Science for our Nation's Energy Future

Energy Frontier Research Centers
Principal Investigators' Meeting

October 26 - 27, 2015
Washington, D.C.

Washington Marriott
Wardman Park

U.S. DEPARTMENT OF ENERGY | Office of Science

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Pre-Meeting Event

Sunday, October 25, 2015

4:00 – 6:00 PM **Early Registration in the mezzanine outside the Thurgood Marshall Ballroom**

2:30 – 7:30 PM **Classical Concert at the National Gallery of Art Followed by Dinner (students and postdocs only)**

Agenda Day 1

Monday, October 26, 2015
8:30 AM – 6:30 PM

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

7:30 – 8:20 AM **Women in Energy Science Breakfast, *Lincoln 5***
- Moderator: Robin Hayes, Program Manager in DOE Office of Basic Energy Sciences
- Pat Dehmer, Acting Director of the DOE Office of Science
- Cynthia Friend, Professor at Harvard University and Director of the IMASC EFRC
- Sunita Satyapal, Director of the DOE Fuel Cell Technologies Office

Plenary Session

Thurgood Marshall Ballroom

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

8:30 – 8:45 AM **Welcome**
Pat Dehmer, Acting Director of the DOE Office of Science

8:45 – 9:15 AM **Perspectives on Science and Energy in the US DOE**
Lynn Orr, DOE Undersecretary for Science and Energy

9:15 – 9:45 AM **Current and Future Energy Landscape**
David Daniels, Chief Energy Modeler of the U.S. Energy Information Administration

9:45 – 10:15 AM **BESAC Report: Challenges at the Frontiers of Matter and Energy**
George Crabtree, Senior Scientist, Distinguished Fellow at Argonne National Laboratory

10:15 – 10:45 AM **Break**

10:45 – 11:15 AM **Stakeholder Perspective on the Role of EFRCs in Energy Science Research**
Eric Isaacs, Provost of the University of Chicago

11:15 AM – 11:40 **Announce finalists of the Student and Postdoctoral Researcher Competition and winners of the Poetry of Science Contest**
Andrew Schwartz, Team Lead of the EFRCs

11:40 – 1:10 PM **Lunch (buffet lunch provided)**

12:00 – 1:00 PM **“Learn at Lunch” Sessions**

1. **Scientific Communication in the Age of Social Media, *Lincoln 5***
    - **Marshall Brennan**, Graduate Student at University of Illinois
    - **Bethany Brookshire**, Science education writer at Science News
    - **Yury Gogotsi**, Professor at Drexel University and member of the FIRST EFRC
    - **Eric Schulze**, Molecular biologist and host of ‘Ask Smithsonian Online’
2. **Career Panel, *Lincoln 3/4***
    - **Kumar Challa**, Managing Director IMASC EFRC, Harvard University
    - **Robin Hayes**, Program Manager, Department of Energy, Basic Energy Sciences
    - **Alex Martinson**, Principle Investigator and Chemist, Argonne National Laboratory
    - **Maureen McCann**, Professor of Biological Sciences at Purdue University and Director of the C3Bio EFRC
    - **Hunter McDaniel**, CEO and Founder of UbiQD LLC, former member of the CASP EFRC

1:10 – 2:50 PM **Parallel Talks Session I**

A. Energy Storage, *Thurgood Marshall E/N*
B. Solar Energy Conversion, *Thurgood Marshall S/W*
C. Control at the Level of Electrons, *Lincoln 2*
D. Carbon Sequestration, *Lincoln 6*
E. Materials and Chemistry by Design, *Lincoln 5*
F. Catalysis, *Lincoln 3/4*

2:50 – 3:20 PM **Break**

3:20 – 5:00 PM **Parallel Talks Session II**

A. Energy Storage, *Thurgood Marshall E/N*
B. Solar Energy Conversion, *Thurgood Marshall S/W*
E. Materials and Chemistry by Design, *Lincoln 5*
F. Catalysis, *Lincoln 3/4*
G. Synthesis of Functional Matter, *Lincoln 2*
H. Bioscience, *Lincoln 6*

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

6:30 PM **Adjourn**

6:30 – 7:30 PM **Science Trivia Night (students and postdocs only), *Lincoln 3/4 and Lincoln 5***

Agenda Day 2

Tuesday, October 27, 2015
8:30 AM – 5:00 PM

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

8:30 – 10:10 AM **Parallel Talks Session III**

A. Energy Storage, *Thurgood Marshall E/N*
B. Solar Energy Conversion, *Thurgood Marshall S/W*
E. Materials and Chemistry by Design, *Lincoln 5*
F. Catalysis, *Lincoln 3/4*
I. Separations, *Lincoln 2*
H. Bioscience, *Lincoln 6*

10:10 – 10:40 AM **Break**

10:40 – 12:00 PM **Parallel Talks Session IV**

B. Solar Energy Conversion, *Thurgood Marshall S/W*
C. Control at the Level of Electrons, *Lincoln 2*
D. Carbon Sequestration, *Lincoln 6*
E. Materials and Chemistry by Design, *Lincoln 5*
F. Catalysis, *Lincoln 3/4*
J. Mesoscale Science, *Thurgood Marshall E/N*

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

12:20 – 1:20 PM **“Learn at Lunch” Sessions**

1. **EFRCS and Industry: Experiences, Challenges, and Opportunities, *Lincoln 5***
    - **Dionisios Vlachos**, Professor at the University of Delaware and Director of the CCEI EFRC
    - **Mahdi Abu-Omar**, Professor at Purdue University and Associate Director of the C3Bio EFRC
    - **Tobin Marks**, Professor at Northwestern University and member of the ANSER and CEES EFRCs
    - **Ted Calverley**, Fellow at Dow Chemical and member of the ICDC EFRC
2. **Science Policy Panel, *Lincoln 3/4***
    - **Diana Bauer**, Director, Office of Energy Systems Analysis and Integration at DOE Office of Energy Policy and Systems Analysis (EPSA)
    - **Paul Doucette**, Executive Director of Government Relations at Battelle
    - **Matt Hourihan**, Director of the R&D Budget and Policy Program at the American Association for the Advancement of Science (AAAS)

1:30 – 3:10 PM **Parallel Talks Session V**

A. Energy Storage, *Thurgood Marshall E/N*
B. Solar Energy Conversion, *Thurgood Marshall S/W*
D. Carbon Sequestration, *Lincoln 6*
E. Materials and Chemistry by Design, *Lincoln 5*
F. Catalysis, *Lincoln 3/4*
G. Synthesis of Functional Matter, *Lincoln 2*

3:10 – 5:00 PM **Poster Session II, *Exhibition Hall C (Lincoln Rooms)***
4:00 PM **Announce winners of the *Graduate Student and Postdoctoral Researcher Competition, Area outside Lincoln 5***

5:00 PM **Adjourn**

WOMEN IN ENERGY SCIENCE SPEAKER BIOGRAPHIES

Pat Dehmer – Dr. Dehmer is Acting Director and Deputy Director for Science Programs in the DOE Office of Science. In this capacity, Dr. Dehmer is the senior career science official in the Office of Science. From 1995 to 2007, Dr. Dehmer served as the Director of the Office of Basic Energy Sciences (BES) in the Office of Science. Before coming to DOE, she was a Distinguished Fellow at Argonne National laboratory. Dr. Dehmer is a fellow of the American Physical Society and the American Association for the Advancement of Science. She was awarded the Meritorious Presidential Rank Award in 2000 and 2008 and the Distinguished Presidential Rank Award in 2003.

Cynthia Friend – Dr. Friend is a Professor of Chemistry and Materials Science at Harvard University, Director of the Rowland Institute at Harvard, and Director of the Integrated Mesoscale Architectures for Sustainable Catalysis (IMASC) EFRC. She served as the Associate Laboratory Director of SLAC National Accelerator Laboratory from 2011-12. Dr. Friend is a fellow of the American Chemical Society and the American Association for the Advancement of Science and is an expert on surface chemistry and heterogeneous catalysis. She was awarded the George C. Olah Award in Hydrocarbon Chemistry from the American Chemical Society in 2009, the Hanse-Wissenschaftskolleg Fellowship in 2008, and the Alexander von Humboldt Senior Research Award in 2007.

Sunita Satyapal – Dr. Satyapal is the Director of the Fuel Cell Technologies Office in the DOE Office of Energy Efficiency and Renewable Energy (EERE), where she manages approximately $100 million per year in research, development and demonstration activities. For several years she has coordinated hydrogen and fuel cell activities across DOE, with other agencies, and with international stakeholders, including with seventeen countries and the European Commission, through the International Partnership for Hydrogen and Fuel Cells in the Economy. In addition to her time at DOE, she has more than 20 years of experience in academia, industry, and government, including managing industry research groups of 15 to 50 scientists and engineers at United Technologies in Connecticut. She has numerous publications and 10 patents.

PLENARY SPEAKER BIOGRAPHIES

George Crabtree – Dr. Crabtree holds the ranks of Senior Scientist, Distinguished Fellow and Director of the Joint Center for Energy Storage Research (JCESR), an Energy Innovation Hub, at Argonne National Laboratory and is a Professor of Physics, Electrical, and Mechanical Engineering at University of Illinois at Chicago. He is a co-chair of the 2015 BESAC Report: *Challenges at the Frontiers of Matter and Energy*. He has won numerous awards for his research, including the Kammerlingh Onnes Prize in 2003 for his work on the physics of vortices in high temperature superconductors, the University of Chicago Award for Distinguished Performance at Argonne twice, the U.S. Department of Energy's Award for Outstanding Scientific Accomplishment in Solid State Physics four times, and an R&D 100 Award for his pioneering development of Magnetic Flux Imaging Systems. He is a Fellow of the American Physical Society, a charter member of ISI's Highly Cited Researchers in Physics, and a Member of the U.S. National Academy of Sciences.

David Daniels – Dr. Daniels has been the Chief Energy Modeler of the EIA since 2012, where he works to ensure internal consistency across EIA's disparate modeling and analytic products. Prior to 2012, Dr. Daniels served as Chief Scientist of Digital Sandbox, a security analytics software company, where he developed the terrorism risk analysis methodology used by the Department of Homeland Security to allocate over $20B in grants to states and urban areas. He has also worked as a consultant for Booz Allen Hamilton, where he primarily provided technical support to a number of DARPA programs, and for The Boston Consulting Group, a commercial strategy consulting firm. His academic background is in experimental high energy particle physics, having earned his M.Sc. from Oxford and his Ph.D. from Harvard.

Eric Isaacs – Dr. Isaacs has extensive experience in universities, national laboratories, and industry. Since 2014, he has served as the Provost of the University of Chicago. Previously, he was founding Director of Argonne's Center for Nanoscale Materials, then Deputy Laboratory Director for programs, and ultimately the Director of Argonne National Laboratory for five years. He also spent 15 years at Bell Laboratories in various capacities, including Director of Semiconductor Physics Research and Materials Physics Research. He is a fellow of the American Physical Society and has served on the Basic Energy Sciences Advisory Committee.

Lynn Orr – Dr. Orr, the Under Secretary for Science and Energy, is the principal advisor to the Secretary and Deputy Secretary on clean energy technologies and science and energy research initiatives. Dr. Orr is the inaugural Under Secretary for the office, which was created to closely integrate DOE's basic science, applied research, technology development, and deployment efforts. Prior to joining the Department of Energy, Dr. Orr was Professor Emeritus in the Department of Energy Resources Engineering at Stanford University. He served as the founding director of the Precourt Institute for Energy at Stanford University from 2009 to 2013 and the founding director of the Stanford Global Climate and Energy Project from 2002 to 2008. Early in his career, he worked at the New Mexico Institute of Mining and Technology, Shell Development Company Bellaire Research Center, and the U.S. Environmental Protection Agency. He is a member of the National Academy of Engineering and has served on the Basic Energy Sciences Advisory Committee.

