel I. Gonzalez[1], Jarad A. Mason[1], Dianne J. Xiao[1], Douglas A. Reed[1], Matthew T. Kapelewski[1], Eric D. Bloch[1], Simon J. Teat[2], Kevin J. Gagnon[2], Gregory Y. Morrison[2], Wendy L. Queen[2], Jeffrey R. Long[1,2]

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PI-I-2: THEORY AND REALIZATION OF SYNTHESIS ROUTES FOR MnO_2 AND TiO_2 POLYMORPHS

[EFRC – CNGMD] Lauren Garten[1], Daniil Kitchaev[2], Praneetha Selvarasu[1], John Perkins[1], David Ginley[1], Wenhao Sun[3], Kirill Popov[3], Shyam Dwaraknath[3], Kristin Persson[3], Gerbrand Ceder[3], John Mangum[4], Brian Gorman[4], Laura Schelhas[5], Michael Toney[5], Zamyla Chan[6], Daniel Nocera[6], James Haggerty[7], Okan Agirseven[7], Janet Tate[7], William Tumas[1]

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PI-I-3: COMPUTATIONAL SYNTHESIS OF LAYERED MATERIALS USING CHEMICAL VAPOR DEPOSITION AND LIQUID PHASE EXFOLIATION

[CMS – MAGICS] Priya Vashishta[1], Sungwook Hong[1], Rajiv K. Kalia[1], Aravind Krishnamoorthy[1], Subodh Tiwari[1], Chunyang Sheng[1], Guoqing Zhou[1]

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PI-I-4: DESIGN STRATEGIES FOR SHAPE PERSISTENT POROUS ORGANIC CAGES

[EFRC – UNCAGE-ME] Guanghui Zhu[1], Yang Liu[1], Luis Flores[2], Christopher W. Jones[1], David Dixon[2], David S. Sholl[1], Ryan P. Lively[1]

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PI-I-5: SOLVOTHERMAL SYNTHESIS OF FORBIDDEN SULFIDES AND DIMENSIONAL STRUCTURE SCREENING

[EFRC – CES] Insung Han[1], Zhelong Jiang[1], Hong Zhang[2], Huaping Sheng[2], Ankita Bhutani[1], Lucas K. Wagner[1], Dean J. Miller[2], Daniel P. Shoemaker[1]

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PI-I-6: FABRICATION OF POROUS MATERIALS FOR GAS SEPARATION AND CO_2 CAPTURE

[EFRC – CGS] Shuai Yuan[1], Gregory Day[1], Feng Xue[2], Michael Tsapatsis[2], Hong-Cai Zhou[1]

[1]Texas A&M University; [2]University of Minnesota

PI-I-7: EFFECTS OF CHEMICAL COMPLEXITY ON INTRINSIC PROPERTIES AND LATTICE DISTORTION

[EFRC – EDDE] Hongbin Bei[1], Fuxiang Zhang[1], Ke Jin[1], Yang Tong[1], Shijun Zhao[1], Haizhou Xue[3], Gihan Velişa[1], J.C. Neuefeind[2], Brian C. Sales[1], G. Malcolm Stocks[1], Ke An[2], William J. Weber[1,3], Yanwen Zhang[1]

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J. MATERIALS AND CHEMISTRY BY DESIGN

PI-I-1: STOCHASTIC GW

[CMS – C2SEPEM] Vojtech Vlceck[3], Daniel Neuhauser[3], Eran Rabani[1, 2]
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PI-I-2: ELECTRON RATCHETS: THEORY AND EXPERIMENT

[EFRC – CBES] Ofer Kedem[1], Bryan Lau[1], Daniel Kwasnieski[1], Mark A. Ratner[1], Emily A. Weiss[1]
Northwestern University[1]

PI-I-3: ENHANCING THE SUPERCONDUCTING CRITICAL CURRENT THROUGH DESIGNED HETEROGENEITY

[EFRC – CES] U. Welp[1], A. E. Koshelev[1], W. –K. Kwok[1], M. P. Smylie[1,2], D. J. Miller[1], H. P. Sheng[1], A. Glatz[1,3], I. A. Sadovskyy[1,4], Y. Zhang[5], M. W. Rupich[6], S. Sathyamurthy[6], S. Fleshler[6], S. Eley[7], L. Civale[7], A. Kayani[8], P. M. Niraula[8], J.H. Kwon[0], J. M. Zuo[9]
[1]Argonne National Laboratory, [2]University of Notre Dame, [3]Northern Illinois University, [4]University of Chicago, [5]SuperPower Corp., [6]American Superconductor Corp., [7]Los Alamos National Laboratory, [8]Western Michigan University, Kalamazoo, [9]University of Illinois-Urbana Champaign

PI-I-4: COMBINING THEORY AND EXPERIMENT TO REALIZE NEW FUNCTIONAL MATERIALS

[EFRC – CNGMD] Vladan Stevanovic[1], David Ginley[2], Prashun Gorai[1], John Mangum[1], Brian Gorman[1], Lauren Garten[2], John Perkins[2], Riley Brandt[3], Jeremy Poindexter[3], Rachel Kurchin[3], Robert Hoye[3], Tonio Buonassisi[3], Shyam Dwaraknath[4], Kristin Persson[4], Laura Schelhas[5], Michael F. Toney[5], William Tumas[2]
[1]Colorado School of Mines; [2]National Renewable Energy Laboratory; [3]Massachusetts Institute of Technology; [4]Lawrence Berkeley National Laboratory; [5]SLAC National Accelerator Laboratory

PI-I-5: ULTRAFAST PUMP-PROBE EXPERIMENTS TO DETERMINE OPTICALLY INDUCED STRUCTURAL TRANSFORMATIONS IN 2D MATERIALS AND THEIR VALIDATION USING QUANTUM MOLECULAR DYNAMICS

[CMS – MAGICS] David Fritz[1], Uwe Bergmann[1], [1]Ming-Fu Lin, Clemens Wegener[1], Aravind Krishnamoorthy[2], Lindsay Bassman[2], Hiroyuki Kumazoe[2], Aiichiro Nakano[2], Priya Vashishta[2], Vidya Kochat[3], Chandrashekar Tiwari[3], Pulickel Ajayan[3]
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PI-I-6: SINTER-RESISTANT PLATINUM CATALYST SUPPORTED BY METAL-ORGANIC FRAMEWORK

[EFRC – ICDC] In Soo Kim[1], Zhanyong Li[2], Jian Zheng[3], Ana Platero-Prats[4], Andreas Mavrandonakis[5], Steven Pellizzeri[6], Magali Ferrandon[1], Leighanne C. Gallington[4], Thomas Webber[5], Nicolaas A. Vermeulen[2], R. Lee Penn[5], Rachel B. Getman[6], Christopher J. Cramer[5], Karena W. Chapman[4], Donald M. Camaioni[3], John L. Fulton[3], Johannes A. Lercher[7], Omar K. Farha[2], Joseph T. Hupp[2], Alex B. F. Martinson[1]
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PI-I-7: NMR STUDIES OF CARBON DIOXIDE SORPTION IN METAL-ORGANIC FRAMEWORKS

[EFRC – CGS] Alexander C. Forse[1], Phillip J. Milner[1], Rebecca L. Siegelman[1], Jeffrey D. Martell[1], Miguel I. Gonzalez[1], Jeffrey R. Long[1,2], Jeffrey A. Reimer[1,2]
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PI-I-8: VALIDATION AND APPLICATIONS OF MICCOM CODES: MATERIALS FOR ENERGY CONVERSION

[CMS – MICCoM] Maria Chan[1], Yi Xia[1], James Hodges[2], Mercouri Kanatzidis[2], Marton Voros[1], Siyoung Kim[3], Marcello Puligheddu[3], Choo Wooje[3], Dmitri Talapin[1,3], Marco Govoni [1,3], Francois Gygi[4], Monica Olvera de la Cruz[2], Giulia Galli[1,3]

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PI-I-9: DEGRADATION AND STABILITY OF MIL-125 AND MIL-125 DERIVATIVES: A STUDY ON THE FACTORS CONTRIBUTING TO MOF STABILITY

[EFRC—UNCAGE-ME] Ian M. Walton[1], Chu Han[1], William P. Mountfield III[1], Alex C. Elder[1], Krista Walton[1]

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PI-I-10: CHARGE TRANSPORT IN MESOSCALE ASSEMBLIES OF QUANTUM DOTS

[EFRC – CASP] Juliette Micone[1], Daniel B. Straus[2], Andrew F. Fidler[3], Kan Fu[1], Jason Tolentino[1], Ashley R. Marshall[4], Ting Chen[7], Marton Voros[5], Justin C. Johnson[4], Andrew Shabaev[6], Matt Law[1], Cherie R. Kagan[2], Matthew C. Beard[4], Giulia Galli[5], Alexander L. Efros[6], Uwe R. Kortshagen[7], Victor I. Klimov[3]

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PI-I-11: TUNABLE EXCITONS IN BILAYER GRAPHENE

[CMS – C2SEPEM] Long Ju[4], Lei Wang[3], Ting Cao[2], Takashi Taniguchi[5], Kenji Watanabe[5], James Hone, Steven G. Louie[1, 2], Farhan Rana[4], Jiwoong Park[4], Feng Wang[1, 2], Paul McEuen[4]

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PI-I-12: CONSTRUCTION OF A TWO-DIMENSIONAL MATERIALS DATABASE FOR FUNCTIONAL MATERIAL DISCOVERY AND DESIGN

[EFRC – CCDM] Q. Yan[1], H. Banjade[1], J. Pan[1], H. Peng[1], J.P. Perdew[1]

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PI-I-13: NOVEL OPTIMIZATION TECHNIQUES FOR MANY-BODY WAVEFUNCTIONS

[CMS – CPSFM] Luning Zhao[1], Eric Neuscamman[1]

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PI-I-14: COMBINED EXPERIMENTAL AND COMPUTATIONAL EFFORTS FOR THE CHARACTERIZATION OF METAL-MODIFIED METAL-ORGANIC FRAMEWORKS

[EFRC – ICDC] Ana E. Platero-Prats[1], Wei-Guang Liu[2], Manuel A. Ortuño[2], Leighanne C. Gallington[1], Takaaki Ikuno[3], In Soo Kim[4], Jian Zheng[5], Aaron B. League,[2] Varinia Bernales,[2] Jingyun Ye[2], Aleksei Vjunov[5], Neil M Schweitzer[6], Zhanyong Li[6], Aaron W. Peters[6], Maricruz Sanchez-Sanchez[3], Andrey A. Yakovenko[1], Dale R. Pahls[2], Layla Mehdi[5], Timothy C. Wang[6], Andrew J. Stevens[5], Alice Dohnalkova[5], Mahalingam Balasubramanian[1], John L. Fulton[5], Donald M. Camaioni[5], Debmalya Ray[2], Joseph T. Hupp[6], Omar K. Farha[6,7], Donald G. Truhlar[2], Alex B. F. Martinson[4], Christopher J. Cramer[2], Johannes A. Lercher[3,5], Laura Gagliardi[2], Karena W. Chapman[1]

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PI-I-15: VALIDATION AND APPLICATIONS OF MICCOM CODES: MATERIALS FOR ENERGY CONVERSION

[CMS – MICCoM] Maria Chan[1], Yi Xia[1], James Hodges[2], Mercouri Kanatzidis[2], Marton Voros[1], Siyoung Kim[3], Marcello Puligheddu[3], Choo Wooje[3], Dmitri Talapin[1,3], Marco Govoni [1,3], Francois Gygi[4], Monica Olvera de la Cruz[2], Giulia Galli[1,3]

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PI-I-16: FIRST PRINCIPLES ELECTRON TRANSPORT SIMULATIONS OF THERMOELECTRIC MATERIALS

[EFRC – S^{3}TEC] Jiawei Zhou[1], Te-Huan Liu[1], Qichen Song[1], Jun Mao[2], Ran He[2], Hangtian Zhu[2], Jing Shuai[2], Bolin Liao[1], Zhifeng Ren[2], Liang Fu[1], David Singh[3], Gang Chen[1]

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PI-I-17: CENTER FOR NEXT GENERATION OF MATERIALS BY DESIGN

[EFRC – CNGMD] William Tumas[1], Gerbrand Ceder[2], David Ginley[1], John Perkins[1], Stephan Lany[1], Andriy Zakutayev[1], Kristin Persson[2], Alexie Kolpak[3], Tonio Buonassisi[3], Roy Gordon[4], Daniel Nocera[4], Brian Gorman[5], Vladan Stevanovic[5], Janet Tate[6], Michael Toney[7]

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PI-I-18: SOFTWARE FOR COMPUTATIONAL MATERIALS SCIENCE: METASCALABLE REACTIVE MOLECULAR DYNAMICS AND QUANTUM MOLECULAR DYNAMICS, AND DATA ANALYTICS

[CMS – MAGICS] Lindsay Bassman[1], Aiichiro Nakano[1], Subodh Tiwari[1], Chunyang Sheng[1], Kuang Liu[1], Rajiv K. Kalia[1], Priya Vashishta[1], Oleg Prezhdo[1], Muratahon Aykol[2], Patrick Huck[2], Kristin Persson[2], Saber Naserifar[3], William Goddard[3], David J. Singh[4]

[1]*University of Southern California*; [2]*Lawrence Berkeley National Laboratory, University of California Berkeley*; [3]*California Institute of Technology;* [4]*University of Missouri*

PI-I-19: ADVANCED LIGHT MANAGEMENT WITH STRUCTURED SURFACES

[EFRC – LMI] Seyedeh Mahsa Kamali[1], Soo Jin Kim[2], Ehsan Arbabi[1], Majid Esfandyarpour[2], Amir Arbabi[1], Ju-Hyung Kang[2], Yu Horie[1], Pengyu Fan[2], Mohammad Sadegh Faraji-Dana[1], Mehmet Mutlu[2], Andrei Faraon[1], Mark L. Brongersma[2]

[1]California Institute of Technology; [2]Stanford University

PI-I-20: STUDY OF NANOSTRUCTURED COMPOSITES Nd(Ti,Zr)O/Si(B)CO FOR OPTICAL AND NUCLEAR WASTE STORAGE APPLICATION

[EFRC – CAST] Vanessa Proust

Florida State University

PI-I-21: COMPOSITIONAL EFFECTS ON ENERGY DISSIPATION AND DEFECT DYNAMICS IN CONCENTRATED SOLID SOLUTION ALLOYS

[EFRC – EDDE] William J. Weber[1,2], Shijun Zhao[2], Eva Zarkadoula[2], Mohammad W. Ullah[2], Gihan Velişa[2], Neila Sellami[2], Hongbin Bei[2], Lumin Wang[3], Yanwen Zhang[1]

[1]University of Tennessee-Knoxville; [2]Oak Ridge National Laboratory; [3]University of Michigan-Ann Arbor

PI-I-22: COVALENT-SUPRAMOLECULAR HYBRID POLYMERS AND MUSCLE-INSPIRED ANISOTROPIC ACTUATORS

[EFRC – CBES] Stacey M. Chin[1], Christopher V. Synatschke[1], Shuangping Liu[1], Rikkert J. Nap[1], Igal Szleifer[1], Monica Olvera de la Cruz[1], Samuel I. Stupp[1]

Northwestern University[1]

POSTER SESSION II: TUESDAY, JULY 25, 2017; 3:30 – 5:00 PM, *EXHIBITION HALL C*

A. BIOSCIENCE

PII-A-1: LIGHT HARVESTING IN CYANOBACTERIA: PROTECTIVE MECHANISMS AND RESPONSES TO NUTRIENT AVAILABILITY

[EFRC – PARC] Hui-Yuan Steven Chen[1], Michelle Liberton[1], Daniel A. Weisz[1], Jaclyn Murton[2], Aparna Nagaragan[1], Amelia Nguyen[1], Harmony A. Hancock[2], Haijun Liu[1], Hao Zhang[1], Jerilyn A. Timlin[2], Michael L. Gross[1], Dariusz M. Niedzwiedzki[1], Himadri B. Pakrasi[1]
[1]Washington University in St. Louis; [2]Sandia National Laboratories

PII-A-2: PHYSICAL AND THERMODYNAMIC DETERMINANTS OF NON-FLAVIN BASED ELECTRON BIFURCATION

[EFRC – BETCy] Jacob H. Artz[1,2], Jonathan L. Yuly[3], Michael W.W. Adams[4], Gerrit J. Schut[4], Diep M.N. Nguyen[4], Monika Tokmina-Lukaszewska[1], Brian Bothner[1], Oleg A. Zadvornyy[1,2], David N. Beratan[3], Paul W. King[5], John W. Peters[1,2]
[1]Montana State University; [2]Washington State University; [3]Duke University; [4]University of Georgia; [5]National Renewable Energy Laboratory

PII-A-3: TRANS-DISCIPLINARY STRUCTURAL ANALYSIS PROVIDES INSIGHT INTO FUNCTION AND VARIATION OF THE PLANT CELLULOSE SYNTHESIS COMPLEX

[EFRC – CLSF] Candace H. Haigler[1], B. Tracy Nixon[2], Juan Du[2], Jonathan K. Davis[1], Jason N. Burris[1], Abhishek Singh[1], Yaroslava G. Yingling[1], Hugh O'Neill[3], Eric M. Roberts[4], Arielle M. Chaves[5], Alison W. Roberts[5]
[1]North Carolina State University; [2]The Pennsylvania State University; [3]Oak Ridge National Laboratory; [4]Rhode Island College; [5]University of Rhode Island

PII-A-4: MULTI-SCALE MODELING AND STRUCTURAL CHARACTERIZATION OF BIOMASS FROM ENERGY CROPS

[EFRC – C3Bio] Bryon S. Donohoe[1], Matheus Benatti[2], Lintao Bu[1], Jacob Hinkle[1], Jiliang Liu[3], Yan Zheng[3], Peter Ciesielski[1], Michael F. Crowley[1], Michael E. Himmel[1], Lee Makowski[3], Maureen C. McCann[2]
[1]National Renewable Energy Lab; [2]Purdue University; [3]Northeastern University

PII-A-5: REMODELING AND ENERGY TRANSFER OF PHOTOSYNTHETIC COMPLEXES IN FAR-RED LIGHT

[EFRC – PARC] Ming-Yang Ho[1], Dariusz M. Niedzwiedzki[2], Robert E. Blankenship[2], Donald A. Bryant[1]
[1]The Pennsylvania State University; [2]Washington University in St. Louis

PII-A-6: PRODUCTION AND ORGANIZATION OF CELLULOSE MICROFIBRILS IN PRIMARY AND SECONDARY CELL WALLS

[EFRC – CLSF] Shundai Li[1], Xiaoran Xin[1], Yunzhen Zheng[2], Tian Zhang[1], Shixin Huang[1], Sai Venkatesh Pingali[2], Seong Kim[1], Hugh O'Neill[2], Daniel J. Cosgrove[1], Ying Gu[1]
[1]The Pennsylvania State University; [2]Oak Ridge National Laboratory

B. CARBON SEQUESTRATION

PII-B-1: PORE-SCALE SIMULATION OF THE PROCESSES ASSOCIATED WITH THE INJECTION AND SEQUESTRATION OF CO_2 IN THE SUBSURFACE

[EFRC – NCGC] Cyprien Soulaine[1], Hamdi A. Tchelepi[1], Moataz Abu AlSaud[1], Sophie Roman[1], Sergi Molins Rafa[2], Carl I. Steefel[2], Jiamin Wan[2], Tetsu K. Tokunaga[2]

[1]Stanford University; [2]Lawrence Berkeley National Laboratory

PII-B-2: IMPACT OF BRINE/CO_2 MIXTURES ON THE TRANSPORT AND MECHANICAL PROPERTIES OF MT. SIMON ROCK SAMPLES

[EFRC – GSCO2] Zhuofan Shi[1], Maria Gabriela Davila Ordonez[2], Ange-Therese Akono[2], Jennifer Druhan[2], Kristian Jessen[1], Theodore Tsotsis[1]

[1]University of Southern California, [2]University of Illinois at Urbana-Champaign

PII-B-3: DISCRETE ELEMENT MODELING OF ROCK MECHANICAL ALTERATION DUE TO CO_2 – CHARGED BRINE

[EFRC – CFSES] Zhuang Sun[1], D. Nicolas Espinoza[1], Matthew T. Balhoff[1], Thomas Dewers[2]

[1]The University of Texas at Austin; [2]Sandia National Laboratories

PII-B-4: FLOW, REACTION AND SEALING BEHAVIORS OF FRACTURED SHALE CAP-ROCKS IN CO_2 SEQUESTRATION

[EFRC – NCGC] Michael C. Cheshire[1], Andrew G. Stack[1], Lawrence M. Anovitz[1], Victoria DiStefano[1], David R. Cole[2], Alexander A. Swift[2], Catherine A. Peters[3], Sassan Hajirezaie[3], Benjamin Gilbert[4]

[1]Oak Ridge National Laboratory; [2]The Ohio State University; [3]Princeton University; [4]Lawrence Berkeley National Laboratory

PII-B-5: UNIVERSAL LINEAR TIME-DEPENDENCE OF PERMEABILITY THROUGH DISSOLVING FRACTURES INDUCED BY ACIDIC FLUID

[EFRC – CFSES] Lichun Wang[1], M. Bayani Cardenas[1]

[1]The University of Texas at Austin

PII-B-6: POROMECHANICAL ASPECTS OF RESERVOIR ROCK-CO_2 INTERACTION

[EFRC – GSCO2] Ali Tarokh[1], Roman Makhnenko[1,] Victor Vilarrasa[2]

[1]University of Illinois at Urbana-Champaign, [2]Spanish National Research Council

PII-B-7: MULTISCALE PORE FEATURES AND ASSOCIATED FLUID BEHAVIOR IN CO_2 SEALS AND RESERVOIRS

[EFRC – NCGC] Alexander A. Swift[1], Bohyun Hwang[1], Tanya Whitmer[1], Deepansh J. Srivastava[1], Philip J. Grandinetti[1], Julia Sheets[1], Lawrence Anovitz[2], Timothy J. Kneafsey[3], David R. Cole[1]

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C. Catalysis

PII-C-1: One-step thermochemical saccharification of lignocellulosic biomass
[EFRC – CCEI] Sunitha Sadula[1], Abhay Athaley[2], Weiqing Zheng[1], Marianthi Ierapetritou[2], Basudeb Saha[1]
[1]University of Delaware; [2]Rutgers University

PII-C-2: Dynamic Nature of Nanoporous NiCu in reducing and oxidizing conditions
[EFRC – IMASC] Nare Janvelyan,[1] Cheng Hao Wu,[2] Matthijs A. van Spronsen,[1] Miquel B. Salmeron,[2] Robert J. Madix,[1], Cynthia M. Friend.[1]
[1]Harvard University; [2]Lawrence Berkeley National Laboratory

PII-C-3: Water Oxidation and CO_2 Reduction Catalysis for Solar Fuels Production
[EFRC – UNC] Ying Wang[1], Sergio Gonell-Gómez[1], Matthew V. Sheridan[1], Benjamin D. Sherman[1], Matthew R. Kita[1], Alexander J. M. Miller[1], Cynthia K. Schauer[1], James T. Muckerman[2], Thomas J. Meyer[1]
[1]University of North Carolina at Chapel Hill; [2]Brookhaven National Laboratory