STUDENT AND POSTDOC ORGANIZED EVENTS

SOCIAL EVENTS

Students and Postdoctoral Researchers Only

CLASSICAL CONCERT AT THE NATIONAL GALLERY OF ART AND DINNER

Sunday, October 25, 2015, 2:30 – 7:30 PM

ENERGY FRONTIER RESEARCH CENTERS TRIVIA NIGHT

Monday, October 26, 2015, 6:30 – 7:30 PM; Lincoln 3/4 and Lincoln 5

LEARN AT LUNCH SESSIONS

Open to All

SCIENTIFIC COMMUNICATION IN THE AGE OF SOCIAL MEDIA

Monday, October 26, 2015, 12:00 – 1:00 PM; Lincoln 5

- **Marshall Brennan**, Graduate Student at University of Illinois
- **Bethany Brookshire**, Science education writer at Science News
- **Yury Gogotsi**, Professor at Drexel University and member of the FIRST EFRC
- **Eric Schulze**, Molecular biologist and host of ‘Ask Smithsonian Online’

CAREER PANEL

Monday, October 26, 2015, 12:00 – 1:00 PM; Lincoln 3/4

- **Kumar Challa**, Managing Director IMASC EFRC, Harvard University
- **Robin Hayes**, Program Manager, Department of Energy, Basic Energy Sciences
- **Alex Martinson**, Principle Investigator and Chemist, Argonne National Laboratory
- **Maureen McCann**, Professor of Biological Sciences at Purdue University and Director of the C3Bio EFRC
- **Hunter McDaniel**, CEO and Founder of UbiQD LLC, former member of the CASP EFRC

EFRCS AND INDUSTRY: EXPERIENCES, CHALLENGES AND OPPORTUNITIES

Tuesday, October 27, 2015, 12:20 – 1:20 PM; Lincoln 5

- **Dionisios Vlachos**, Professor at the University of Delaware and Director of the CCEI EFRC
- **Mahdi Abu-Omar**, Professor at Purdue University and Associate Director of the C3Bio EFRC
- **Tobin Marks**, Professor at Northwestern University and member of the ANSER and CEES EFRCs
- **Ted Calverley**, Fellow at Dow Chemical and member of the ICDC EFRC

SCIENCE POLICY PANEL

Tuesday, October 27, 2015, 12:20 – 1:20 PM; Lincoln 3/4

- **Diana Bauer**, Director, Office of Energy Systems Analysis and Integration at DOE Office of Energy Policy and Systems Analysis (EPSA)
- **Paul Doucette**, Executive Director of Government Relations at Battelle
- **Matt Hourihan**, Director of the R&D Budget and Policy Program at the American Association for the Advancement of Science (AAAS)

COMMITTEE MEMBERS

Each EFRC was invited to nominate a student or postdoc to an EFRC-wide committee that would plan events for early career scientists at the 2015 EFRC PI Meeting.

Katie Van Aken	Drexel University	Fluid Interface Reactions, Structures and Transport Center (FIRST)
Laurent Beland	Oak Ridge National Laboratory	Energy Dissipation to Defect Evolution (EDDE)
David Bierman	Massachusetts Institute of Technology	Solid-State Solar-Thermal Energy Conversion Center (S^3TEC)
Hayden Black	Georgia Tech	Center for Solar Fuels (UNC)
Kirsten Chojnicki	Sandia National Laboratories	Center for Frontiers of Subsurface Energy Security (CFSES)
Laura Fernandez	University of Minnesota	Inorganometallic Catalyst Design Center (ICDC)
Andrew Fidler	Los Alamos National Laboratory	Center for Advanced Solar Photophysics (CASP)
Khim Karki	Brookhaven National Laboratory	NorthEast Center for Chemical Energy Storage (NECCES)
Sarah Kiemle	Penn State	Center for Lignocellulose Structure and Formation (CLSF)
Karen Kihlstrom	Argonne National Laboratory	Center for Emergent Superconductivity (CES)
Molly Koehle	University of Delaware	Catalysis Center for Energy Innovation (CCEI)
Mya Le	University of California, Irvine	Nanostructures for Electrical Energy Storage (NEES)
Rebecca Lindquist	Northwestern University	Argonne-Northwestern Solar Energy Research Center (ANSER)
Haylie Lobeck	University of Notre Dame	Materials Science of Actinides (MSA)
Cara Lubner	National Renewable Energy Laboratory	Center for Biological Electron Transfer and Catalysis (BETCy)
Charles Monson	University of Illinois at Urbana-Champaign	Center for Geologic Storage of CO_2 ($GSCO_2$)
Priya Murria	Purdue University	Center for Direct Catalytic Conversion of Biomass to Biofuels (C3Bio)
Bruno G. Nicolau	University of Illinois at Urbana-Champaign	Center for Electrochemical Energy Science (CEES)
Michael Pegis	Yale	Center for Molecular Electrocatalysis (CME)
Parthiban Santhanan	Stanford	Light-Material Interactions in Energy Conversion (LMI)
Sally Tracy	Caltech	Energy Frontier Research in Extreme Environments (EFree)
Pramey Upadhyaya	University of California Los Angeles	Spins and Heat in Nanoscale Electronic Systems (SHINES)
Matt Wolak	Temple University	Center for the Computational Design of Functional Layered Materials (CCDM)
Branko Zugic	Harvard University	Integrated Mesoscale Architectures for Sustainable Catalysis (IMASC)

CLASSICAL CONCERT AT THE NATIONAL GALLERY OF ART AND DINNER

Sunday, October 25, 2015, 2:30 – 7:30 PM

Students and Postdoctoral Researchers Only

COMMITTEE MEMBERS

- **Haylie Lobeck**, University of Notre Dame, MSA
- **Hayden Black**, Georgia Tech, UNC
- **Molly Koehle**, University of Delaware, CCEI
- **Cara Lubner**, National Renewable Energy Laboratory, BETCy

Join us for a trip to the National Gallery of Art to attend a classical concert performed by the National Gallery of Art Orchestra. The music by European composers Jean Sibelius (1865-1957) and Carl Nielsen (1865-1931) will be featured.

A group of us will be meeting at the Washington Marriott Wardman Park Hotel (2:30pm) where we will travel (via subway) to the concert together. The doors open at 3:00pm and the concert starts at 3:30pm. Afterwards, enjoy dinner with a group of your peers at one of the selected restaurants near the Gallery.

If you would just like to join us for dinner, we will meet in the Sculpture Garden (in front of the Pavilion Café) at the National Gallery of Art at 6:00pm before heading to the restaurants. We will divide off into smaller groups based on interest in restaurants.

The concert is free of charge, but you will need to provide your own subway ticket and meal costs.

If you have questions, feel free to contact event coordinators Haylie Lobeck (hlobeck@nd.edu) or Molly Koehle (makoehle@gmail.com).

NGA:*http://www.nga.gov/content/ngaweb/calendar/concerts.html?category=Concerts&pageNumber=1*
Sculpture Garden Map: *https://www.nga.gov/feature/sculpturegarden/general/map.shtm*

Important Addresses

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

National Gallery of Art – 6th & Constitution Ave NW, Washington, DC 20565
Sunday hours – 11am-6pm

Hotel → National Gallery of Art

- Take the red line (direction Glenmont) to *Judiciary Square Metro Station*
- Walk West on E St NW towards 5th St
- Turn Left onto 6th St NW
- The National Gallery of Art will be straight ahead on Constitution Ave NW

(Total walking 11 mins ~0.5 miles)

Restaurants close to National Gallery of Art /Judiciary Square Metro Stop

Daikaya Ramen Shop
Description: ramen and noodle bowl, limited vegetarian option
Price: $$
Location: 705 6th Street NW
Sunday hours: 11am – 10pm
www.daikaya.com

District Taco
Description: tacos and burritos
Price: $
Location: 1309 F Street NW
Sunday hours: 10am – 9pm
www.districttaco.com

District of Pi
Description: pizza, vegan and gluten free options
Price: $$
Location: 910 F Street NW
Sunday hours: 11am – 10pm
www.pi-dc.com

Plan B Burger
Description: fancy burgers, sandwiches
Price: $$
Location: 801 Pennsylvania Ave NW
Sunday hours: 11am – 12am
www.planbburger.com

Grand Trunk
Description: Indian, Pakistani
Price: $
Location: 641 Indiana Ave NW
Sunday hours: 11am – 11pm
www.grandtrunk.us

Vapiano
Self-serve Italian
Price: $$
623 H St NW
Sunday hours: 12-10pm
vapianointernational.com

Cava Mezze
Fast casual Mediterranean
Price: $$
707 H St NW
Sunday hours: 11am – 10pm
cavagrill.com

Matchbox
Pizza, American, lots of vegetarian options
Price: $$
713 H St NW
Sunday hours: 10am -10:30 pm
matchboxrestaurants.com

Teaism
Description: Teas, Asian influence café food, vegetarian options
Price: $$
Location: 400 8th St. NW
Sunday hours: 9am – 9pm
https://www.teaism.com

ENERGY FRONTIER RESEARCH CENTERS TRIVIA NIGHT

Monday, October 26, 2015, 6:30 – 7:30 PM
Lincoln 3/4 & Lincoln 5
Students and Postdoctoral Researchers Only

COMMITTEE MEMBERS

- **Sarah Kiemle**, Penn State, CLSF
- **Sally Tracy**, Caltech, Efree
- **Parthiban Santhanan**, Stanford, LMI
- **Michael Pegis**, Yale, CME
- **Charles Monson**, University of Illinois at Urbana-Champaign, GSCO2
- **Mya Le**, University of California Irvine, NEES

Please come out for a fun and energy-filled night of trivia and camaraderie. Teams of 6-10 people will compete in 4 rounds of science based quiz questions with prizes, so bring your competitive streak. It is a great catalyst for students and postdocs to get together and meet peers at other EFRCs in a fun and informal setting. Preregistration is not required.

SCIENTIFIC COMMUNICATION IN THE AGE OF SOCIAL MEDIA

Monday, October 26, 2015, 12:00 – 1:00 PM
Lincoln 5
Open to All

COMMITTEE MEMBERS

- **Bruno G. Nicolau**, University of Illinois at Urbana-Champaign, CEES
- **Matt Wolak**, Temple University, CCDM
- **Khim Karki**, Brookhaven National Laboratory, NECCES

PANELISTS

- **Marshall Brennan**, Graduate Student at University of Illinois
- **Bethany Brookshire**, Science education writer at Science News
- **Yury Gogotsi**, Professor at Drexel University and member of the FIRST EFRC
- **Eric Schulze**, Molecular biologist and host of 'Ask Smithsonian Online'

DESCRIPTION

Younger generations have shown decreasing interest in television and printed media as their source of news and slowly shifted their focus to online only sources. Most interactions now take place in blogs, social networks and Youtube channels. This has greatly reduced the entry price to become a science communicator. In the current climate science communicators have an unprecedented ease to interact with audiences, tailor content and act as opinion formers. These are exciting times which provide researches with many opportunities to define how their work will be presented to the public. It is therefore of utmost importance that bridges are built between this new generation of science communicators and the scientists conducting work in world leading research institutions. This panel intends to provide an environment where both new media science communicators and scientists can give some insight into their work and their expectations from each other.

SPEAKER BIOGRAPHIES

Marshall R. Brennan – Marshall Brennan received his PhD in inorganic chemistry under the supervision of Prof Alison Fout at the University of Illinois at Urbana-Champaign in October 2015. In 2014 he was voted by C&EN as one the "Top 20 Chemists to Follow on Twitter." Marshall is a regular contributor to the journal Nature Chemistry and his blog Colorblind Chemistry; in addition he can be found on Twitter as @Organometallica.

Bethany Brookshire – Dr. Bethany Brookshire has a B.S. in biology and a B.A. in philosophy from The College of William and Mary, and a Ph.D. in physiology and pharmacology from Wake Forest University School of Medicine. She is a staff writer for Science News, the guest editor of *The Open Laboratory Anthology of Science Blogging, 2009*, and the winner of the Society for Neuroscience Next Generation Award and the Three Quarks Daily Science Writing Award, among others. She blogs at Eureka! Lab and at Scicurious.

Yury Gogotsi - Dr. Yury Gogotsi is a Distinguished University Professor and Trustee Chair in the Department of Materials Science and Engineering at Drexel University. He is the founding Director of the A.J. Drexel Nanomaterials Institute and Associate Editor of ACS Nano. He received his MS (1984) and

PhD (1986) degrees from Kiev Polytechnic and a DSc degree from the Ukrainian Academy of Science in 1995. Dr. Gogotsi is a member of the Fluid Interface Reactions, Structures and Transport Center (FIRST) EFRC. He has co-authored 2 books, edited 13 books, obtained more than 50 patents and authored more than 400 peer-reviewed papers, being recognized as Highly Cited Researcher by Thomson-Reuters in 2014.