PII-C-4: High Throughput Integration of Multifunctional Catalyst Coatings with Light Absorbers
[Hub – JCAP] Joel A. Haber[1], Aniketa Shinde[1], Dan Guevarra[1], Guiji Liu[2], Guo Li[2], Lan Zhou[1], Santosh K. Suram[1], Qimin Yan[2], Ian D. Sharp[2], Francesca M. Toma[2], Jeffery B. Neaton[2], John M. Gregoire[1]
[1]California Institute of Technology; [2]Lawrence Berkeley National Laboratory

PII-C-5: Electrocatalytic Oxidation and Production of Hydrogen: Strategies for Lowering the Overpotential
[EFRC – CME] Eric. S. Wiedner[1], Geoffrey M. Chambers[1], Christina M. Klug[1], Aaron M. Appel[1], Molly O'Hagan[1], R. Morris Bullock[1]
[1]Pacific Northwest National Laboratory

PII-C-6: Energetics of [FeS] Cluster Assemblies and Influence on Catalysis
[EFRC – BETCy] S. Garrett Williams[1], Paul W. King[2], Jacob Artz[3,4], David W. Mulder[2], Michael W. Ratzloff[2], Carolyn E. Lubner[2], Oleg A. Zadvornyy[3,4], Axl X. LeVan[3], Michael W.W. Adams[5], John W. Peters[3,4], Anne K. Jones[1]
[1]Arizona State University; [2]National Renewable Energy Laboratory; [3]Montana State University; [4]Washington State University; [5]University of Georgia

PII-C-7: QM Derived Mechanism for CO_2RR and OER; Design and testing of improved catalysts
[Hub – JCAP] Hai Xiao[1], Tao Cheng[1], Saber Naserifar[1], Yufeng Huang[1], Robert Nielsen[1], William A. Goddard[1]
[1]California Institute of Technology

PII-C-8: Low-Overpotential Oxygen Reduction with Co-Based Molecular Electrocatalysts
[EFRC – CME] Yu-Heng Larry Wang[1], Colin W. Anson[1], James B. Gerken[1], Zach Goldsmith[2], Patrick Schneider[2], Michael L. Pegis[3], James M. Mayer[3], Sharon Hammes-Schiffer,[2] Shannon S. Stahl[1]
[1]University of Wisconsin-Madison; [2]University of Illinois at Urbana-Champaign; [3]Yale University

PII-C-9: Systems-level molecular mapping of biomass-derived molecules to fuels and chemicals
[EFRC – C3Bio] Taufik Ridha, Emre Gencer, Yiru Li, Mohit Tawarmalani, W. Nicholas Delgass, Fabio H. Ribeiro, Rakesh Agrawal
Purdue University

PII-C-10: Novel Synthesis of Designed Nanoporous Catalytic Materials

[EFRC – IMASC] Tanya Shirman,[1] Zhen Qi,[2] Elijah Shirman,[1] Judith Lattimer,[1] Mathilde Luneau,[1] Nare Janvelyan,[1] Cynthia Friend,[1] Juergen Biener,[2] Joanna Aizenberg[1]

[1]Harvard University; *[2] Lawrence Livermore National Laboratory*

PII-C-11: Catalytic Hydrodeoxygenation of High-Carbon Furylmethanes to Renewable Jet-fuel Range Alkanes

[EFRC – CCEI] Sibao Liu[1], Saikat Dutta[1], Weiqing Zheng[1], Nicholas S. Gould[1], Ziwei Cheng[1], Bingjun Xu[1], Basudeb Saha[1], Dionisios G. Vlachos[1]

[1]University of Delaware

PII-C-12: Fine Tuning the Activity of Metal-Organic Framework-Supported Cobalt Catalysts for Oxidative Dehydrogenation of Propane

[EFRC – ICDC] Zhanyong Li[1], Aaron W. Peters[1], Matt Simons[2], Ana E. Platero-Prats[3], Varinia Bernales[2], Manuel A. Ortuño[2], Karena W. Chapman[3], Neil M. Schweitzer[1], Jian Liu[1], Chung-Wei Kung[1], Matthew R. DeStefano[1], Hyunho Noh[1], Christopher J. Cramer[2], Laura Gagliardi[2], Joseph T. Hupp[1], Omar K. Farha[1,4]

[1]Northwestern University, [2]University of Minnesota, [3]Argonne National Laboratory, [4]King Abdulaziz University

PII-C-13: Enhancing rates of polysaccharide conversion using cellulose decrystallization

[EFRC – C3Bio] Nathan S. Mosier[1], Chien-Yuan Lin[2], Hao Lou[3], Anna T. Olek[1], Tânia M. Shiga[4], Haibing Yang[1], Ximing Zhang[1], Weihua Xiao[5], Bryon S. Donohoe, Lee Makowski[6], Maureen C. McCann[1], Mahdi M. Abu-Omar[3], Nicholas C. Carpita[1]

[1]Purdue University; *[2]National Renewable Energy Lab[3]; University of California Santa Barbara; [4]University of São Paulo; [5]China Agricultural University*, *[6]Northeastern University*

PII-C-14: Integrated Design and Analysis of Chemical Production from biomass Feedstocks

[EFRC – CCEI] Abhay Athaley[1], Basudeb Saha[2], Marianthi Ierapetritou[1]

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

PII-C-15: Solvent Effects on Interfacial Electron Transfer Reactions and Implications for Catalysis

[EFRC – CCDM] R.C. Remsing[1], N. H. Attanayake[1], E. Borguet[1], Q. Kang[1], M. L. Klein[1], I. G. McKendry[1], S. L. Shumlas[1], D. R. Strongin[1], C. Thenuwara[1], A. L. Vernisse[1], M. J. Zdilla[1]

[1]*Temple University*

PII-C-16: Catalytic N_2 Reduction to Silylamines using Molecular Iron and Chromium Complexes

[EFRC – CME] Demyan E. Prokopchuk[1], Alexander J. Kendall[1], Eric S. Wiedner[1], Eric D. Walter[2], Codrina V. Popescu[3], Nicholas A. Piro[4], R. Morris Bullock[1], Michael T. Mock[1]

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D. ENERGY STORAGE

PII-D-1: ATOMISTIC TO MESOSCOPIC VIEW OF LI-S BATTERIES: A MULTI-MODAL APPROACH

[Hub – JCESR] Vijay Murugesan[1], Nav Nidhi Rajput[2], Elizabeth C. Miller[3], Kee Sung Han[1], Michael F. Toney[3], Kristin A. Persson[2], Karl T. Mueller[1]

[1]Pacific Northwest National Laboratory; [2]Lawrence Berkeley National Laboratory; [3]Stanford Synchrotron Radiation Lightsource, SLAC National Accelerator Laboratory

PII-D-2: DESIGNING ELECTRODE INTERPHASES FOR MG-BASED BATTERY SYSTEM

[EFRC – NEES] Emily Sahadeo[1], Jaehee Song[2], Chuan-Fu Lin[1], Karen Gaskell[1], Gary Rubloff[1], Sang Bok Lee[1]

[1]University of Maryland; [2]Samsung Electronics

PII-D-3: PROBING THE LI INSERTION MECHANISM OF SPINEL STRUCTURED MATERIALS: INSIGHTS GAINED FROM A COMBINED EXPERIMENTAL AND DENSITY FUNCTIONAL THEORY APPROACH

[EFRC – m2M] Lei Wang[1], Haoyue Guo[1], Yue Ru Li[1], Yiman Zhang[1], Coray McBean[1], Shihui Zou[1], Alexander Brady[1], Paul Smith[1], Christopher Pelliccione[2], Jiefu Yin[1], Megan Scofield[1], Jing Li[1], Eric Stach[2], Amy Marschilok[1], Kenneth Takeuchi[1], Esther Takeuchi[1], Stanislaus Wong[1], Ping Liu[2].

[1]Stony Brook University, [2]Brookhaven National Laboratory

PII-D-4: PHOTO-ACCELERATED FAST CHARGING OF LITHIUM-ION BATTERIES

[EFRC – CEES] Anna Lee[1], Márton Vörös[1], Wesley M. Dose[1], Jens Niklas[1], Oleg Poluektov[1], Richard D. Schaller[1], Hakim Iddir[1], Victor A. Maroni[1], Eungje Lee[1], Brian Ingram[1], Larry A. Curtiss[1], Christopher S. Johnson[1]

[1]*Argonne National Laboratory*

PII-D-5: BEYOND THERMODYNAMICS IN MG-ION BATTERIES: UNDERSTANDING INTERFACIAL DYNAMICS THROUGH THE SYNERGY BETWEEN EXPERIMENT AND THEORY

[Hub – JCESR] Ethan J. Crumlin[1], Yi Yu[1], Carlos Valero-Vidal[1], Artem Baskin[2], Nathan T. Hahn[3], Kevin R. Zavadil[3], Bryan W. Eichhorn[4], David Prendergast[2], Pietro P. Lopes[5], Krista L. Hawthorne[5], Sang-Don Han[5], Brian J. Ingram[5], Justin G. Connell[5], Nenad M. Markovic[5]

[1]Advanced Light Source, Lawrence Berkeley National Laboratory; [2]Molecular Foundry, Lawrence Berkeley National Laboratory; [3]Sandia National Laboratories; [4]University of Maryland; [5]Argonne National Laboratory

PII-D-6: INVESTIGATION OF LAYERED AND SPINEL STRUCTURES: INSIGHTS FROM CONTINUUM MODELING AND DENSITY FUNCTIONAL THEORY

[EFRC – m2M] Christianna Lininger[1], Nicholas Brady[1], Kevin Knehr[1], Xiaobing Hu[2], Lijun Wu[2], Christina Cama[3], Qing Zhang[3], Andrea Bruck[3], David Bock[2], Yimei Zhu[2], Alan West[1], Mark Hybertsen[2], Amy Marschilok[3], Kenneth Takeuchi[3], Esther Takeuchi[3].

[1]Columbia University, [2]Brookhaven National Laboratory, [3]Stony Brook University

PII-D-7: QUANTUM CAPACITANCE, DIELECTRIC SCREENING, AND EDGE EFFECTS IN CARBON SUPERCAPACITORS AND BEYOND

[EFRC – FIRST] Cheng Zhan[1], Justin Neal[1], Pengfei Zhang[2], Sheng Dai[2], Jianzhong Wu[1], Peter Cummings[3], De-en Jiang[1]

[1]University of California at Riverside; [2]Oak Ridge National Laboratory; [3]Vanderbilt University

PII-D-8: Nanofluidic Battery: Electrochemical Transport Near Electrodes Under Nanoscale Confinement

[EFRC – NEES] Sylvia X. Li[1], Nam Kim[2], Kim McKelvey[3], Chanyuan Liu[4], Henry White[3], Sang Bok Lee[2], Gary Rubloff[2], Mark Reed[1]

[1]Yale University; [2]University of Maryland; [3]University of Utah; [4]Lam Research

PII-D-9: Stabilizing the Li Metal Anode in Li-S Batteries with Novel Electrolytes and Protective Coatings

[Hub – JCESR] Brian D. Adams[1], Hui Wang[1], Kee Sung Han[1], Karl T. Mueller[1], Emily V. Carino[2], Justin G. Connell[2], Tylan Watkins[3], Kyle C. Klavetter[3], Lin Chen[2], Jeffery W. Elam[2], Nitin Kumar[4], Donald J. Siegel[4], Ji-Guang Zhang[1], Kevin R. Zavadil[3]

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PII-D-10: Insight into Realizing the Full 2 Li^+ Capacity of Multi-electron Li_xVOPO_4

[EFRC – NECCES] Shawn Sallis[1], Jatinkumar Rana[1], Linda W Wangoh[1], Kamila M. Wiaderek[2], Yuh-Chieh Lin[3], Yong Shi[1], Carrie Siu[1], Natasha A. Chernova[1], Jinghua Guo[4], Lu Ma[2], Tianpin Wu[2], Tien-Lin Lee[5], Shyue Ping Ong[3], Karena W. Chapman[2], M. Stanley Whittingham[1], Louis F. J. Piper[1]

[1]Binghamton University; [2]Argonne National Laboratory, [3]University of California, San Diego; [4]Lawrence Berkeley National Laboratory; [5]Diamond Light Source Ltd., Harwell Science and Innovation Campus

PII-D-11: Asynchronous Stress and Strain in Li-ion Composite Cathodes

[EFRC – CEES] Kimberly E. Lundberg[1], Ömer Özgur Çapraz[1], Sonika Rajput[1], Robert E. Warburton[2], Siddharth Deshpande[2], Jeffrey Greeley[2], Nancy R. Sottos[1], Andrew A. Gewirth[1]

[1]University of Illinois, [2]Purdue University

PII-D-12: Differentiating Ion & Electron Transport in Mesoscale Architectures

[EFRC – NEES] Singyuk Hou[1], Tao Gao[1], Xiaogang Li[1], Chaoji Chen[1], Liangbing Hu[1], Chunsheng Wang[1]

[1]University of Maryland

PII-D-13: Ion Transport and Electron Transfer in Tunnel Structured Materials: Factors Influencing Electrochemistry

[EFRC – m2M] Paul Smith[1], Xiaobing Hu[2], Jianping Huang[1], Altug Poyraz[2], Bingjie Zhang[1], Lijun Wu[2], Seung-Yong Lee[2], Shaobo Cheng[2], Feng Xu[2], Qingping Meng[2], Jessica Durham[1], Merzuk Kaltak[1], Christopher Pelliccione[2], Maria Fernandez-Serra[1], Mark Hybertsen[2], Esther Takeuchi[1], Amy Marschilok[1], Yimei Zhu[1], Kenneth J. Takeuchi[1].

[1]Stony Brook University, [2]Brookhaven National Laboratory

PII-D-14: Organic-Inorganic Hybrid Electrode Materials for Static and Flowable Pseudocapacitive Energy Storage

[EFRC – FIRST] Muhammad Boota[1], Katherine Van Aken[1], Kelsey Hatzell[2], Haoxiang Luo[2], Peter Cummings[2], Naresh C. Osti[3], Alexander Kolesnikov[3], Eugene Mamontov[3], Yury Gogotsi[1]

[1]Drexel University; [2]Vanderbilt University; [3]Oak Ridge National Laboratory

PII-D-15: TOWARDS ULTRA LOW COST ELECTROCHEMICAL COUPLES FOR GRID STORAGE

[Hub – JCESR] Liang Su[1], Menghsuan Sam Pan[1], Longjun Li[2], Miranda Baran[2], Chun Yuen Kwok[3], Parvin Adeli[3], Zheng Li[1], Andres F. Badel[1], Linda Jing[1], Stephanie L. Eiler[1], Brett A. Helms[2], Linda F. Nazar[3], Fikile R. Brushett[1], Yet-Ming Chiang[1]

[1]Massachusetts Institute of Technology; [2]Lawrence Berkeley National Laboratory; [3]University of Waterloo

PII-D-16: ADVANCING OPERANDO TOOLS TO PROBE MULTISCALE COMPLEXITY IN CHEMICAL ENERGY STORAGE

[EFRC – NECCES] Hao Liu[1], Ieuan D. Seymour[2], Philip Reeves[2], Nicole M. Trease[2], David M. Halat[2], Khim Karki[3,4], Mark Wolf[5], Brian May[5], Eric A. Stach[3], Guangwen Zhou[4], Jordi Cabana[5], Clare P. Grey[2], Peter J. Chupas[6], Karena W. Chapman[1]

[1]Argonne National Laboratory; [2]University of Cambridge; [3]Binghamton University; [4]Brookhaven National Laboratory; [5]University of Illinois-Chicago; [6]Argonne National Laboratory

E. NUCLEAR ENERGY AND WASTE

PII-E-1: LOCAL STRUCTURE DISTORTION IN URANIUM OXIDE SYSTEMS

[EFRC – MSA] Raul I. Palomares[1], Lei Zhang[2], Joerg Neuefeind[3], Jie Lian[4], Alexandra Navrotsky[5], Maik Lang[1]

[1]University of Tennessee; [2]University of Notre Dame; [3]Oak Ridge National Laboratory; [4]Rensselaer Polytechnic Institute; [5]University of California-Davis

PII-E-2: CONSTRUCTION, ACTIVATION, AND REACTIVITY OF URANIUM-ELEMENT MULTIPLE BONDS

[EFRC – CAST] Ezra Coughlin

Purdue University

PII-E-3: QUANTIFYING PHENOMENA LEADING TO AGGREGATION AND OTHER RESPONSE DYNAMICS THAT COUPLE ACROSS SCALES

[EFRC – IDREAM] Jaehun Chun[1], Larry Anovitz[3], Nigel Browning[1], James De Yoreo[1], Lance Edens[2], Layla Mehdi[1], Jeff Morris[4], Elias Nakouzi[1], Alex Robertson[1], Greg Schenter[1], David Semrouni[2], Andrew Stack[3], Xin Zhang[1]

[1]Pacific Northwest National Laboratory, [2]Washington State University, [3]Oak Ridge National Laboratory, [4]The City University of New York

PII-E-4: ICME DESIGN OF NOVEL CORROSION-RESISTANT HIGH-ENTROPY ALLOYS

[EFRC – WastePD] Tianshu Li,[1] Jayendran Srinivasan,[2] Pin Lu,[3] Orion Swanson,[1] James Saal,[3] Gregory B. Olson,[3] John R. Scully,[2] Gerald S. Frankel [1]

[1]Ohio State University; [2]University of Virginia; [3]QuesTek Innovations LLC;

PII-E-5: REACTION PATHWAYS IN NANO-SCALE REDUCTION ALLOYING FROM IN-SITU X-RAY DIFFRACTION

[EFRC – CHWM] Rob Koch[2], Scott Misture[2], Simerjeet Gill[3], Lynne Ecker[3], Guangfang Li[1], Hui Wang[1]

[1]University of South Carolina (lead institution); [2]Alfred University; [3]Brookhaven National laboratory

PII-E-6: *F*-ELEMENT COORDINATION COMPLEXES IN THE GAS PHASE: ELUCIDATING METAL-LIGAND INTERACTIONS

[EFRC – CAST] John Gibson

Lawrence Berkeley National Laboratory

PII-E-7: LIGAND EXCHANGE KINETICS OF THE NEPTUNYL ION AND IMPLICATIONS OF *F*-ELEMENT CHEMISTRY
[EFRC – MSA] Corey D. Pilgrim[1], Harris E. Mason[2], Mavrik Zavarin[2], William H. Casey[1]
[1]University of California-Davis; [2]Lawrence Livermore National Laboratory

PII-E-8: EFFECTS OF COMPOSITIONAL COMPLEXITY ON MICROSTRUCTURAL EVOLUTION IN NI-CONTAINING SINGLE-PHASE FCC ALLOYS
[EFRC – EDDE] Taini Yang[1], Chenyang Lu[1], Ke Jin[2], Gihan Velişa[2], Yanwen Zhang[2], Hongbin Bei[2], Lumin Wang[1]
[1]University of Michigan-Ann Arbor; [2]Oak Ridge National Laboratory

PII-E-9: ATOMIC PROBE TOMOGRAPHY ANALYSIS AND DFT MODELING OF CRYOGENICALLY-PREPARED SPECIMENS
[EFRC – WastePD] Daniel E. Perea,[1] Dan K. Schreiber,[1] Wolfgang Windl,[2] James E. Evans,[1] Joseph V. Ryan,[1] John D. Vienna[1]
[1]Pacific Northwest National Laboratory; [2]Ohio State University

PII-E-10: UNDERSTANDING THE ROLES OF SOLVENT DYNAMICS, CHEMICAL REACTIVITY, SOLUTE ORGANIZATION, AND PRE-NUCLEATION SPECIES IN EXTREME SYSTEMS
[EFRC – IDREAM] Carolyn Pearce[1], Aurora Clark[2], Sue Clark[1], Andy Felmy[2], Trent Graham[2], Jianzhi Hu[1], Joseph Kasper[3], AJ Krzysko[2], Xiaosong Li[3], Ernesto Martinez-Baez[2], Katherine Page[4], Kevin Rosso[1], David Semrouni[2], Andrew Stack[4], Hsui-Wen Wang[4], David Wesolowski[4], Xin Zhang[1], Tiecheng Zhou[2]
[1]Pacific Northwest National Laboratory, [2]Washington State University, [3]University of Washington, [4]Oak Ridge National Laboratory

PII-E-11: A MOLECULAR DYNAMICS STUDY OF U20 NANOCLUSTERS IN AQUEOUS SOLUTION
[EFRC – MSA] Kenneth Newcomb[1], Edward J. Maginn[1]
[1]University of Notre Dame

PII-E-12: FIRST PRINCIPLES DETERMINATION OF STABILITY LAYER ADHESION IN AU-CU NANOPARTICLES
[EFRC – CHWM] Shubham Pandey[1], Simon R. Phillpot[1]
[1]University of Florida

F. QUANTUM MATERIALS

PII-F-1: ABOVE 400 K PERPENDICULAR MAGNETIC PHASE IN TOPOLOGICAL INSULATOR SURFACE STATES INDUCED BY PROXIMITY COUPLING
[EFRC – SHINES] Chi Tang[1], Cui-Zu Chang[2,3], Gejian Zhao[4], Yawen Liu[1], Zilong Jiang[1], Chao-Xing Liu[3], Martha R. McCartney[4], David J. Smith[4], Tingyong Chen[4], Jagadeesh S. Moodera[2], Jing Shi[1]
[1]University of California, Riverside; [2]Massachusetts Institute of Technology; [3]The Pennsylvania State University; [4]Arizona State University

PII-F-2: GUTZWILLER QUANTUM MOLECULAR DYNAMICS SIMULATIONS OF CORRELATED ELECTRON MATERIALS
[CMS – CDMFTS] Gia-Wei Chern[1], Jun Liu[1], Kipton Barros[2], Cristian Batista[3,4], Gabriel Kotliar[5,6]
[1]University of Virginia; [2]Los Alamos National Lab; [3]University of Tennessee; [4]Oak Ridge National Lab; [5]Rutgers University;[6] Brookhaven National Lab

PII-F-3: QUANTUM MONTE CARLO INVESTIGATION OF ANTIFERROMAGNETIC FEO
[CMS – CPSFM] Joshua Townsend[1], Luke Shulenburger[1], Thomas Mattsson[1], Ken Esler[2], Ronald Cohen[3]
[1]Sandia National Laboratories; [2]Stone Ridge Technology; [3]Carnegie Institution

PII-F-4: ACCURATE FIRST-PRINCIPLE STRUCTURES AND ENERGIES OF DIVERSELY BONDED SYSTEMS FROM AN EFFICIENT DENSITY FUNCTIONAL
[EFRC – CCDM] J. Sun[1], M.L. Klein[2], H. Peng[2], J. P.Perdew[2], R. C. Remsing[2], A. Ruzsinszky[2], Z. Sun[2], X. Wu[2]
[1]*University of Texas-El Paso,* [2]*Temple University*

PII-F-5: NON-TRIVIAL TOPOLOGICAL SURFACE STATES IN SmB_6 THIN FILMS
[EFRC – SHINES] Tao Liu[1], Yufan Li[2], Lei Gu[3], Junjia Ding[4], Houchen Chang[1], P. A. Praveen Janantha[1], Valentyn Novosad[4], Axel Hoffmann[4], Ruqian Wu[3], C. L. Chien[2], Mingzhong Wu[1]
[1]Colorado State University; [2]Johns Hopkins University; [3]University of California, Irvine; [4]Argonne National Laboratory

PII-F-6: GENERATION OF SOFT PSEUDOPOTENTIALS FROM AND FOR CORRELATED METHODS
[CMS – CPSFM] Chandler Bennett[1], Cody Melton[1], Luke Shulenburger[2], Lubos Mitas[1]
[1]North Carolina State University; [2]Sandia National Laboratories