Eric Schulze – Dr. Eric Schulze is a molecular biologist, host of 'Ask Smithsonian Online', and speechwriter. He is the co-founder and executive creative director at @thirstdc, a creative communities agency that brings together speakers and participants from fields of science, technology, fashion, music, the arts, and beyond. Eric also hosts and writes for the popular event, "The Periodic Table," a dinner and show that tells the story of humanity through the science of food. Dr. Schulze writes, lectures, and presents frequently on the subject of human creativity, science communication, and the science of food. He can be reached on Twitter at @SciencEric.

CAREER PANEL

Monday, October 26, 2015, 12:00 – 1:00 PM
Lincoln 3/4
Open to All

COMMITTEE MEMBERS

- **Priya Murria**, Purdue University, C3Bio
- **Andrew Fidler**, Los Alamos National Laboratory, CASP
- **Rebecca Lindquist**, Northwestern University, ANSER
- **Pramey Upadhyaya**, University of California Los Angeles, SHINES

PANELISTS

- **Kumar Challa**, Managing Director IMASC EFRC, Harvard University
- **Robin Hayes**, Program Manager, Department of Energy, Basic Energy Sciences
- **Alex Martinson**, Principle Investigator and Chemist, Argonne National Laboratory
- **Maureen McCann**, Professor of Biological Sciences at Purdue University and Director of the C3Bio EFRC
- **Hunter McDaniel**, CEO and Founder of UbiQD LLC, former member of the CASP EFRC

DESCRIPTION

The career panel will explore the multitude of career opportunities available to Ph.D. scientists. The session aims to inform and provide insights to students and postdocs attending the EFRC meeting about life along various professional paths including possibilities beyond the typical government, academia, and industry molds. Following introductions of the speakers and some general prepared questions we will allow for questions from the audience.

SPEAKER BIOGRAPHIES

Kumar Challa – Dr. Challa became the managing director for the Integrated Mesoscale Architectures for Sustainable Catalysis (IMASC) EFRC at Harvard University this year following his work since 2002 as a group leader and director in Nanofabrication and Nanomaterials at the Center for Advanced Microstructures and Devices in Baton Rouge, LA. He received his Ph.D. in chemistry from the Sri Sathya Sai Institute in Prashantinilayam, India and has several years of industry and research and development experience. Additionally, Dr. Challa is the founder of Millifluidica LLC (www.millifluidica.com), a company that provides custom lab-on-a-chip solutions for chemical applications, and serves as the editor-in-chief of Nanotechnology Reviews. Dr. Challa's broad experience will inform participants about industrial and applied science research and the challenges and opportunities associated with managing large research organizations.

Robin Hayes – Dr. Hayes is a program manager at the Department of Energy, Office of Basic Energy Sciences. She earned her Ph.D. in physical chemistry from the University of California, Los Angeles in 2004 and gained almost five years of research experience at New York University. From 2009 to 2011, Dr. Hayes worked as an AAAS Science and Technology Policy fellow where she helped to launch the Energy Frontier Research Centers. Dr. Hayes can provide insight into the transition from research to science policy and the job opportunities provided by the government.

Alex Martinson – Dr. Martinson is a principle investigator in the Surface Chemistry group within the Materials Science Division at Argonne National Laboratory (ANL) and a participant in the Argonne-Northwestern Solar Energy Research (ANSER) and Inorganometallic Catalyst Design Center (ICDC) EFRCs. He earned his Ph.D. in physical chemistry from Northwestern University in 2008 and then conducted his postdoctoral studies at ANL as a Director's Fellow. His continued research at ANL focuses on the design and fabrication of novel surface chemistries for solar energy conversion and catalysis. He will offer perspective on the opportunities provided by the national laboratories.

Maureen McCann – Professor McCann is the director of the Center for Direct Catalytic Conversion of Biomass to Biofuels (C3Bio) EFRC, Director of the Purdue Energy Center, and Professor of Biological Sciences at Purdue University. She received her Ph.D. in botany in 1990 from the University of East Anglia. Dr. McCann worked as a postdoctoral researcher and then project leader at the John Innes Centre, a UK government funded research institute, until coming to Purdue in 2003. Her research focuses on the molecular machinery of the plant cell wall and the potential for biofuels production from lignocellulosic biomass. Professor McCann's extensive experience in both academia and research institutes will provide insight into the attributes and experiences that academic institutions are currently looking for in new hires.

Hunter McDaniel – Dr. McDaniel obtained his Ph.D. in materials science and engineering from the University of Illinois at Urbana-Champaign in 2011 then worked at Los Alamos National Laboratory as a postdoctoral research associate until 2014. He is now the CEO and Founder of UbiQD LLC (www.ubiqd.com), a startup company seeking to bring non-toxic quantum dots as a general use fluorophore to the market. A former member of the Center for Advanced Solar Photophysics (CASP) EFRC, Dr. McDaniel will provide perspective on the role of entrepreneurship in bringing state of the art science to the marketplace.

EFRCS AND INDUSTRY: EXPERIENCES, CHALLENGES AND OPPORTUNITIES

Tuesday, October 27, 2015, 12:20-1:20 PM
Lincoln 5
Open to All

COMMITTEE MEMBERS

- **Laurent Beland**, Oak Ridge National Laboratory, EDDE
- **Katie Van Aken**, Drexel University, FIRST
- **Branko Zugic**, Harvard University, IMASC

PANELISTS

- **Dionisios Vlachos**, Professor at the University of Delaware and Director of the CCEI EFRC
- **Mahdi Abu-Omar**, Professor at Purdue University and Associate Director of the C3Bio EFRC
- **Tobin Marks**, Professor at Northwestern University and member of the ANSER and CEES EFRCs
- **Ted Calverley**, Fellow at Dow Chemical and member of the ICDC EFRC

DESCRIPTION

Panelists from EFRCs involved with industrial partners, including startups, share their experiences, and provide insights into challenges and opportunities involved in industry-EFRC partnerships. Each panelist will give a short presentation, followed by a panel discussion, which will include questions from the audience.

SPEAKER BIOGRAPHIES

Dionisios Vlachos – Professor Vlachos is the Elizabeth Inez Kelley Professor of Chemical and Biological Engineering and a joint Professor of Physics and Astronomy at of the University of Delaware. He is also the Director of the Catalysis Center for Energy Innovation (CCEI) EFRC, which focuses on developing innovative heterogeneous catalytic technologies to transform lignocellulosic biomass materials into fuels and chemicals. The CCEI EFRC is involved with over twelve industrial partners. He received his Bachelor’s degree from the National Technical University of Athens and his Ph.D. from the University of Minnesota.

Mahdi Abu-Omar – Professor Mahdi Abu-Omar is currently the R. B. Wetherill Professor of Chemistry and Professor of Chemical Engineering at Purdue University and the Associate Director of the Center for Direct Catalytic Conversion of Biomass to Biofuels (C3Bio) EFRC. Dr. Abu-Omar is the founder of Spero Energy, which is developing cost competitive processes for the conversion of abundant non-food biomass to high value chemicals (HVCs) and renewable fuels. He has also served on the faculty at UCLA (1997-2003). He holds a B.S. in chemistry from Hampden-Sydney College in Virginia and a Ph.D. from Iowa State University.

Tobin Marks – Professor Marks is Professor of Chemistry and Material Science at Northwestern University and member of the Argonne-Northwestern Solar Energy Research (ANSER) Center and Center for Electrochemical Energy Science (CEES) EFRCs. In addition to serving on the advisory boards of many scientific companies, he is a co-founder of Polyera Corporation, which is developing next-generation technologies that enable both novel electronics form factors and advanced electronics manufacturing processes. His recognitions include the 2006 U.S. National Medal of Science, the 2008 Principe de

Asturias Prize, the 2009 the MRS Von Hippel Award, the 2011 Dreyfus Prize in the Chemical Sciences, and the 2012 NAS Award in the Chemical Sciences. He has served on the NAS Board on Chemical Sciences and Technology and the DOE Council on Chemical Sciences. Professor Marks received his B.S. in Chemistry from the University of Maryland (1966) and his Ph.D. from the Massachusetts Institute of Technology (1971).

Ted Calverley – Dr. Calverley is a fellow in the Inorganic Materials and Heterogeneous Catalysis discipline of Core R&D at The Dow Chemical Company, current President of the Michigan Catalysis Society, and member of the Inorganometallic Catalyst Design Center (ICDC) EFRC. His role at Dow includes managing and setting technical direction for projects within Core R&D including process development for new products, catalyst discovery and development and novel separations technologies. Since joining Dow in 1990, Ted's work has been generally focused on the development, scale up, design and optimization of new and existing commercial reaction systems using a combination of experimental and modeling approaches. Dr. Calverley received his BASc (chemical engineering) from the University of Waterloo and his Ph.D. from McMaster University.

SCIENCE POLICY PANEL

Tuesday, October 27, 2015, 12:20 – 1:20pm
Lincoln 3/4
Open to All

COMMITTEE MEMBERS

- **Laura Fernandez**, University of Minnesota, ICDC
- **Karen Kihlstrom**, Argonne National Laboratory, CES
- **David Bierman**, Massachusetts Institute of Technology, S3TEC
- **Kirsten Chojnicki**, Sandia National Laboratories, CFSES

PANELISTS

- **Diana Bauer**, Director, Office of Energy Systems Analysis and Integration at DOE Office of Energy Policy and Systems Analysis (EPSA)
- **Paul Doucette**, Executive Director of Government Relations at Battelle
- **Matt Hourihan**, Director of the R&D Budget and Policy Program at the American Association for the Advancement of Science (AAAS)

DESCRIPTION

The panel is geared toward helping all meeting attendees understand how their work fits into the larger pictures of energy security and sustainability and federally funded research. The panel will be asked questions related to budget, prioritization of research directions, and the impact of scientific research on the economy. The session will end with questions from audience members.

SPEAKER BIOGRAPHIES

Diana Bauer is the Director of Energy Systems Analysis and Integration within the Office of Energy Policy and Systems Analysis (EPSA) at the U.S. Department of Energy (DOE). She led the DOE team that published The Water-Energy Nexus: Challenges and Opportunities in 2014. She currently co-chairs DOE's Water-Energy Tech Team (WETT). Dr. Bauer has a PhD in Mechanical Engineering from the University of California at Berkeley and a BSE in Mechanical Engineering from Princeton University.

Paul Doucette is Executive Director of Government Relations at Battelle, the world's largest non-profit independent research and development organization, and a co-chair of the Energy Sciences Coalition (ESC), a broad based coalition of organizations representing scientists, engineers and mathematicians in universities, industry and national laboratories who are committed to supporting and advancing the scientific research programs of the DOE Office of Science. He worked as a senior advisor and legislative director in the office of U.S. Rep. Judy Biggert (R-IL), who was a senior member of the House Science and Technology Committee and co-chaired the House Research and Development Caucus. He holds a bachelor's degree in public administration from Drake University in Des Moines, Iowa.

Matt Hourihan is the Director of the R&D Budget and Policy Program at the American Association for the Advancement of Science (AAAS). Prior to joining AAAS, he served as a clean energy policy analyst at the Information Technology & Innovation Foundation (ITIF). He earned a masters degree in public policy with a focus on science and technology policy at George Mason University, and a B.A. in journalism from Ithaca College.