PII-F-7: UNRAVELLING THE COMPLEXITIES OF THE HIGH TC SUPERCONDUCTOR PHASE DIAGRAMS
[EFRC – CES] Hu Miao[1], Nader Zaki[1], Peter Johnson[1], Peter Sprau[1], Seamus Davis[1], Mark Dean[1], John Tranquada[1], Genda Gu[1], Michael Norman[2]
[1]Brookhaven National Laboratory, [2]Argonne National Laboratory

PII-F-8: STRUCTURE AND PHASE STABILITY OF SOLID LI AT I ATM AND HIGH PRESSURE
[EFRC – EFree] Sabri Elatresh[1], Stanimir Bonev[2], Neil Ashcroft[1], Roald Hoffmann[1]
[1]Cornell University, [2]Lawrence Livermore National Laboratory

PII-F-9: MAGNONIC HOLOGRAPHIC IMAGING OF MAGNETIC MICROSTRUCTURES
[EFRC – SHINES] D. Gutierrez[1], H. Chiang[1], T. Bhowmick[1], A.D. Volodchenkov[1], M. Ranjbar[1], G. Liu[1], C. Jiang[1], C. Warren[1], M. Balinskiy[1], Y. Khivintsev[2,3], Y. Filimonov[2,3], J. Garay[4], R. Lake[1], A.A. Balandin[1], A. Khitun[1]
[1]University of California, Riverside; [2]Kotelnikov Institute of Radioengineering and Electronics of Russian Academy of Sciences, Russia; [3]Saratov State University, Russia; [4]University of California, San Diego

PII-F-10: LARGE SCALE SIMULATIONS OF FERMIONIC SYSTEMS INTERACTING WITH CLASSICAL DEGREE OF FREEDOM
[CMS – CDMFTS] Cristian Batista[1], Zhentao Wang[1], Kipton Barros[2]
[1]University of Trennessee;[2] Los Alamos National Lab

H. SOLAR ENERGY CONVERSION

PII-H-1: PROBING PHOTOCATHODE MATERIALS AND INTERFACES TO ENABLE TANDEM DYE SENSITIZED PHOTOELECTROSYNTHESIS CELLS

[EFRC – UNC] Taylor H. Moot, Lesheng Li, Shannon M. McCullough, Bing Shan, Aaron D. Taggart, Lenzi J. Williams, Chiung-Wei Huang, Olexandr Isayev, Alexander Tropsha, Rene Lopez, Joanna M. Atkin, John M. Papanikolas, Thomas J. Meyer, Yosuke Kanai, James F. Cahoon

University of North Carolina at Chapel Hill

PII-H-2: PROGRAMING EXCITONIC CIRCUITS WITH DNA NANOASSEMBLIES

[EFRC – CE] Etienne Boulais[2], Nicolas P. D. Sawaya[1], Remi Veneziano[2], Alessio Andreoni [3,4], Su Lin [3,4], James Banal[2], Wei Jia Chen[2], John Ogren[2], Neal Woodbury[3], Hao Yan[3], Gabriela Schlau-Cohen[2], Alan Aspuru-Guzik[1], Mark Bathe[2]

[1]Harvard University, [2]Massachusetts Institute of Technology; [3]Arizona State University

PII-H-3: DESIGN AND INVESTIGATION OF NOVEL MATERIALS USING ULTRAFAST SPECTROSCOPY TO DETERMINE THE EFFECTS OF AGGREGATION ON THE PHOTOPHYSICS OF ORGANIC SEMICONDUCTING POLYMERS

[EFRC – ANSER] Thomas J. Fauvell[1,2], Nicholas D. Eastham[1], Zhengxu Cai[3], Thomas J. Aldrich[1], Eric Manley[1,2], Robert P. H. Chang[1], Tobin J. Marks[1], Luping Yu[3], Lin X. Chen[1,2]

[1]Northwestern University, [2]Argonne National Laboratory, [3]University of Chicago

PII-H-4: CARRIER MULTIPLICATION IN SEMICONDUCTOR NANOCRYSTALS FOR PHOTOVOLTAICS AND PHOTOCHEMISTRY

[EFRC – CASP] Matthew C. Beard[1], Yong Yan[1], Ryan W. Crisp[1], Jing Gu[1], Boris D. Chernomordik, Gregory F. Pach[1], Ashley R. Marshall[1], John A. Turner[1], Marton Voros[2], Federico Giberti[2], Nicholas P. Brawand[2], Giulia Galli[2], Jianbo Gao[1,3], Andrew F. Fidler[3], Istvan Robel[3], Victor I. Klimov[3]

[1]National Renewable Energy Laboratory; [2]University of Chicago; [3]Los Alamos National Laboratory

PII-H-5: METASTABLE MATERIALS FOR SOLAR ENERGY

[EFRC – EFree] Michael Guerette[1], Venkata Bhadram[1], Konstantin Lokshin[2], Steve Juhl[3], Lakshmi Krishna[4], Hanyu Liu[1], En-shi Xu[5] Nasim Alem[3], Tianshu Li[5], P.Craig Taylor[4], Timothy Strobel[1]

[1]Carnegie Institution of Washington, [2]University of Tennessee, [3]Pennsylvania State University, [4]Colorado School of Mines, [5]George Washington University

PII-H-6: ELECTROLUMINESCENT REFRIGERATION ENABLED BY EFFICIENT LIGHT-EMITTING DIODES AND PHOTOVOLTAICS

[EFRC – LMI] T. Patrick Xiao[1], Kaifeng Chen[2], Parthiban Santhanam[2], Shanhui Fan[2], Eli Yablonovitch[1]

[1]Lawrence Berkeley National Laboratory; [2]Stanford University

PII-H-7: ADVANCED ARCHITECTURES AND NEW METHODS FOR PHOTOELECTROCHEMICAL ENERGY STORAGE

[Hub – JCAP] Gideon Z. Segev[1], Jeffrey W. Beeman[1], Chang-Ming Jiang[1], Jason K. Cooper[1], Ian D. Sharp[1]

[1]Lawrence Berkeley National Laboratory

PII-H-8: A SPEED LIMIT FOR TRIPLET EXCITON TRANSFER IN SOLID-STATE PBS NANOCRYSTAL-SENSITIZED PHOTON UPCONVERSION

[EFRC – CE] Lea Nienhaus[1], Mengfei Wu[1], Nadav Geva[1], James J. Shepherd[1], Mark W.B. Wilson[1], Vladimir Bulovic[1], Troy Van Voorhis[1], Marc A. Baldo[1], Moungi G. Bawendi[1]
[1]Massachusetts Institute of Technology

PII-H-9: PHOTOELECTROCHEMICAL REDUCTION OF CO_2 USING SUPRAMOLECULAR ASSEMBLIES OF RYLENEDIIMIDE CHROMOPHORES AND RE(DIIMINE)$(CO)_3$ CATALYSTS

[EFRC – ANSER] Nathan T. La Porte[1], Jose F Martinez[1], Svante Hedström[2], Benjamin Rudshteyn[2], Victor S. Batista[2], Michael R. Wasielewski[1]
[1]Northwestern University; [2]Yale University

PII-H-10: STRATEGIES TO ACHIEVE FULL SPECTRUM CONTROL AND CONVERSION USING LUMINESCENT CONCENTRATORS AND UPCONVERTERS

[EFRC – LMI] Mikayla A. Anderson[1], Michelle L. Solomon[2], Yuan Yao[2], Gururaj V. Naik[1], Junwen He[2], Alex J. Welch[1], Lu Xu[2], Justin A. Briggs[1], Hanxiao Su[2], Jennifer A. Dionne[2], Ralph Nuzzo[1]
[1]University of Illinois at Urbana-Champaign; [2]Stanford University

PII-H-11: ACCESSING THE PHOTOPHYSICS OF WATER OXIDATION PHOTOANODES

[EFRC – UNC] Renato N. Sampaio, Ke Hu, Degao Wang, Michael S. Eberhart, Seth L. Marquard, M. Kyle Brennaman, Yusuke Tamaki, Thomas J. Meyer, Gerald J. Meyer.
University of North Carolina at Chapel Hill

PII-H-12: HIGH-PERFORMANCE LUMINESCENT SOLAR CONCENTRATORS USING ENGINEERED QUANTUM DOTS

[EFRC – CASP] Hongbo Li[1], Kaifeng Wu[1], Jaehoon Lim[1], Hyung-Jun Song[1], Kirill A. Velizhanin[1], Samantha Ehrenberg[2], Uwe R. Kortshagen[2], Victor I. Klimov[1]
[1]Los Alamos National Laboratory; [2]University of Minnesota

PII-H-13: LAYERED LANTHANIDE CATECHOLATES FOR LASER APPLICATIONS

[EFRC – CE] Grigorii Skorupskii[1], Cole Perkinson[1], Kristopher Williams[1], Ju Li[1], Mircea Cotlet[1], William A. Tisdale[1], Marc A. Baldo[1], Mircea Dincă[1]
[1]Massachusetts Institute of Technology

I. SYNTHESIS SCIENCE

PII-I-1: UNDERSTANDING STRUCTURE, METAL DISTRIBUTION, AND WATER ADSORPTION IN MIXED-METAL MOF-74

[EFRC – UNCAGE-ME] Joshua D. Howe[1], Cody R. Morelock[1], Yang Jiao[1], Karena W. Chapman[2], Krista S. Walton[1], David S. Sholl[1]
[1]Georgia Institute of Technology, [2]Argonne National Laboratory

PII-I-2: DISCOVERY AND CHARACTERIZATION OF NOVEL 2D MATERIALS AND LATERAL HETEROJUNCTIONS

[CMS – MAGICS] Vidya Kochat[1], Amey Apte[1], Chandrashekar Tiwari[1], Pulickel Ajayan[1], Pankaj Rajak[2], Aravind Krishnamoorthy[2], Hiroyuki Kumazoe[2], Rajiv K. Kalia[2], Malancha Gupta[2], David Singh[3]
[1]*Rice University*; **[2]***University of Southern California*; **[3]***University of Missouri*

PII-I-3: SYNTHESIS AND CHARACTERIZATION OF SOFT DONOR LIGANDS FOR ADVANCED *F* ELEMENT SEPARATIONS

[EFRC – CAST] Christopher Dares
Florida International University

PII-I-4: MIXED MATRIX MEMBRANES BASED ON TWO-DIMENSIONAL METAL-ORGANIC FRAMEWORKS FOR CO_2 SEPARATION

[EFRC – CGS] Feng Xue[1], Meera Shete[1], Shuai Yuan[2], Jonathan E. Bachman[3], Jeffrey R. Long[3,4], Hong-Cai Zhou[2], Michael Tsapatsis[1]
[1]University of Minnesota; [2]Texas A&M University; [3]University of California, Berkeley; [4]Lawrence Berkeley National Laboratory (LBNL)

PII-I-5: DISCOVERY AND SYNTHESIS OF NOVEL NITRIDES: MATERIALS INFORMATICS, FIRST PRINCIPLES PREDICTIONS AND SYNTHESIS

[EFRC – CNGMD] Gerbrand Ceder[1], Andriy Zakutayev[2], Wenhao Sun[1], Bernardo Orvananos[1], Elisabetta Arca[2], Aaron Holder[2], Yuki Iguchi[2], John Perkins[2], Stephan Lany[2], John Mangum[3], Brian Gorman[3], Laura Schelhas[4], Mike Toney[4], William Tumas[2]
[1]Lawrence Berkeley National Laboratory; [2]National Renewable Energy Laboratory; [3]Colorado School of Mines; [4]SLAC National Accelerator Laboratory

PII-I-6: sp^3 CARBON NANOMATERIALS SYNTHESIZED AT HIGH PRESSURE

[EFRC – EFree] Damian Paliwoda[1], Maria Baldini[2], Shah Najiba[1], Kai Landskron[1]
[1]Lehigh University, [2]Carnegie Institution of Washington

PII-I-7: STRUCTURED GROWTH OF METAL-ORGANIC FRAMEWORK MIL-53(AL) FROM SOLID ALUMINUM CARBIDE PRECURSOR

[EFRC—UNCAGE-ME] Jayraj N. Joshi[1], Robert M. Marti[2], Colton M. Moran[1], Sophia E. Hayes[2], Krista S. Walton[1]
[1]Georgia Institute of Technology, [2]Washington University in St. Louis

J. MATERIALS AND CHEMISTRY BY DESIGN

PII-J-1: ALGORITHMIC AND IMPLEMENTATION IMPROVEMENTS TO FULL-FREQUENCY DEPENDENT GW CALCULATIONS
[CMS – C2SEPEM] Mauro Del Ben[1], Felipe H. da Jornada[1, 2], Chao Yang[1], Jack Deslippe[1], Steven G. Louie[1, 2]
[1]Lawrence Berkeley National Laboratory; [2]University of California, Berkeley

PII-J-2: CLATHRATE COLLOIDAL CRYSTALS: A PROMISING CLASS OF HOST MATERIALS FOR ENERGY CONVERSION
[EFRC – CBES] Haixin Lin[1], Sangmin Lee[2], Lin Sun[1], Matthew Spellings[2], Michael Engel[3], Sharon C. Glotzer[1], Chad A. Mirkin[1]
Northwestern University[1], University of Michigan[2], Friedrich-Alexander University Erlangen-Nürnberg[3]

PII-J-3: DESIGN OF METASTABLE MATERIALS: CONTROLLING COMPOSITION AND STRUCTURE THROUGH ALLOYING
[EFRC – CNGMD] Aaron Holder[1], Janet Tate[2], Sebastian Siol[1], Lauren Garten[1], Stephan Lany[1], John Perkins[1], David. Ginley[1], Andriy Zakutayev[1], Bethany Matthews[2], John Mangum[3], Brian Gorman[3], Laura Schelhas[4], Kevin Stone[4], Michael Toney[4], Xiabing Lou[5], Roy Gordon[5], William Tumas[1]
[1]National Renewable Energy Laboratory; [2]Oregon State University; [3]Colorado School of Mines, [4]SLAC National Accelerator Laboratory; [5]Harvard University

PII-J-4: DIGITAL DATA INFRASTRUCTURE DEVELOPED WITHIN MICCOM
[CMS – MICCoM] Marco Govoni[1,2], Aditya Tanikanti[2], Jonathan Skone[2], Milson Munakami[2], Juan J. de Pablo[1,2], Sharon Glotzer [3], Giulia Galli[1,2]
[1]Argonne National Laboratory; [2]University of Chicago; [3]University of Michigan

PII-J-5: UNIFYING FIRST-PRINCIPLES CALCULATIONS AND CONTINUUM MODELING OF NANOSCALE HEAT TRANSPORT
[EFRC – S^3TEC] Giuseppe Romano[1], Jesus Carrete[3], Natalio Mingo[3], David Broido[2], Alexie M. Kolpak[1]
[1]Massachusetts Institute of Technology, [2]Boston College, [3]CEA Laboratory for Innovation in New Energy Technologies and Nanomaterials (LITEN)

PII-J-6: USABILITY AND CODE DEVELOPMENT SUPPORT
[CMS – CDMFTS] Hubertus van Dam[1], Ran Adler[2], Sangkook Choi[1]
[1]Brookhaven National Lab; [2]Rutgers University

PII-J-7: MAGNETOELASTIC COLLOID MEMBRANES: BUCKLING AND BOWING IN DYNAMIC FIELDS
[EFRC – CBES] Chase Brisbois[1], Mykola Tasinkevych[1], Pablo Vazques-Montejo[1], Joshua Dempster[1], Monica Olvera de la Cruz[1]
Northwestern University[1]

PII-J-8: THE INFLUENCE OF INTRINSIC FRAMEWORK FLEXIBILITY ON ADSORPTION IN NANOPOROUS MATERIALS
[EFRC – CGS] Matthew Witman[1], Sanliang Ling[2], Sudi Jawahery[1], Peter Boyd[3], Maciej Haranczyk[4,5], Ben Slater[2], Berend Smit[1,3]
[1]University of California, Berkeley; [2]University College London, United Kingdom; [3]École Polytechnique Fédérale de Lausanne (EPFL), Switzerland; [4]Lawrence Berkeley National Laboratory (LBNL); [5]IMDEA Materials Institute, Spain

PII-J-9: Bimetallic Catalysts on Metal-Organic Framework and Nanocast Silica Supports

[EFRC – ICDC] Camille M. May[1], Sai P. Desai[1], Anthony B. Thompson[1], Leighanne Gallington[2], Dale R. Pahls[1], Varinia Bernales[1], Thomas Webber[1], Timothy Wang[3], Omar K. Farha[3], Joseph T. Hupp[3], Karena W. Chapman[2], Laura Gagliardi[1], R. Lee Penn[1], Connie C. Lu[1], Andreas Stein[1]

[1]University of Minnesota, [2]Argonne National Laboratory, [3]Northwestern University

PII-J-10: QBOX AND WEST: IMPLEMENTATION, VALIDATION AND INNOVATION

[CMS – MICCoM] Francois Gygi[1], Marco Govoni[2,3], Ma He[3], Huihuo Zheng[2], Peter Scherpelz[3], Ryan McAvoy[3], Han Yang[3], Christopher Knight[2], Nicholas Brawand[3], Giulia Galli[1,2]

[1]University of California Davis; [2]Argonne National Laboratory; [3]University of Chicago

PII-J-11: Computational Investigation on the Acid Gas Adsorption Using Porous Carbon Structures

[EFRC – UNCAGE-ME] Difan Zhang[1,2], Michael R. Dutzer[3], Tao Liang[2], Krista S. Walton[3], David S. Sholl[3], Suresh K. Bhatia[4], Susan B. Sinnott[2]

[1]University of Florida, [2]Pennsylvania State University, [3]Georgia Institute of Technology, [4]University of Queensland (UQ), Australia

PII-J-12: Effects of molecular packing in organic crystals on singlet fission with ab initio many-body perturbation theory

[CMS – C2SEPEM] Jonah B. Haber[1, 2], Sivan Refaely-Abramson[1, 2], Felipe H. da Jornada[1, 2], Brendan D. Folie[1], Naomi S. Ginsberg[1, 2], Steven G. Louie[1, 2], Jeffrey B. Neaton[1, 2]

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

PII-J-13: The Role of Interfaces and Defects within Quantum Dots and Quantum Dot Films

[EFRC – CASP] Matthew C. Beard[1], Joseph M. Luther[1], Justin C. Johnson[1], Gregory F. Pach[1], Marton Voros[2], Nicholas Brawand[2], Giulia Galli[2], Daniel Straus[3], Cherie Kagan[3]

[1]National Renewable Energy Laboratory; [2]University of Chicago; [3]University of Pennsylvania

PII-J-14: In Situ TEM Study of Microstructure Evolution in Concentrated Solid Solution Alloys Under High Energy Electron Beam Irradiation

[EFRC – EDDE] Shi Shi[1], Mo-Rigen He[1], Shuai Wang[1], Ke Jin[2], Hongbin Bei[2], Kazuhiro Yasuda[3], Syo Matsumura[3], Kenji Higashida[3], Ian M. Robertson[1]

[1]University of Wisconsin-Madison; [2]Oak Ridge National Laboratory; [3]Kyushu University, Japan

PII-J-15: SSAGES AND COPSS: IMPLEMENTATION, VALIDATION, AND INNOVATION

[CMS – MICCoM] Hythem Sidky[1], Yamil J. Colón[2,3], Benjamin J. Sikora[1], Cody Bezik[2], Federico Giberti[2], Ashley Guo[2], Julian Helfferich[2], Xikai Jiang[3], Joshua Lequieu[2], Jiyuan Li[2], Joshua Moller[2], Michael Quevillon[1], Mohammad Rahimi[2], Hadi Ramezani-Dakhel[2], Vikramjit Rathee[1], Daniel Reid[2], Emre Sevgen[2], Vikram Thapar[2], Michael Webb[2,3], Justin Wozniak[3], Xujun Zhao[3], Nicola J. Ferrier[3], Olle G. Heinonen[3], Giulia Galli[2], François Gygi[4], Monica Olvera de la Cruz[5], Juan de Pablo[2,3], Jonathan K. Whitmer[1]

[1]University of Notre Dame; [2]University of Chicago; [3]Argonne National Laboratory; [4]University of California—Davis; [5]Northwestern University

PII-J-16: Colloidal Rollers based on Magnetic Janus Particles

[EFRC – CBES] Wenjie Fei[1], Michelle M. Driscoll[2], Paul M. Chaikin[2], Kyle J.M. Bishop[1]

Columbia University[1], New York University[2]

PII-J-17: RECENT PROGRESS IN HALF-HEUSLER THERMOELECTRIC MATERIALS

[EFRC – S^3TEC] Jun Mao[1], Shashwat Anand[2], Jifeng Sun[3], Jiawei Zhou[4], Gang Chen[4], David Singh[3], Jeffrey Snyder[2], Zhifeng Ren[1].

[1]University of Houston, [2]Northwestern University, [3]University of Missouri-Columbia, [4]Massachusetts Institute of Technology

PII-J-18: PROBING ATOMIC STRUCTURE DEFECTS IN 2D MATERIALS FOR ENERGY APPLICATIONS

[EFRC – FIRST] Xiahan Sang[1], Yu Xie[1], Dundar Yilmaz[2], Mohamed Alhabeb[3], Kichul Yoon[2], Roghayyeh Lotfi[2], Babak Ansori[3], Paul R.C. Kent[1], Adri Van Duin[2], Raymond R. Unocic[1]

[1]Oak Ridge National Laboratory; [2]Penn State University; [3]Drexel University

PII-J-19: POLARIZED OPTICAL METAMATERIALS BASED ON PEROVSKITE SUPRAMOLECULAR NANOCOMPOSITES VIA DIRECT INK WRITING

[EFRC – LMI] Nanjia Zhou[1], Carissa N. Eisler[2,3], Yehonadav Bekenstein[2], Claas W. Visser[1], Dandan Zhang[2], Xiaoguang Wang[1], Joanna Aizenberg[1], Peidong Yang[2,3], Adam M. Schwartzberg[3], A. Paul Alivisatos[2,3], Jennifer A. Lewis[1]

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

PII-J-20: SELF-CONSISTENT GW AND POSSIBLE VERTEX TERM CALCULATIONS UNDER MANY-BODY PERTURBATION THEORY

[CMS – C2SEPEM] Lin-Wang Wang[1], Wei Hu[1], Chao Yang[1]

[1]Lawrence Berkeley National Laboratory

PII-J-21: COMPUTATION OF THE UNIFYING THREAD IN HIGH TEMPERATURE SUPERCONDUCTORS FROM FIRST PRINCIPLES QUANTUM MONTE CARLO

[EFRC – CES] Awadhesh Narayan, Brian Busemeyer, Lucas K. Wagner

University of Illinois, Urbana Champaign

PII-J-22: VIRTUAL REALITY FOR MATERIALS SIMULATIONS: REAL-TIME IMMERSIVE VISUALIZATION OF MOLECULAR PROCESSES

[CMS – MAGICS] Brandon Horton[1], Anders Hafreager[1], Aravind Krishnamoorthy[1], Aiichiro Nakano[1]

[1]*University of Southern California*

GRADUATE STUDENT AND POSTDOCTORAL TEAM SCIENCE CONTEST

(From left) Gihan Kwon, Nathan T. La Porte, Kelly L. Materna, Benjamin Rudshteyn, Jiyun Hong