2015 EFRC PI MEETING – GRAPHIC AGENDA FOR MONDAY, OCTOBER 26, 2015

		A. Energy Storage	**B. Solar Energy Conversion**	**C. Control at the Level of Electrons**	**D. Carbon Sequestration**	**E. Materials and Chemistry by Design**	**F. Catalysis**
Room		*Thurgood Marshall E/N*	*Thurgood Marshall S/W*	*Lincoln 2*	*Lincoln 6*	*Lincoln 5*	*Lincoln 3/4*
Chair		*Craig Henderson*	*Christopher Fecko*	*Jim Rhyne*	*James Rustad*	*Tim Fitzsimmons*	*Mike Markowitz*
I-1	**1:10**	[**CEES**] Christopher Wolverton *Northwestern University* Why Not Both? High-Capacity Hybrid Li-ion/Li-oxygen Batteries	[**CASP**] Ashley Marshall** *NREL; University of Colorado* Understanding and Improving the Chemistry of Lead Chalcogenide Quantum Dots for PV	[**CES**] Ulrich Welp *ANL* Rapid Enhancement of the Critical Current of High-Performance Superconducting Wires	[**NCGC**] Ian C. Bourg *Princeton University* Microstructural Constraints on the Energy Technology Uses of Fine-Grained Sedimentary Rocks	[**IMASC**] E. Kaxiras *Harvard University* Multiscale Modeling of Surface Reactivity in Nanoporous Alloys	[**BETCy**] Michael Adams *University of Georgia* Electron Bifurcation in Managing Efficient Conversion of Electrochemical Potential into Chemical Bonds
I-2	**1:30**	[**NECCES**] Shyue Ping Ong *UC San Diego* An Integrated First Principles and Experimental Approach to Enabling Multi-Electron Lithium-Ion Battery Cathode	[**CE**] Marc Baldo *MIT* Exciton Fission and Fusion	[**EFree**] Ivan Naumov *Carnegie Institution of Washington* Transitions Between Insulating, Metallic and Superconducting States in Low-Z Materials	[**CFSES**] Anastasia G. Ilgen *SNL* Mancos Shale-Brine-CO_2 Interactions and the Long-term Stability of Shale Caprock	[**CME**] Simone Raugei *PNNL* Toward Design of Molecular Electrocatalysts by Computations	[**ICDC**] Omar K. Farha *Northwestern University; King Abdulaziz University* Single-site Nickel Hydrogenation Catalyst Supported on a Metal-Organic Framework Produced via ALD
I-3	**1:50**	[**NEES**] Chunsheng Wang *University of Maryland* Sulfides for Li-ion Batteries and Beyond	[**CASP**] Joseph M. Luther *NREL* Improving the Understanding of Quantum Dot Solar Cells by Modifying the Chemistry of PbS and PbSe Quantum Dots	[**CES**] Daniel Shoemaker *University of Illinois* Directed Synthesis and Fast Characterization of Correlated-Electron Materials for the Center for Emergent Superconductivity	[**NCGC**] Jonathan Ajo-Franklin *LBNL* Self-Sealing or Self-Enhancing? Observations of Fracture Evolution during CO_2 Induced Dissolution at *In-situ* …	[**CCEI**] Tyler R. Josephson** *University of Delaware* Revealing the Sugar Isomerization Mechanism on Homogeneous Sn-Silicate Catalysts	[**CME**] Molly O'Hagan *PNNL* Using Second-Coordination Sphere Strucutral Dynamics to Control H_2 Production Rates in $[Ni(PR_2NR'_2)_2]^{2+}$ Catalysts
I-4	**2:10**	[**m2M**] Alan C. West *Columbia University* Investigations of Mesoscale Transport Processes in Magnetite	[**CBES**] Emily Weiss *Northwestern University* Electron Ratchets	[**SHINES**] Chia-Ling Chien *Johns Hopkins University* Observation of p-Wave Superconductivity in Epitaxial Bi/Ni Bilayers	[**GSCO2**] Kristian Jessen *University of Southern California* Mass Transfer and Sorption in the Context of CO_2 Storage in Saline Formation	[**FIRST**] Peter T. Cummings *Vanderbilt University* Understanding and Predicting the Interfacial Structure and Dynamics in Capacitive Energy Systems Utilizing …	[**BETCy**] Anne Jones *Arizona State University* Defining Determinants of Catalytic Bias in Enzyme Catalyzed Proton-Coupled Electron Transfer Reactions
I-5	**2:30**	[**NEES**] Eleanor I. Gillette *University of Maryland* 3D Structure, Kinetics and Rate Performance in V_2O_5 Cathodes	[**CE**] William Tisdale *MIT* Exciton Dynamics in Hybrid 0D/2D Systems	[**CES**] Sean Vig** *University of Illinois* Characterization of the Low-Energy Bosonic Modes in $Bi_2Sr_2CaCu_2O_{8+x}$ with Incipient Charge Order	[**NCGC**] Lauren Beckingham# *LBNL* The Role of Advanced Reactive Surface Area Characterization in Improving Predictions of Mineral Reaction Rates …	[**UNCAGE-ME**] David A. Dixon *University of Alabama* Molecular and Dissociative Adsorption of Water on $(TiO_2)_n$ Clusters	[**CBES**] Samuel Stupp *Northwestern University* Center for Bio-Inspired Energy Science

2:50 – 3:20 PM **Break**

** Graduate Student Finalist; # Postdoctoral Researcher Finalist

2015 EFRC PI MEETING – GRAPHIC AGENDA FOR MONDAY, OCTOBER 26, 2015

		A. Energy Storage	**B. Solar Energy Conversion**	**G. Synthesis of Functional Matter**	**H. Bioscience**	**E. Materials and Chemistry by Design**	**F. Catalysis**
Room		*Thurgood Marshall E/N*	*Thurgood Marshall S/W*	*Lincoln 2*	*Lincoln 6*	*Lincoln 5*	*Lincoln 3/4*
Chair		*Jane Zhu*	*Christopher Fecko*	*Raul Miranda*	*Robert Stack*	*Mark Pederson*	*Viviane Schwartz*
II-1	**3:20**	[**FIRST**] Boris Dyatkin** *Drexel University* Probing Supercapacitor Carbon-Electrolyte Structure and Ion Dynamics with Neutrons	[**CASP**] Victor I. Klimov *LANL* Luminescent Solar Concentrators Using Engineered Quantum Dots	[**CNGMD**] David Ginley, Kristin Persson *NREL; UC Berkeley; LBNL* Approach to the Targeted Identification and Synthesis of Transition Metal Oxide Polymorphs	[**CLSF**] Daniel Cosgrove *Penn State University* Primary Cell Wall Structure in Plants: New Concepts, Some Remaining Enigmas	[**CCDM**] Jianwei Sun *Temple University* Testing and Applications of the SCAN MetaGGA, an Accurate and Efficient Nonempirical Density Functional	[**IMASC**] Branko Zugic[#] *Harvard University* Dynamic Evolution of Nanoporous Gold Catalysts During Activation and Selective Oxidation Reactions
II-2	**3:40**	[**m2M**] Esther S. Takeuchi *Stony Brook University* Probing the Limits of Electron and Ion Transport over Multiple Length Scales	[**LMI**] Harry A. Atwater *Caltech* Architecting Infrared Absorption and Emission – Control of both Amplitude and Phase	[**CBES**] Kyle Bishop *Penn State University* Shape Directed Dynamics of Active Colloids	[**C3Bio**] Nich Carpita *Purdue University* Structure and Synthesis of Cellulose	[**CES**] Lucas Wagner *University of Illinois* Searching for New Correlated Materials for Superconductivity	[**ICDC**] Connie C. Lu *University of Minnesota* Uniform Heterobimetallic Active Sites in Metal-Organic Frameworks
II-3	**4:00**	[**NECCES**] Aziz Abdellahi** *MIT* The Effect of Cation Disorder on the Li Intercalation Voltage of Transition Metal Oxides	[**S3TEC**] Marin Soljacic *MIT* Nanophotonics in Material-Systems of Large Sizes	[**MSA**] Peter C. Burns *University of Notre Dame* Aggregation and Solubility of Clusters of Actinides in Water	[**CLSF**] Venu Gopal Vandavasi[#] *ORNL* Structural Studies of Plant Cellulose Synthase Support 18 Synthases in the Cellulose Synthesis Complex	[**CNGMD**] William Tumas, Gerbrand Ceder *NREL; UC Berkeley; LBNL* Incorporating Metastabilty into Materials by Design	[**CGS**] Jeffrey A. Reimer *UC Berkeley* NMR Studies of Heterogeneity, Dynamics, and Phase Equilibria in MOFs
II-4	**4:20**	[**m2M**] Yimei Zhu *BNL* The Role of Structural Defects in $Ag_xMn_8O_{16-y}$ Hollandite Nanorods for Energy Storage	[**LMI**] Ralph G. Nuzzo *University of Illinois; Caltech* Optical Materials and Architectures for Ultrahigh-Efficiency Photovoltaics	[**EFree**] Stephen Juhl *Penn State University* Dispersion and High-Resolution Transmission Electron Microscopy of Carbon Nanothreads	[**C3Bio**] Bryon Donohoe *NREL* Altered Lignin Biosynthesis Tailors Plant Cell Wall Architecture for Efficient Catalytic Conversions to Fuels …	[**ICDC**] Laura Gagliardi, Joseph T. Hupp *University of Minnesota; Northwestern University* Inorganometallic Catalyst Design Center	[**IMASC**] Robert J. Madix *Harvard University* Probing Active Sites on npAuAg Alloy
II-5	**4:40**	[**FIRST**] Nina Balke *ORNL* Tracking Ions in Electrochemical Capacitors across Different Time and Length Scales	[**PARC**] Andrew Shreve *University of New Mexico* Energy Harvesting Using Random Assemblies of Chromophores	[**MSA**] Katlyn Turner** *Stanford University* Structural Evolution of Uranyl Peroxide Nano-Cage Fullerene: U60, at Elevated Pressures	[**CLSF**] Jochen Zimmer *University of Virginia* Mechanism of Cellulose Synthesis and Membrane Translocation	[**CGS**] Berend Smit *UC Berkeley* How to Quantify Similarity in Nanoporous Materials	[**ICDC**] Alex Martinson *ANL* Atomic Layer Deposition (ALD) in Metal Organic Frameworks (MOFs)

5:00 – 6:30 PM **Poster Session I (odd # posters), Exhibition Hall C**
6:30 – 7:30 PM **Science Trivia Night (students and postdocs only)**

**** Graduate Student Finalist; # Postdoctoral Researcher Finalist

2015 EFRC PI MEETING – GRAPHIC AGENDA FOR TUESDAY, OCTOBER 27, 2015

		A. Energy Storage	**B. Solar Energy Conversion**	**I. Separations**	**H. Bioscience**	**E. Materials and Chemistry by Design**	**F. Catalysis**
Room		*Thurgood Marshall E/N*	*Thurgood Marshall S/W*	*Lincoln 2*	*Lincoln 6*	*Lincoln 5*	*Lincoln 3/4*
Chair		*Lane Wilson*	*Mark Spitler*	*Larry Rahn*	*Stephen Herbert*	*Jim Davenport*	*Michael Sennett*
III-1	**8:30**	[**NECCES**] Y. Shirley Meng *UC San Diego* Understanding the Layered Oxides for High-Voltage Intercalation in Alkaline Ion Batteries	[**ANSER**] Gary Brudvig *Yale University* Water-Oxidation Catalysts for Solar Fuel Production	[**MSA**] May Nyman *Oregon State University* Cluster-based Uranium Separation using Green Chemistry Principles	[**PARC**] Kaitlyn Faries** *Washington University in St. Louis* Expanding the Range of Light Absorbers for Bacterial Photosynthesis: YFP-Enhanced Charge Separation at the …	[**CCDM**] Liping Yu *Temple University* Designing Functional Two-Dimensional Materials by Bending	[**IMASC**] M. Flytzani-Stephanopoulos *Tufts University* Selective Methanol Dehydrogenation to Formaldehyde Across a Continuum of Structures: From Single Crystals to …
III-2	**8:50**	[**CEES**] Tim Fister *ANL* Interfacial Control of Oxide Conversion Reactions in Thin Film Battery Electrodes	[**FIRST**] Joel Rosenthal *University of Delaware* Insights into the Molecular Dynamics at the Cathode/Electrolyte Interface of Electrocatalyst Materials for CO_2 Reduction in …	[**CGS**] Jeffrey R. Long *UC Berkeley* Carbon Dioxide Capture in Diamine-Appended Metal-Organic Frameworks	[**BETCy**] Anne-Frances Miller *University of Kentucky* Flavins are Single-Molecule Switches that Couple Electron Transfer, Proton Transfer, Conformational Gating …	[**CE**] Jing Kong *MIT* Two Dimensional Transition Metal Dichalcogenide Materials through Chemical Vapor Deposition Synthesis	[**CCEI**] Michael Tsapatsis *University of Minnesota* Advances in Materials Synthesis for Biomass Conversion
III-3	**9:10**	[**NECCES**] Louis Piper *Binghamton University* Electrochemical Evolution of the Surface and Subsurface Properties of Layered Nickel-Rich Oxide Cathodes	[**ANSER**] Rebecca J. Lindquist** *Northwestern University* Incorporation of Perylene-3,4-dicarboximides into Photoanodes and Photocathodes for Solar Fuels	[**UNCAGE-ME**] Krista S. Walton *Georgia Tech* In situ IR Spectroscopic Investigation of Acid Gas Adsorption on MOF-Derived Ceria and Titania	[**PARC**] Volker Urban *ORNL* Neutron Scattering Studies of Photosynthetic Antenna Systems	[**CCDM**] Arun Bansil *Northeastern University* Spin-Polarization, Topological, Water-Splitting and Photo-Catalytic Properties of Ultrathin Films of Transition Metal …	[**ICDC**] Samuel O. Odoh# *University of Minnesota* Metal-Organic Framework Nodes as Nearly Ideal Supports for Molecular Catalysts: NU-1000- and UiO-66-Supported Iridium Complexes for Ethylene …
III-4	**9:30**	[**FIRST**] Michael Naguib *ORNL* 2D Transition Metal Carbides (MXenes) for Electrochemical Capacitors	[**CCDM**] Linyou Cao *North Carolina State University* Design of Multifunctional Two-Dimensional Materials: Toward Ideal Photocatalysts for Solar Water Splitting	[**CCEI**] J. Ilja Siepmann *University of Minnesota* Understanding Unique Diffusion Behavior in Hierarchical Zeolites	[**CBES**] Anna Balazs *University of Pittsburgh* Designing Self-regulating Microcapsules that Harness Chemical Energy to Undergo Bimimetic Collective Motion	[**CE**] Mircea Dinca *MIT* Two-Dimensional Charge Transport in Metal-Organic Frameworks	[**UNCAGE-ME**] Uma Tumuluri# *ORNL* Acid Gas Interaction with Oxide Nanoshapes with Well-defined Surface Facets
III-5	**9:50**	[**NEES**] Yue Qi *Michigan State University* Understanding the Science at Complex Interfaces for Nano-Structured Battery Design	[**UNC**] Gerald J. Meyer *University of North Carolina* Dye-Sensitized Water Oxidation in Photoelectrosynthesis Cells	[**Efree**] Max Murialdo** *Caltech* Anomalous Surface Thermodynamics of Gas Adsorption on Zeolite-Templated Carbon	[**PARC**] Aparna Nagarajan *Washington University* Phycobilisome Degradation in a Fast Growing Cyanobacterium	[**SHINES**] Nathaniel Gabor *UC Riverside* Spatio-Temporal Imaging of Spin, Valley, and Thermal Energy in Two-Dimensional Materials	[**IMASC**] Cynthia Friend *Harvard University* Informing Catalyst Design through Fundamental Studies