H-I-6: THE PYRIDINE ALKOXIDE LIGAND WORKS FOR WATER OXIDATION CATALYSTS BOTH IN THEORY AND IN PRACTICE

[EFRC – ANSER] Benjamin Rudshteyn,[1] Kelly L. Materna,[1] Nathan T. La Porte,[2] Katherine J. Fisher,[1] Ke R. Yang,[1] Svante Hedstrom,[1] Jose F. Martinez,[2] Gihan Kwon,[3] Jiyun Hong,[2] David M. Tiede,[3] Lin X. Chen,[2,3] Michael R. Wasielewski,[2] Robert H. Crabtree,[1] Gary W. Brudvig,[1] Victor S. Batista[1]

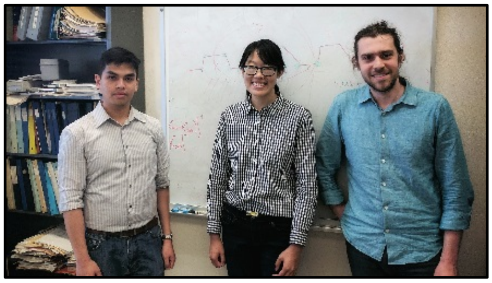
[1]Yale University, [2]Northwestern University, [3]Argonne National Laboratory

(From left) Jonathan Yuly, Diep Nguyen

A-III-1: MECHANISTIC INSIGHTS INTO ENERGY CONSERVATION BY FLAVIN-BASED ELECTRON BIFURCATION

[EFRC – BETCy] D. Nguyen[1], J. Yuly[2], C. Lubner[3], D. Jennings[4], D. Mulder[3], G. Schut[1], O. Zadvornyy[5], J. Hoben[6], P. Zhang[1], M. Tokmina-Lukaszewska[7], L. Berry[7], G. Lipscomb[1], B. Bothner[7], A. Jones[4], A. Miller[6], P. King[3], D. Beratan[2], M. Adams[1], J. Peters[5,7]

[1]University of Georgia, [2]Duke, [3]National Renewable Energy Laboratory, [4]Arizona State, [5]Washington State, [6]University of Kentucky, [7]Montana State



(From left) Iqbal B. Utama, Diana Y. Qiu, Felipe H. da Jornada

F-I-1: ENVIRONMENTAL SCREENING EFFECTS IN 2D MATERIALS: RENORMALIZATION OF THE BANDGAP, ELECTRONIC STRUCTURE, AND OPTICAL SPECTRA

[CMS – C2SEPEM] Diana Y. Qiu, Felipe H. da Jornada, M. Iqbal B. Utama, Feng Wang, Steven G. Louie

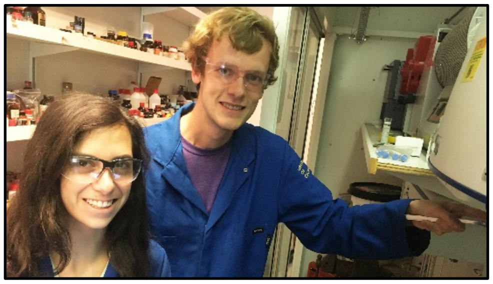
Lawrence Berkeley National Laboratory / University of California, Berkeley

(From left on top) Robert Warburton, Bruno Nicolau, Kendra Letchworth-Weaver;
(From left on bottom) Xiao Chen, Kan-Sheng Chen

D-III-1: UNDERSTANDING AND CONTROLLING THE REACTIVITY OF $LiMn_2O_4$-ELECTROLYTE INTERFACES

[EFRC – CEES] Robert Warburton[1], Bruno Nicolau[2], Kendra Letchworth-Weaver[4], Kan-Sheng Chen[3], Aaron Petronico[2], Laila Jaber-Ansari[3], Xiao Chen[4], Yasaman Ghadar,[4] Maria Chan[4], Ralph Nuzzo[2], Andrew Gewirth[2], Jeffrey P. Greeley[1], Mark Hersam[3], Paul Fenter[4]

[1]Purdue University, [2]University of Illinois, [3]Northwestern University, [4]Argonne National Laboratory

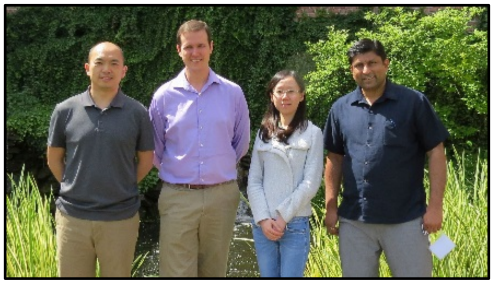


(From left) Rebecca Siegelman, Alexander Forse

G-II-4: RATIONAL DESIGN OF NEW MATERIALS FOR CARBON DIOXIDE CAPTURE

[EFRC – CGS] Rebecca L. Siegelman,[1] Alexander C. Forse,[1] Phillip J. Milner,[1] Thomas M. McDonald,[1] Miguel I. Gonzalez,[1] Tomče Runčevski,[1] Jeffrey D. Martell,[1] Jarad A. Mason,[1] Jung-Hoon Lee,[1,2] Bess Vlaisavljevich,[1] Walter S. Drisdell,[2] Jeffrey B. Kortright,[2] David Prendergast,[2] Jeffrey B. Neaton,[1,2,3] Berend Smit, Jeffrey A. Reimer,[1] Jeffrey R. Long[1,2]

[1]University of California, Berkeley; [2]Lawrence Berkeley National Laboratory; [3]Kavli Energy NanoSciences



(From left) Hui Yang, Jason Burris, Xiaoran Xin, Abhishek Singh

A-II-1: THE NANOMACHINE THAT SYNTHESIZES CELLULOSE IN PLANTS

[EFRC – CLSF] Abhishek Singh[1], Yaraslova Yingling[1], Jason N. Burris[1], Jonathan K. Davis[1], Alison W. Roberts[2], Candace H. Haigler[1], Xiaoran Xin[3], Ying Gu[3], Hui Yang[3], James D. Kubicki[4], Jochen Zimmer[5]

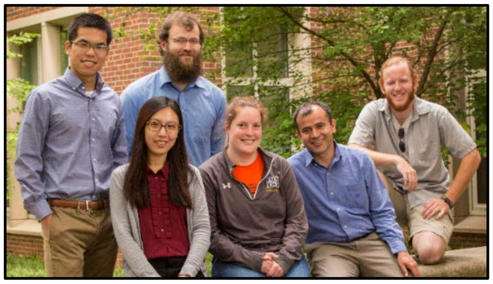
[1]North Carolina State University, [2]University of Rhode Island, [3]Pennsylvania State University, [4]University of Texas at El Paso, [5]University of Virginia

(From left) Shijun Zhao, Taini Yang, Shi Shi

I-II-3: EFFECTS OF ALLOY COMPLEXITY ON DEFECT PRODUCTION AND MICROSTRUCTURAL EVOLUTION IN CONCENTRATED ALLOYS

[EFRC – EDDE] Shijun Zhao[1], Taini Yang[2], Shi Shi[3], Chenyang Lu[2], Eva Zarkadoula[1], Hongbin Bei[1], Lumin Wang[2], Ian Robertson[3], Yanwen Zhang[1]

[1]Oak Ridge National Laboratory; [2]University of Michigan; [3]University of Wisconsin-Madison



(Standing from left) Yu Zhang, Matt Thompson; (Seated from left) Kun Liu, Katie Van Aken, Naresh Osti, Justin Neal

D-I-3: UNDERSTANDING ROOM TEMPERATURE IONIC LIQUIDS AND THEIR PERFORMANCE IN SUPERCAPACITORS

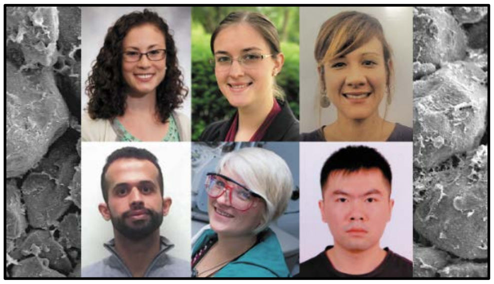
[EFRC – FIRST] Justin Neal[1], Kun Liu[1], Naresh Osti[2], Matthew W. Thompson[3], Katherine Van Aken[4], Yu Zhang[3]

[1]University of California, Riverside, [2]Spallation Neutron Source, Oak Ridge National Laboratory, [3]Vanderbilt University, [4]Drexel University

B-IV-3: Geochemical Reactions During Geological Carbon Sequestration Can Decrease Fracture Toughness of Reservoir Rock and Contribute to Microseismic Events

[EFRC – GSCO2] L Dalton[1], MG Davila Ordonez[2], S Fuchs[3], P Kabir[2], Z Shi[4], MK Tkach[1], A Akono[2], DM Crandall[1], J Druhan[2], AL Goodman[1], K Jessen[4], T Tsotsis[4], CJ Werth[3]

[1]National Energy Technology Laboratory, [2]University of Illinois at Urbana-Champaign, [3]University of Texas at Austin, [4]University of Southern California



(Top from left) Laura Dalton, Samantha Fuchs, Gabriela Dávila; (Bottom from left) Pooyan Kabir, Mary Tkach, Zhuofan Shi

C-I-3: Post-functionalized Metal–Organic Frameworks for Catalysis

[EFRC – ICDC] Manuel A. Ortuño,[1] Zhanyong Li,[2] Ana E. Platero-Prats,[3] Karena W. Chapman,[3] Joseph T. Hupp,[2] Omar. K. Farha,[2] Christopher J. Cramer,[1] Laura Gagliardi[1]

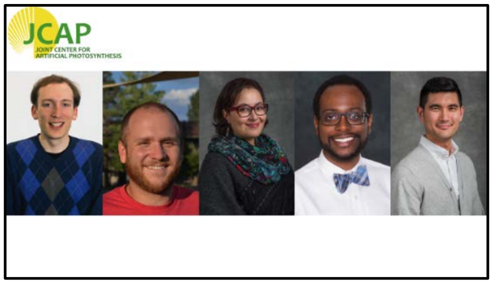
[1]University of Minnesota; [2]Northwestern University; [3]Argonne National Laboratory

(From left) Manual A. Ortuna, Ana E. Platero-Prats, Zhanyong Li

J-I-1: Materials Discovery, Theory, and Characterization of Intermetallics for Electrochemical CO_2 Reduction

[Hub – JCAP] Jeremy T. Feaster[1,4], Daniel A. Torelli[2,4], Zachary W. Ulissi[1,4], Maryam Farmand[3,4], Sean W. Fackler[3,4], J.W. Beeman[3], A. Mehta[1], R. Davis[1], A.T. Landers[1,4], J.C. Lin[1,4], D.C. Higgins[1,4], S.A. Francis[2,4], J.C. Crompton[2,4], A. Javier[2,4], J.R. Thompson[2], M.T. Tang[1,4], J. Xiao[1,4], X. Liu[1,4], M. Karamad[1], R. Sandberg[1,4], K. Chan[1,4], C. Hahn[1,4], B.S. Brunschwig[2,4], M.P. Soriaga[2,4], W.S. Drisdell[3,4], J. Yano[3,4], T.F. Jaramillo[1,4], N.S. Lewis[2,4], J.K. Nørskov[1,4]

[1]Stanford/SLAC, [2]Caltech, [3]LBNL, [4]JCAP



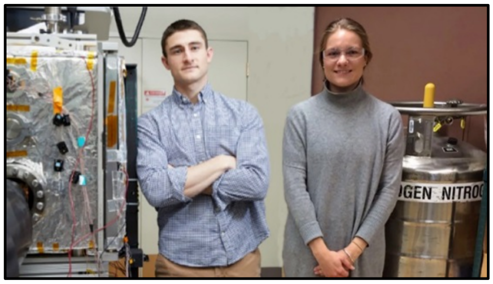
(From left) Zachary W. Ulissi, Daniel A. Torelli, Maryam Farmand, Jeremy T. Feaster, Sean W. Fackler