** Graduate Student Finalist; # Postdoctoral Researcher Finalist

2015 EFRC PI MEETING – GRAPHIC AGENDA FOR TUESDAY, OCTOBER 27, 2015

10:10 – 10:40AM Break

		J. Mesoscale Science	B. Solar Energy Conversion	C. Control at the Level of Electrons	D. Carbon Sequestration	E. Materials and Chemistry by Design	F. Catalysis
Room		*Thurgood Marshall E/N*	*Thurgood Marshall S/W*	*Lincoln 2*	*Lincoln 6*	*Lincoln 5*	*Lincoln 3/4*
Chair		*Philip Wilk*	*Refik Kortan*	*Michael Pechan*	*P. Thiyagarajan*	*John Vetrano*	*Wade Sisk*
IV-1	**10:40**	[**EDDE**] Yanwen Zhang *ORNL* Influence of Chemical Disorder on Energy Dissipation and Defect Evolution in Advanced Alloys - Progress toward Structural Materials by …	[**ANSER**] Mercouri Kanatzidis *Northwestern University* Lead Free Inorganic-Organic Hybrid Perovskites: Chemistry and Solar Cells	[**MSA**] Albert Migliori *LANL* Precision Plutonium Thermodynamics-Equilibria, Kinetics, and Complications	[**NCGC**] Andrew G. Stack *ORNL* Pore-Size Dependent Mineral Reactions in Porous Media	[**CNGMD**] Lauren Garten[#] *NREL* Predicting and Controlling Polymorphism in Transition Metal Oxides	[**CCEI**] Eyas Mahmoud *University of Delaware* Diels-Alder and Dehydration Reactions of Biomass-Derived Furan and Acrylic Acid for the Synthesis of Benzoic Acid
IV-2	**11:00**	[**CLSF**] Candace Haigler *North Carolina State University* Leveraging Empirical and Computationally Modeled Structures to Explore Plant Cellulose Synthase Protein Function	[**CNGMD**] Riley Brandt, Vladan Stevanovic *MIT; Colorado School of Mines* Perovskite Inspired Search for New PV Materials	[**S3TEC**] Bolin Liao *MIT* Understanding Electron Transport in Thermoelectrics from First-principles	[**GSCO2**] Kenneth T. Christensen *University of Notre Dame; Kyushu University* Pore-Scale Phenomena Affecting Transport and Fate of Supercritical CO_2 in Geological Reservoirs: Flow Dynamics, …	[**EDDE**] Ian M. Robertson *University of Wisconsin* Damage Production in Single-Phase Concentrated Solid Solution Alloys	[**C3Bio**] Maureen McCann *Purdue University* Delivering Fit-for-Purpose Biofuels
IV-3	**11:20**	[**MSA**] Maik Lang *University of Tennessee* Advanced Characterization Techniques for Actinide Materials	[**ANSER**] Tobin Marks *Northwestern University* Interface Science of Soft Matter Solar Cells	[**SHINES**] Javier Garay *UC Riverside* Producing Nanocrystalline Magnetic Insulators for Spin and Thermal Conductivity Studies	[**CFSES**] Tip Meckel *UT Austin* Constraining the Influence of Meso-scale Heterogeneity on CO_2 Saturation Resulting from Buoyant Flow using …	[**CNGMD**] Janet Tate, Aaron Holder *Oregon State University; NREL* Metastable Heterostructural Alloys	[**CCEI**] Alexander V. Mironenko *University of Delaware* Metal/Lewis Bifunctional Catalysts for Low Temperature Upgrade of Biomass
IV-4	**11:40**	[**CLSF**] Christopher Lee *Penn State University* Probing the Architecture of Plant Cell Wall In-between the Nanoscopic and Macroscopic Length Scales with Sum-Frequency-Generation (SFG) Vibration Spectroscopy	[**EFree**] Timothy A. Strobel *Carnegie Institution of Washington* Materials for Solar Energy Conversion Using Extreme Conditions: An Overview	[**CES**] J.C. Seamus Davis *BNL* Interplay of d-Symmetry Cooper Pairs and d-Symmetry Density Waves within the Cuprate Pseudogap Phase	[**UNCAGE-ME**] Christopher W. Jones *Georgia Tech* Neutron Scattering Links CO_2 Adsorption Performance to Polymer Morphology in Silica/PEI Composite Adsorbents	[**EDDE**] Laurent K Béland *ORNL* Modeling Primary Damage Production and Evolution in Concentrated NiFe	[**C3Bio**] Mahdi Abu-Omar *Purdue University* Selective Conversion of Lignin First in Total Utilization of Biomass to Make Fuels and Chemicals

12:00 – 1:30 PM Lunch

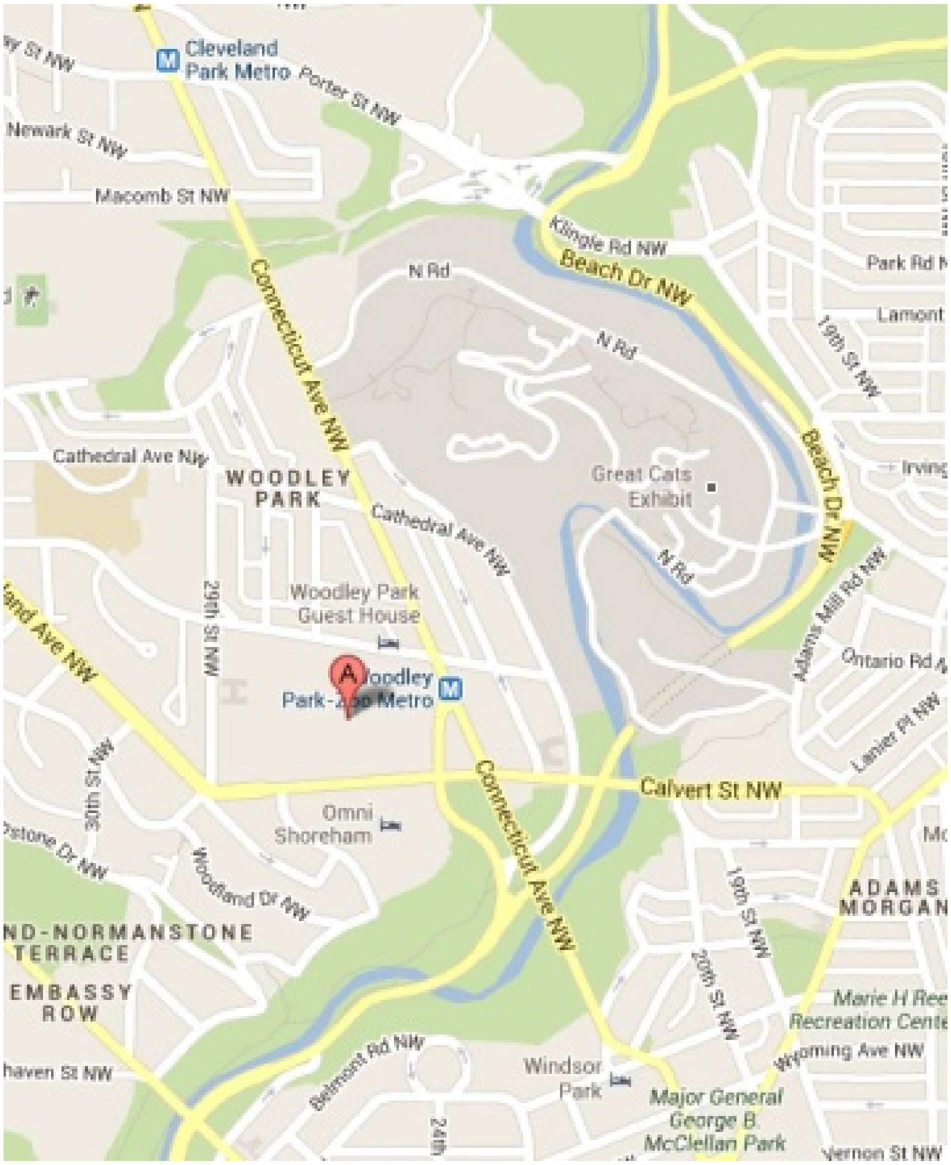
2015 EFRC PI MEETING – GRAPHIC AGENDA FOR TUESDAY, OCTOBER 27, 2015

		A. Energy Storage	**B. Solar Energy Conversion**	**G. Synthesis of Functional Matter**	**D. Carbon Sequestration**	**E. Materials and Chemistry by Design**	**F. Catalysis**
Room		*Thurgood Marshall E/N*	*Thurgood Marshall S/W*	*Lincoln 2*	*Lincoln 6*	*Lincoln 5*	*Lincoln 3/4*
Chair		*Craig Henderson*	*George Maracas*	*Bonnie Gersten*	*P. Thiyagarajan*	*Matthias Graf*	*Robert Stack*
V-1	**1:30**	[**CEES**] Mark Hersam *Northwestern University* Suppressing Manganese Dissolution from Lithium Manganese Oxide Cathodes with Single-Layer Graphene	[**CASP**] Alexander L. Efros *George Mason; NRL* Modeling of the Electronic Structure of Semi-conductor Nanocrystals, and Carrier Transport in Nanocrystal Arrays	[**CGS**] Lorenzo Maserati[#] *LBNL* Ultrafast Synthesis Metal-Organic Frameworks Critical for Energy-Efficient CO_2 Capture	[**CFSES**] Thomas Dewers *SNL* Geomechanics and Research Challenges for Geologic Carbon Storage	[**S3TEC**] Gang Chen *MIT* Probing and Understanding Thermal Transport and Energy Conversion In Nanostructures	[**BETCy**] Lance Seefeldt *Utah State University* Unraveling Nitrogenase Energy Conversion and Electron Transfer
V-2	**1:50**	[**NEES**] A. Alec Talin *SNL* The Challenge of 3D All Solid State Li-ion Battery	[**UNC**] Thomas J. Meyer *University of North Carolina* Systems and Assemblies for Applications in Dye-Sensitized Photo-electrosynthesis Cells	[**LMI**] Jennifer A. Lewis *Harvard University* Printing Functional Materials	[**NCGC**] Carl I. Steefel *LBNL* Pore-Scale and Continuum Modeling of Fracture Evolution and Mineral Trapping during CO_2 Sequestration	[**EDDE**] G. Malcolm Stocks *ORNL* Extreme Chemical Complexity: A Route to the Control of Energy Dissipation and Defect Evolution in Structural Materials for Intense …	[**UNCAGE-ME**] Israel E. Wachs *Lehigh University* Defects Matter: Co-precipitated and Impregnated Supported WO_3/TiO_2 and V_2O_5-WO_3/TiO_2 Catalysts for …
V-3	**2:10**	[**m2M**] Kenneth J. Takeuchi *Stony Brook University* Structure-Function Relationships of Electroactive Materials Modulated by Synthetic …	[**CASP**] Matt Law *UC Irvine* Charge Transport in Mesoscale Assemblies of Quantum Dots	[**CGS**] Michael Tsapatsis *University of Minnesota* Advances in 2-Dimensional Porous Layers for Gas Separation Membranes	[**GSCO2**] Michael Jordan *SINTEF Petroleum Research* Improved Quantification of Reservoir Parameters from Seismic Data	[**S3TEC**] David Broido *Boston College* Phonon Thermal Transport in Thermoelectric Materials from First Principles	[**CME**] Michael T. Mock *PNNL* Exploring the Role of Pendant Amines in Metal Complexes for N_2 Reduction and NH_3 Oxidation
V-4	**2:30**	[**CEES**] Nancy R. Sottos *University of Illinois* Electrochemical Stiffness in Lithium-ion Batteries – A New Concept for Understanding Electrode Response	[**UNC**] John M. Papanikolas *University of North Carolina* Ultrafast Dynamics in Molecular Assemblies for Solar Energy Conversion	[**EFree**] Yiqun Liu *Lehigh University* Synthesis of Periodic Mesoporous Silica With Crystalline Pore Walls	[**CFSES**] Marc A. Hesse *UT Austin* Constraints on Long-term Safety of Geological CO_2 Storage from Natural Analogues	[**LMI**] Austin J. Minnich *Caltech* Spectrally Selective Semiconductor Absorbers for Solar Thermal Energy Conversion	[**ANSER**] Alex Martinson *ANL* Atomic Layer Epitaxy of Fe_2O_3 for New Frontiers in Photo-Assisted Water Oxidation
V-5	**2:50**	[**NECCES**] Karena Chapman *ANL* Advancing Operando Tools to Probe Multiscale Complexity in Chemical Energy Storage	[**PARC**] Jonathan Lindsey *North Carolina State University* Biohybrid Light-Harvesting Architectures - Blending Chemistry and Biology	[**UNC**] James F. Cahoon *University of North Carolina* Designing Photocathode Materials For Dye-Sensitized Photo-electrosynthesis Cells	[**GSCO2**] Volker Oye *NORSAR* Induced Seismicity Due to Low Pressure-Gradient Fluid Injections: Linking Laboratory-Scales with Field-Scale Observations	[**SHINES**] Jing Shi *UC Riverside* Topological Spin Seebeck Effect in Topological Insulator/Yttrium Iron Garnet Heterostructures	[**CME**] James M. Mayer *Yale University* Molecular Catalysts for the Oxygen Reduction Reaction (ORR)

3:10 – 5:00 Poster Session II (even # posters), Exhibition Hall C; 4:00 Announce winners of the *Graduate Student and Postdoctoral Researcher Competition*

** Graduate Student Finalist; # Postdoctoral Researcher Finalist

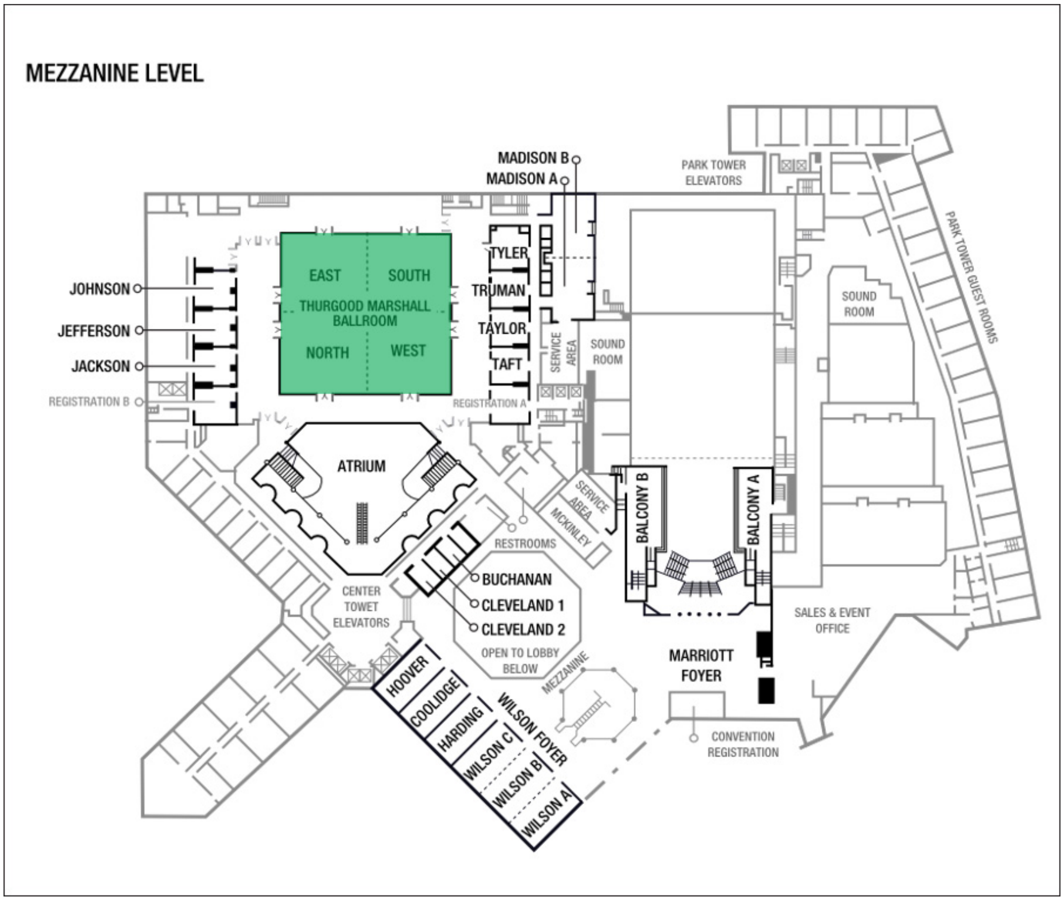
HOTEL MAPS



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

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

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


MEZZANINE LEVEL
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MADISON A
PARK TOWER ELEVATORS
PARK TOWER GUEST ROOMS
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HARDING
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WILSON B
WILSON A
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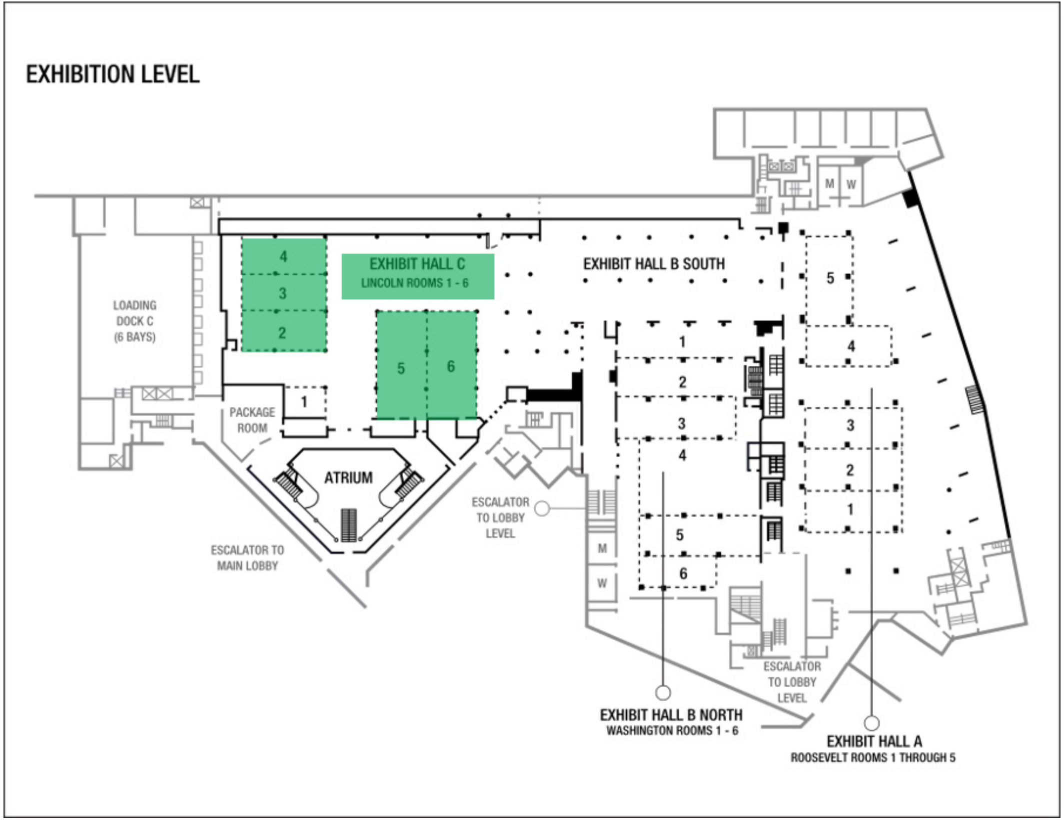
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TALK ABSTRACTS

A. ENERGY STORAGE

SESSION I: MONDAY, OCTOBER 26, 2015; 1:10 – 2:50 PM; THURGOOD MARSHALL E/N

1:10 PM

A-I-1: WHY NOT BOTH? HIGH-CAPACITY HYBRID LI-ION/LI-OXYGEN BATTERIES

[CEES] Chun Zhan[1], Chi Kai Lin[1], Jun Lu[1], Alper Kinaci[1], Zhenpeng Yao[2], Fernando Castro[2], Zhenzhen Yang[1], Jinsong Wu[2], Xiaoping Wang[1], Liang Li[1], Vic Maroni[1], Roy Benedek[1], Vinayak Dravid[2], Chris Wolverton[2], Maria Chan[1], Christopher Johnson[1], Khalil Amine[1], Michael Thackeray[1]
[1]Argonne National Laboratory; [2]Northwesterm University

Lithium ion batteries are now the standard power source for many applications, while lithium oxygen batteries hold promise for a significant future increase in energy storage capacity. 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 lithium-ion and lithium-oxygen electrochemistries to deliver high energy storage capacities several times that of typical Li-ion batteries. A prototypical hybrid material, Li_5FeO_4 (LFO), contains an unusually high Li to transition metal ratio, giving it a theoretical capacity of over 800 mAh/g. Experiments carried out in CEES indicate the possibility of hybrid energy storage using LFO, but the fundamental mechanisms of reactions remain unclear. In this talk, we will discuss extensive characterization of electrochemical, structural, vibrational, and electronic properties of LFO, as well as corresponding first principles predictive modeling of the reaction mechanisms. We will also discuss high throughput computational searches for other promising hybrid materials, as well as challenges and opportunities for new hybrid materials.

1:30 PM

A-I-2: AN INTEGRATED FIRST PRINCIPLES AND EXPERIMENTAL APPROACH TO ENABLING MULTI-ELECTRON LITHIUM-ION BATTERY CATHODE

[NECCES] Shyue Ping Ong[1], Yul-Chieh C. Lin [1], Yiqing Huang[2], Bohua Wen[2,3], Nicholas F. Quackenbush[2], Youngmin Chung[2], Natasha A. Chernova[2], Fredrick Omenya[2], Louis F. J. Piper[2], M. Stanley Whittingham[2]
[1] University of California, San Diego; [2] Binghamton University; [3] Massachusetts Institute of Technology

Today's commercial lithium-ion battery cathodes function on the basis of a single-electron transfer per transition metal. In order to attain significantly higher capacities, particularly in polyanionic compounds with higher voltages, achieving reversible multi-electron transfer per transition metal is necessary. In this talk, we will discuss the efforts of the Northeast Center for Chemical Energy Storage (NECCESS), an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Award Number DE-SC0012583, to identify crystal structures that can reversibly intercalate two lithium ions and understand the implications to the crystal lattice and its stability of inserting those two lithium ions. Specifically, we will present results from our combined first principles and experimental investigations into the thermodynamics, kinetics and electronic structure of ε-$VOPO_4$ (theoretical capacity of 318 mAh/g) over two Li insertion. We find that density functional theory, X-ray photoelectron spectroscopy and cyclic voltammetry all provide evidence of two-phase behavior during the first Li insertion and multiple intermediate phases during the second

Li insertion. We will also show that ε-$VOPO_4$ and its lithiated compounds show extremely good thermal stability relative to other well-known cathodes, and discuss our findings on the ionic and electronic limitations in this material.