D-II-1: Thermodynamic Stability, Voltage and Diffusion Kinetics of Li$_x$VOPO$_4$ (x=0,1,2) Vanadyl Phosphate Polymorphs: Joint First-principles and Experimental Study

[EFRC – NECCES] Yuh-Chieh Lin,[1] Iek-Heng Chu,[1] Marc V. Hidalgo,[2] Carrie Siu,[2] Fredrick Omenya,[2] Natasha A. Chernova,[2] Linda W. Wangoh,[2] Shawn Sallis,[2] Louis F. J. Piper,[2] M. Stanley Whittingham,[1] Shyue Ping Ong[1]

[1]University of California San Diego, [2]Binghamton University

(From left) Marc Francis Hidalgo, Yuh-Chieh (Paul) Lin, Shawn Sallis

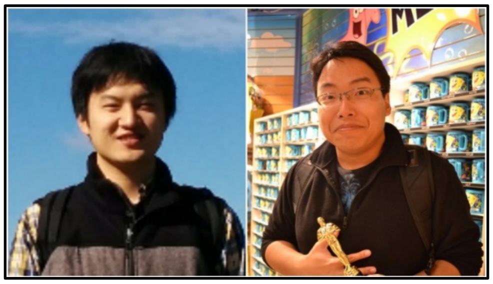


(From left) David Bierman, Veronika Stelmakh

H-III-4: TAILORING THERMAL EMISSION FOR HIGH PERFORMANCE SOLAR THERMOPHOTOVOLTAIC DEVICES

[EFRC – S3TEC] David M. Bierman[1], Veronika Stelmakh[1], Andrej Lenert[1,2], Veronika Rinnerbauer[1,3], Walker R. Chan[1], Ivan Celanovic[1], Marin Soljacic[1], and Evelyn N. Wang[1]

[1]Massachusetts Institute of Technology; [2]Currently at University of Michigan – Ann Arbor; [3] Currently at Johannes Kepler University Linz

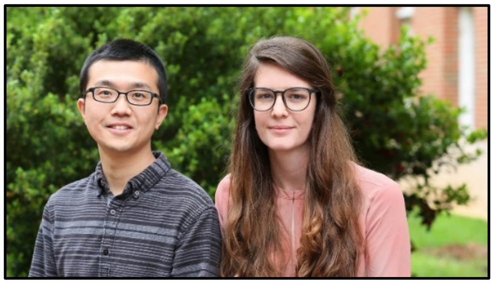


(From left) Xin Ma, Gen Yin

F-IV-1: MAGNETIC SKYRMIONS IN FERROMAGNETIC/HEAVY-METAL MULTI-LAYERS

[EFRC – SHINES] Gen Yin[1], Xin Ma[2], Kang L. Wang[1]. Xiaoqin Li[2]

[1]University of California, Los Angeles, [2]University of Texas at Austin



(From left) Lesheng Li, Taylor Moot

H-IV-1: IDENTIFICATION AND PASSIVATION OF THE DEFECT STATES IN NIO FOR PHOTOVOLTAIC AND SOLAR FUEL APPLICATIONS

[EFRC – UNC] Taylor H. Moot[1], Lesheng Li[1], Aaron D. Taggart[1], Bing Shan[1], Shannon M. McCullough, Carrie L. Donley[1], Thomas J. Meyer[1], Yosuke Kanai[1], James F. Cahoon[1].

[1]University of North Carolina at Chapel Hill.

(From left) Joshua D. Howe, Robert M. Marti

G-II-5: UNDERSTANDING STRUCTURE AND DYNAMICS OF CO_2 ADSORBED IN OPEN-SITE METAL-ORGANIC FRAMEWORKS

[EFRC – UNCAGE-ME] Robert M. Marti[1], Joshua D. Howe[2], Cody R. Morelock[2], Krista S. Walton[2], Mark S. Conradi[1,3] , David S. Sholl[2], Sophia E. Hayes[1]

[1]Washington University, [2]Georgia Institute of Technology, [3]ABQMR

2017 EFRC-HUB-CMS PI MEETING – ACRONYMS AND IDS

Talk ID:	**Letter of Technical Session – Session Block – Number** (e.g. C-I-1 is a Catalysis talk on Monday at 3:00 pm)
Poster ID:	**P Session Block – Letter of Technical Session – Number** (e.g. PII-A-1 is a Biosciences poster on Tue at 3:30 – 5:00 pm)

TYPES OF BASIC ENERGY SCIENCES CENTERS

CMS	Computational Materials Sciences Award
EFRC	Energy Frontier Research Center
Hub	Energy Innovation Hub

BASIC ENERGY SCIENCES CENTERS

[EFRC – ANSER] Argonne-Northwestern Solar Energy Research Center
Michael Wasielewski, Northwestern University
Award Period: 2009 – 2014; 2014 – 2018

[EFRC – BETCy] Center for Biological Electron Transfer and Catalysis
John Peters, Montana State University
Award Period: 2014 – 2018

[CMS – C2SEPEM] Center for Computational Study of Excited-State Phenomena in Energy Materials
Steven Louie, Lawrence Berkeley National Laboratory
Award Period: 2016 – 2020

[EFRC – C3Bio] Center for Direct Catalytic Conversion of Biomass to Biofuels
Maureen McCann; Purdue University
Award Period: 2009 – 2014; 2014 – 2018

[EFRC –CASP] Center for Advanced Solar Photophysics
Victor Klimov, Los Alamos National Laboratory
Award Period: 2009 – 2014; 2014 – 2018

[EFRC – CAST] The Center for Actinide Science and Technology
Thomas Albrecht-Schmitt, Florida State University
Award Period: 2016 – 2020

[EFRC – CBES] Center for Bio-Inspired Energy Science
Samuel Stupp, Northwestern University
Award Period: 2009 – 2014; 2014 – 2018

[EFRC – CCDM] Center for the Computational Design of Functional Layered Materials
John Perdew, Temple University
Award Period: 2014 – 2018

[EFRC – CCEI] Catalysis Center for Energy Innovation
Dionisios Vlachos, University of Delaware
Award Period: 2009 – 2014; 2014 – 2018

[CMS – CDMFTS] Center for Computational Design of Functional Strongly Correlated Materials and Theoretical Spectroscopy
Gabriel Kotliar, Brookhaven National Laboratory
Award Period: 2015 – 2019

[EFRC – CE] Center for Excitonics
Marc Baldo, Massachusetts Institute of Technology
Award Period: 2009 – 2014; 2014 – 2018

[EFRC – CEES] Center for Electrochemical Energy Science
Paul Fenter, Argonne National Laboratory
Award Period: 2009 – 2014; 2014 – 2018

[EFRC – CES] Center for Emergent Superconductivity
Peter Johnson, Brookhaven National Laboratory
Award Period: 2009 – 2014; 2014 – 2018

[EFRC – CFSES] Center for Frontiers of Subsurface Energy Security
Larry Lake, University of Texas at Austin
Award Period: 2009 – 2014; 2014 – 2018

[EFRC – CGS] Center for Gas Separations Relevant to Clean Energy Technologies
Jeffrey Long, University of California, Berkeley
Award Period: 2009 – 2014; 2014 – 2018

[EFRC– CHWM] Center for Hierarchical Wasteform Materials
Hans-Conrad zur Loye, University of South Carolina
Award Period: 2016 – 2020

[EFRC – CLSF] Center for Lignocellulose Structure and Formation
Daniel Cosgrove, Pennsylvania State University
Award Period: 2009 – 2014; 2014 – 2018

[EFRC – CME] Center for Molecular Electrocatalysis
R. Morris Bullock, Pacific Northwest National Laboratory
Award Period: 2009 – 2014; 2014 – 2018

[EFRC – CNGMD] Center for Next Generation of Materials by Design: Incorporating Metastability
William Tumas, National Renewable Energy Laboratory
Award Period: 2014 – 2018

[CMS – CPSFM] Center for Predictive Simulation of Functional Materials
Paul Kent, Oak Ridge National Laboratory
Award Period: 2016 – 2020

[EFRC – EDDE] Energy Dissipation to Defect Evolution
Yanwen Zhang, Oak Ridge National Laboratory
Award Period: 2014 – 2018

[EFRC – EFree] Energy Frontier Research in Extreme Environments
Russell Hemley, Carnegie Institution of Washington
Award Period: 2009 – 2014; 2014 – 2018

[EFRC – FIRST] Fluid Interface Reactions, Structures and Transport Center
David Wesolowski, Oak Ridge National Laboratory
Award Period: 2009 – 2014; 2014 – 2018

[EFRC – GSCO2] Center for Geologic Storage of CO_2
Scott M. Frailey, University of Illinois at Urbana-Champaign
Award Period: 2014 – 2018

[EFRC – ICDC] Inorganometallic Catalyst Design Center
Laura Gagliardi, University of Minnesota
Award Period: 2014 – 2018

[EFRC – IDREAM] Interfacial Dynamics in Radioactive Environments and Materials
Sue Clark, Pacific Northwest National Laboratory
Award Period: 2016 – 2020

[EFRC – IMASC] Integrated Mesoscale Architectures for Sustainable Catalysis
Cynthia Friend, Harvard University
Award Period: 2014 – 2018

[Hub – JCAP] Joint Center for Artificial Photosynthesis
Harry Atwater, California Institute of Technology
Award Period: 2010 – 2015; 2015 – 2020

[Hub – JCESR] Joint Center for Energy Storage Research
Georgy Crabtree, Argonne National Laboratory
Award Period: 2012 – 2017

[EFRC – LMI] Light-Material Interactions in Energy Conversion
Ralph Nuzzo, California Institute of Technology
Award Period: 2009 – 2014; 2014 – 2018

[EFRC – m2M] Center for Mesoscale Transport Properties
Esther Takeuchi, Stony Brook University
Award Period: 2014 – 2018

[CMS – MAGICS] MAterials Genome Innovation for Computational Software
Priya Vashishta, University of Southern California
Award Period: 2015 – 2019

[CMS – MICCoM] Midwest Integrated Center for Computational Materials
Giulia Galli, Argonne National Laboratory
Award Period: 2015 – 2019

[EFRC – MSA] Materials Science of Actinides
Peter Burns, University of Notre Dame
Award Period: 2009 – 2014; 2014 – 2018

[EFRC – NCGC] Center for Nanoscale Controls on Geologic CO_2
Donald DePaolo, Lawrence Berkeley National Laboratory
Award Period: 2009 – 2014; 2014 – 2018

[EFRC – NECCES] NorthEast Center for Chemical Energy Storage
M. Stanley Whittingham, Binghamton University
Award Period: 2009 – 2014; 2014 – 2018

[EFRC – NEES] Nanostructures for Electrical Energy Storage
Gary Rubloff, University of Maryland
Award Period: 2009 – 2014; 2014 – 2018

[EFRC – PARC] Photosynthetic Antenna Research Center
Robert Blankenship, Washington University in St. Louis
Award Period: 2009 – 2014; 2014 – 2018

[EFRC – S3TEC] Solid-State Solar-Thermal Energy Conversion Center
Gang Chen, Massachusetts Institute of Technology
Award Period: 2009 – 2014; 2014 – 2018

[EFRC – SHINES] Spins and Heat in Nanoscale Electronic Systems
Jing Shi, University of California, Riverside
Award Period: 2014 – 2018

[EFRC – UNC] Center for Solar Fuels
Thomas Meyer, University of North Carolina
Award Period: 2009 – 2014; 2014 – 2018

[EFRC – UNCAGE-ME] Center for Understanding and Control of Acid Gas-induced Evolution of Materials for Energy
Krista Walton, Georgia Institute of Technology
Award Period: 2014 – 2018

[EFRC – WastePD] Center for Performance and Design of Nuclear Waste Forms and Containers
Gerald. Frankel, Ohio State University
Award Period: 2016 – 2020

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
SNL	Sandia National Laboratories
SRNL	Savannah River National Laboratory