1:50 PM

A-I-3: SULFIDES FOR LI-ION BATTERIES AND BEYOND

[NEES] Chunsheng Wang[1], Sang Bok Lee[2], Gary W. Rubloff[3,4]
[1] Department of Chemical and Biomolecular Engineering, University of Maryland; [2] Department of Chemistry and Biochemistry, University of Maryland; [3] Department of Materials Science and Engineering, University of Maryland; [4] Institute for Systems Research, University of Maryland

The NEES team has explored numerous sulfide chemistries as potential electrode and electrolyte materials for Li-ion batteries. To reduce the shuttle reaction of high-order lithium polysulfide, we physically traps short-chain S_2 and S_4 into micro-sized porous carbon or chemically bonds sulfurs to Cu, Fe metals in carbon, thus allowing the S_2/C nanocomposite to be stably charged/discharged for more than 4000 cycles with capacity decay per cycle less than 0.0014%. Use of soft porous carbon from wood to replace hard porous carbon from polymer can increase the S_2 loading from 33% to 76% without sacrificing the performance. By collaborating with Saft American Inc., we also prelithiated S_2/C cathode using stabilized lithium metal powders and paired it to commercial graphite to fabricate a C/Li_2S full cell, which provides a stable capacity of around 600 mAh/g for 150 cycles. The NEES team also matched the sulfur cathodes to dendrite-free Mg anode and while incorporating Li-ion in Mg-ion electrolyte as a mediator, which significantly enhanced the cycling stability of Mg/S full cells. The presence of Li-ions in Mg-ion electrolytes also improved the reaction kinetics and cycling stability of titanium sulfide cathodes in Mg-ion batteries. Beyond liquid organic electrolytes, the NEES team also revolutionarily fabricated an interface-free all-solid-state Li-ion battery by using a single sulfide-based solid electrolyte material, $Li_{10}GeP_2S_{12}$ (LGPS), where the Li–S and Ge–S components in LGPS electrolyte could also act as cathode and anode when carbon is mixed into LGPS. This “single material battery” concept could fabricate solid state nano electrochemical devices.

2:10 PM

A-I-4: INVESTIGATIONS OF MESOSCALE TRANSPORT PROCESSES IN MAGNETITE

[m2M] Kevin W. Knehr[1], Nicholas W. Brady[1], Christina A. Cama[2], David C. Bock[3], Zhou Lin[2], Christianna N. Lininger[1], Amy C. Marschilok[2], Kenneth J. Takeuchi[2], Esther S. Takeuchi[2,3] Alan C. West[1]
[1]Columbia University; [2]Stony Brook University; [3]Brookhaven National Laboratory

Magnetite is a model, low-cost inverse spinel material, and its performance may potentially improve with advanced synthesis of nano-sized crystals with a uniform size. However, improvements may only be realized if the materials are assembled effectively into full cells. For example, such crystals may form agglomerates, either during synthesis or during the electrode or cell fabrication. Transport through the agglomerate structures may impede performance, but it can be difficult to determine entirely from scaling arguments which transport resistances may be dominant due to uncertainties in physical properties.

For the case of the magnetite electrodes we have fabricated, open circuit transients in response to galvanostatic interruption exhibit very large time constants. Multi-scale simulations suggest that transport processes on the scale of the agglomerate have a very significant influence on cell performance. The simulations account for transport processes within the micron-sized

agglomerates as well as diffusion within the crystals. Simulation results are compared to discharge data of cathodes comprised of 6, 8, or 32 nm crystals. Furthermore, the simulations are used to investigate the impact of the agglomerate-size distribution on performance. Finally, the simulations are used to test reasons for a maximum in open circuit potential that is observed for cathodes fabricated from 6 and 8 nm crystals at relatively small loadings of lithium.

2:30 PM

A-I-5: 3-D STRUCTURE, KINETICS AND RATE PERFORMANCE IN V_2O_5 CATHODES

[NEES] Eleanor I. Gillette[1], Chanyuan Liu[2,3], Gary Rubloff[2,3], Sang Bok Lee[1]
[1] Department of Chemistry & Biochemistry, University of Maryland; [2] Department of Materials Science and Engineering, University of Maryland; [3] Institute for Systems Research, University of Maryland

Electrode structure can determine the kinetics of electrochemical reactions, with direct consequences for rate performance and electrode durability. Both electronic conductivity and ionic conductivity can be influenced by structural changes and characterizing the structural features of randomly oriented, disordered materials is challenging. Without predictable structural features on the nano- and meso-scales, it is difficult to isolate the impact of structure on energy storage mechanism. Very simple ordered arrays of nanowires or nanotubes have been previously demonstrated, but more complex systems of nanomaterials have not been extensively studied.

In order to understand the consequences of transitioning to less ordered, three-dimensional structures, we demonstrate anodized aluminum oxide template electrodes that can be modified to have increasing numbers of interconnected regions evenly spaced within the aligned nanopores. Atomic layer deposition (ALD) then conformally coats these structures with V_2O_5 to produce electrodes with systematically modulated surface area and disorder. The rate performance of the branched structures is notably improved over their aligned counterparts, and the cycling performance of the two electrodes remains similar, despite the introduction of numerous defect sites in the cross-linked template. Kinetic analysis methods can be used to separate the contributions from faster surface charge storage mechanisms and slower bulk charging mechanisms, in order to understand the origin of rate performance increases.

SESSION II: MONDAY, OCTOBER 26, 2015; 3:20 – 5:00 PM; THURGOOD MARSHALL E/N

3:20 PM – Graduate Student Finalist

A-II-1: PROBING SUPERCAPACITOR CARBON-ELECTROLYTE STRUCTURE AND ION DYNAMICS WITH NEUTRONS

[FIRST] Boris Dyatkin[1], Hsiu-Wen Wang[2], Eugene Mamontov[3], Naresh Osti[3], Katherine Page[3], Ray Unocic[3], Gernot Rother[3], Matthew Thompson[4], Yu Zhang[4], Peter Cummings[4], David Wesolowski[3], Yury Gogotsi[1]
[1]Drexel University; [2]University of Tennessee; [3]Oak Ridge National Laboratory; [4]Vanderbilt University

Electrochemical capacitors (supercapacitors) showcase high energy and power densities and exhibit exceptional promise in electrical energy storage applications including transportation and grid storage systems. Carbide-derived carbon (CDC) electrodes feature high specific surface areas (> 2000 m^2/g) and narrow porosity distributions (0.7 nm d_{av}) and, as a result, offer optimal capacitances. Although simulations and experimental findings have determined the influence of the ion/pore diameter ratio on charge accumulation, most studies have not investigated the interface between pore surfaces and

electrolytes. The influence of surface chemistry and graphitic ordering on capacitance, charge/discharge rates, and electrochemical stability is poorly understood. Furthermore, conventional materials characterization and electrochemical testing approaches are incapable of quantifying essential structural properties and ion dynamics. This insight is vital for the design of the next generation of high-performance supercapacitors.

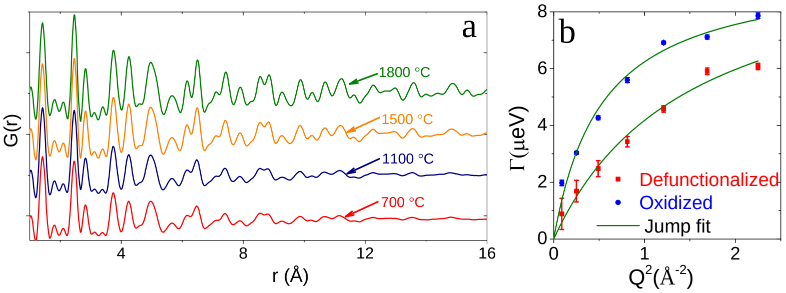


Fig. 1. a) PDF analysis of graphitization and ring prevalence transformations in SiC-CDCs annealed at 700 – 1800 ºC under 10^{-6} torr. b) Cole-Cole fit of energy transfer coefficients of mobilities of [Omim$^+$][TF$_2$N$^-$] RTIL inside of differently functionalized pores of Mo$_2$C-CDC collected using QENS.

We present our findings that rely on a combination of neutron scattering and spectroscopy with Quenched Molecular Dynamics (QMD) to correlate structural and chemical features of porous carbons with capacitance and electrosorption dynamics. We used chemical treatments, such as air oxidation and vacuum annealing, to modify graphitization and surface chemistry of nanoporous CDCs derived from SiC and Mo$_2$C. We relied on neutron diffraction and electron energy loss spectroscopy (EELS) to quantify thermally-driven graphite ring content transformations (5–, 6–, 7–member rings) and prevalent sp^2/sp^3 bonding in CDCs. We used small-angle neutron scattering (SANS) to assess changes in surface roughness and porosities and combined them with Pair Distribution Function (PDF) analysis of X-ray and neutron total scattering data (Fig. 1a) to develop comprehensive structural models of the CDCs. We combined our measurements with computational models to evaluate surface structure, bonding angles, and grain terminations. We filled the pores of differently functionalized CDCs with Room Temperature Ionic Liquid (RTIL) electrolytes and used Quasi-Elastic Neutron Scattering (QENS) and inelastic neutron scattering (INS) to probe the structures of confined ions and their dynamics inside of pores (Fig. 1b). We found that oxygen-rich pores became more ionophilic and showed enhanced mobilities of electrolyte ions, decreased filling densities, and lowered vibrational energies under pore-confinement. We found corresponding improvements in capacitance, higher ion mobility, and lower ionic resistance of electrolytes in oxidized CDCs. We relied on X-Ray PDF analysis to show ion-ion correlation changes and intermolecular interactions confined in defunctionalized vs. oxidized pores. We combined this analysis with MD simulations of electrolyte interactions with functionalized electrode surfaces to correlate electrosorption densities and ion orientations with capacitance and energy densities of these systems.

3:40 PM

A-II-2: PROBING THE LIMITS OF ELECTRON AND ION TRANSPORT OVER MULTIPLE LENGTH SCALES

[m2M] Esther S. Takeuchi[1,2], Lei Wang[1], Yiman Zhang[1], Yue Ru Li[1], Jiefu Yin[1], Megan E. Scofield[1], Coray McBean[1], David C. Bock[1], Christina A. Cama[1], Zhou Lin[1], Stanislaus S. Wong[1,2], Feng Wang[1], Wei Zhang[2], Jing Li[1,2], Eric A. Stach[2], Amy C. Marschilok[1], Kenneth J. Takeuchi[1]
[1]Stony Brook University; [2]Brookhaven National Laboratory

In the context of electrochemical energy storage, battery polarization (i.e. thermodynamic voltage - loaded voltage) under use conditions is a critical determinant of functional energy delivery. Strategies for determination of the factors that contribute to and control polarization at the material and electrode level will be described. The local environment of an electroactive material can significantly influence its functional behavior. Heterostructures combining nanoscale spinel materials and conductive additives were probed where different attachment modalities were explored. The intimate arrangement of the material and the conductive additives was characterized at the particle and the electrode level. The resultant electrochemistry was studied through a variety of electrochemical methods including electrochemical impedance spectroscopy, voltammetry and galvanostatic cycling. The results indicated significant impact of local resistance on the kinetics of the electrochemical reaction and thus, the functional energy delivery of the active material.

4:00 PM – Graduate Student Finalist

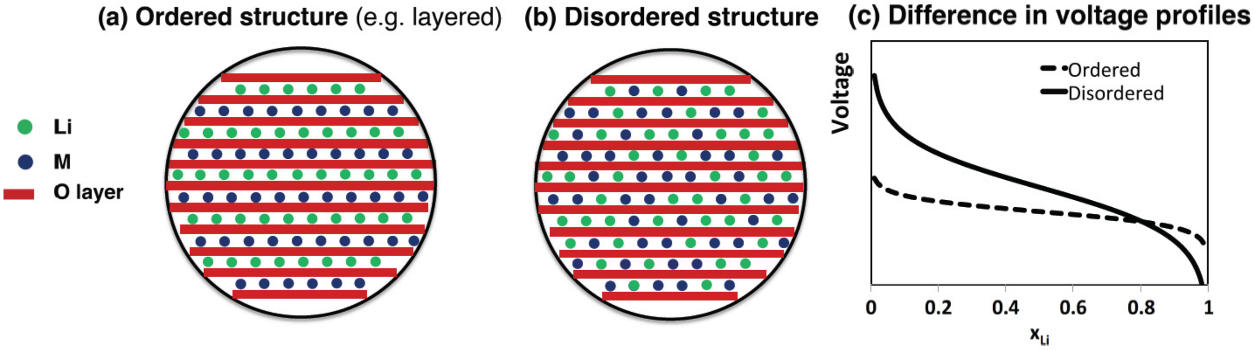
A-II-3: THE EFFECT OF CATION DISORDER ON THE LI INTERCALATION VOLTAGE OF TRANSITION METAL OXIDES

[NECCES] Aziz Abdellahi[1], Alexander Urban[2], Stephen Dacek[1], ShinYoung Kang[1], Pinaki Mukherjee[3], Khim Karki[4], Frederic Cosandey[3], Gerbrand Ceder[2]

[1]Masschusetts Institute of Technology, [2]UC Berkeley [3]Rutgers University, [4]Brookhaven National Laboratory

Cation disorder is a phenomenon that is becoming increasingly important in the field of Li-ion batteries. Disordered Li-excess rocksalts have achieved high-capacity via Li transport through percolating zero-transition-metal pathways[1], paving the way towards a new design space of high-capacity Li-ion battery cathodes. In situ cation-disorder also occurs in a large class of ordered materials, resulting in the formation of disordered bulk or surface phases upon cycling. In particular, commercially relevant NCA ($LiNi_{0.8}Co_{0.15}Al_{0.05}O_2$) particles were shown to undergo surface changes upon delithiation, leading to the formation of disordered rocksalt regions and partially disordered spinel regions at the surface, both with an increased transition metal (TM) to Li ratio [2].

In these cases, cation disorder has a strong impact on the voltage profile of lithium transition metal oxides; altering the average voltage of the Li-intercalation reaction as well as increasing the slope of the voltage profile. Even when cation disorder is limited to the particle surface (such as in the case of NCA), slow Li transport at the disordered surface (which does not have percolating zero-TM pathways) can lead to a voltage profile dominated by the surface redox processes.



In this work, we use first principles methods to understand and quantify the effect of cation-disorder on the Li-insertion voltage of transition metal oxides. In order to isolate the effect of cation-disorder from other effects such as the of Li/TM ratio, we investigate the effect of cation-disorder on the voltage of *stoichiometric* transition metal oxides. Our first principles work is complemented by detailed TEM characterization of NCA surfaces, thus helping clarify the structure and composition of the (partially) disordered phases that form at the surface.

[1] Lee et al., Science, 2014. [2] Hwang et al., *Chemistry of Materials*, 2015.

4:20 PM

A-II-4: THE ROLE OF STRUCTURAL DEFECTS IN $AG_XMN_8O_{16-Y}$ HOLLANDITE NANORODS FOR ENERGY STORAGE

[m2M] Yimei Zhu[1], Lijun Wu[1], Feng Xu[1], Qingping Meng[1], Feng Wang[1], Alexander B. Brady[2], Jianping Huang[2], Jessica L. Durham[2], Eric Dooryhee[1], Mark S. Hybertsen[1], Amy C. Marschilok[2], Kenneth J. Takeuchi[2], Esther S. Takeuchi[1,2]
[1]Brookhaven National Laboratory; [2]Stony Brook University

Hollandites are an intriguing class of sorbents, catalysts, and energy storage materials with a tunnel structure along the longitudinal c-direction, permitting one-dimensional (1D) insertion and deinsertion of ions and small molecules. A seven-fold increase in delivered capacity for $Li/Ag_xMn_8O_{16}$ electrochemical cells was observed upon a small change in silver content (x=1.1 or 1.6). Quantitative electron diffraction and atomic imaging illustrate that the structure of the individual nanorods is consistent with that refined by XRD, however the Ag occupancy varies significantly even within neighboring channels. High-resolution electron energy-loss spectroscopy reveals a large number of oxygen vacancies and low Mn valence-states in the low-Ag (x=1.1) nanorods relative to its high-Ag (x=1.6) counterpart, agreeing with bulk measurements. Furthermore, we found lower Mn oxidation state and more lattice distortion on the surface of the nanorods with respect to their interior. Lithiation pathway in the 1D nanorods was also studied using in-situ microscopy, revealing unexpected non-1D behavior, and Li-ion diffusivity was measured, showing good agreement with bulk measurement and DFT calculations. Our study suggests defects (including surface defects), such as oxygen vacancies as well as Mn valence-states play an important role in Li-ion diffusion and electrochemical reaction kinetics.

4:40 PM

A-II-5: TRACKING IONS IN ELECTROCHEMICAL CAPACITORS ACROSS DIFFERENT TIME AND LENGTH SCALES

[FIRST] Jennifer Black[1], Guang Feng[2], Paul Fenter[3], Ahmet Uysal[3], M. Baris Okatan[1], Sheng Dai[1], Peter Cummings[4], Sergei V. Kalinin[1], Nina Balke[1]
[1]Oak Ridge National Laboratory; [2]Huazhong University of Science and Technology, China;
[3]Argonne National Laboratory; [4]Vanderbilt University

Electrochemical capacitors (ECs) are a vital component of today's electrochemical energy storage, having energy and power densities ideally approaching that of batteries and electrolytic capacitors. Typical ECs utilize porous carbon electrodes and store charge in the electrochemical double layer (EDL) formed at the electrode/electrolyte interface. Electrolytes of high interest are room temperature ionic liquids (RTILs) which are liquid at room temperature and exhibit unique properties such as broad electrochemical stability and as such have found a wide variety of applications over the past number of years, particularly in the field of electrochemistry.

Here, we aim to understand the two most fundamental mechanisms involved in ECs: Ion insertion into the pores of the electrode and the structure and dynamics of the EDL in the RTIL. This is achieved by an integrated approach of experiment and modeling to look at different time and length scales. When ions are inserted into porous electrodes, large volume changes are observed which can be tracked by dilatometry-based techniques. We are using molecular dynamics (MD) to elucidate the origin of strain as function of ion content. The structure of the EDL can be understood through the complementary use of scattering techniques (X-ray) and force spectroscopy atomic force microscopy (AFM). Both approaches deliver a detailed image of the ion layering inside the EDL which can be compared with predictions by MD. The experiments reveal unexpected dynamics and structural defects within the EDL potentially important for performance and lifetime of the capacitor.

SESSION III: TUESDAY, OCTOBER 27, 2015; 8:30 – 10:10 AM; THURGOOD MARSHALL E/N

8:30 AM

A-III-1: UNDERSTANDING THE LAYERED OXIDES FOR HIGH-VOLTAGE INTERCALATION IN ALKALINE ION BATTERIES

[NECCES] Y. Shirley Meng[1], Anderj Singer[1], Sunny Hy[1], Haodong. Liu[1], Oleg Shpyrko[1]
Max Radin[2], Anton Van der Ven[2], Natasha A. Chernova[3], M. Stanley Whittingham[3], Nicole M. Trease[4], Clare P. Grey[4], Brian May[5], Young-Sang Yu[5, 6], Jordi Cabana[5]
[1] University of California, San Diego; [2] University of California, Santa Barbara; [3] Binghamton University; [4] Cambridge University; [5] University of Illinois at Chicago; [6] Advanced Light Source, Lawrence Berkeley National Laboratory

Among all candidates of positive electrode materials for lithium ion batteries, the layered oxides have gained growing research interest in recent years, especially the Ni rich layered oxides and the mixed transition metal (Ni,Co,Mn) layered oxides. They can reach more than 220mAh/g capacity when charged above 4.5V, making them one of the highest energy density positive electrode materials among all known intercalation compounds for cathode materials. Being the source of major capacity improvement, the high voltage operation (>4.5V), on the other hand, also cause unexplained phenomena in these layered oxides. Three critical questions remain unanswered: (1) how can we visualize and quantify the change in structure and chemical content at the atomic level (2) what is the oxygen activity upon high voltage and how does it assist transition metal migration and (3) what are the impact of these high voltage phenomena on rate capability and long-term cycling. A suite of powerful experimental tools and computational tools has been deployed in our EFRC center. To probe the bulk structural change, morphological and chemical changes, we combined X-ray diffraction (XRD), Neutron diffraction (ND), Pair Distribution Function (PDF) analysis, Electron Energy Loss Spectroscopy (EELS) and Transmission X-ray Microscopy (TXM), analytical Transmission Electron Microscopy (TEM). We will reveal and discuss the factors that determining the high voltage stability of oxides materials in alkaline ion batteries.

8:50 AM

A-III-2: INTERFACIAL CONTROL OF OXIDE CONVERSION REACTIONS IN THIN FILM BATTERY ELECTRODES

[CEES] Tim Fister[1], Guennadi Evmenenko[2], Michael Bedzyk[2], Jinsong Wu[2], Vinayak Dravid[2], Handan Yildrim[3], Jeff Greeley[3], Jennifer Esbenshade[4], Kimberly Lundberg[4], Andrew Gewirth[4], Jae Jin Kim[1], Paul Fenter[1]
[1] Chemical Sciences and Engineering Division, Argonne National Laboratory; [2] Material Sciences and Engineering, Northwestern University; [3] School of Chemical Engineering, Purdue University; [4] School of Chemical Sciences, University of Illinois Urbana-Champaign

The electrochemically-driven phase separation of a metal oxide into nanoscale lithia and reduced metal species can provide specific capacities well beyond typical intercalation materials in lithium ion batteries. However, these so-called conversion reactions suffer from severe hysteresis and generally occur at potentials far below that expected from their thermodynamic formation energies. These losses are loosely ascribed to the interfacial component of the reaction which inhibits the formation of each phase. To better understand the nucleation and

growth of the lithium rich and reduced metal components, we have studied model thin films of MOx (M = Ni, Cr, and Fe) using in-situ X-ray reflectivity and electron microscopy. At thicknesses approaching the size of typical conversion products, we find that the phase separation process is converted into a one-dimensional reaction, leading to the formation of a bilayer of metal and Li2O. Intriguingly, the surface is found to lithiate at potentials close to the thermodynamic limit and this phase slowly grows until the onset of 'bulk' 3D lithiation, which is observed at lower potentials. We have also explored using a pre-existing metal layer to seed the reduction of the metal species using a multilayer of alternating M/MOx units. These results show that nucleation does proceed at the interface and that the Li2O product becomes confined between neighboring metal layers. Beyond improving the energy density of such a reaction, such a heterostructure is useful for directing the volume expansion within the reacted oxide, improving its overall reversibility.

9:10 AM

A-III-3: ELECTROCHEMICAL EVOLUTION OF THE SURFACE AND SUBSURFACE PROPERTIES OF LAYERED NICKEL-RICH OXIDE CATHODES

[NECCES] Louis F. J. Piper[1], Shawn Sallis[1], Nathalie Pereira[2], Pinaki Mukherjee[2], Frederic Cosandey[2], Yiqing Huang[1], Nicholas F. Quackenbush[1], M. Stanley Whittingham[1], Glenn G. Amatucci[2]
[1] Binghamton University; [2] Rutgers University

The limitation and degradation of the ionic and electronic transport across the positive electrode/electrolyte interface can potentially reduce the achievable capacity of Li-ion batteries. This is evident for the layered oxides such as those based on nickel that operate outside the stability of today's organic electrolytes. The rise in impedance and capacity fade with cycling has been identified as a result of loss of electrical contact originating from the instability of electrode surface and decomposition of the electrolyte. In this talk, we will discuss the surface and subsurface properties of $LiNi_{0.8}Co_{0.15}Al_{0.05}O_2$ (NCA). NCA provides a model system for correlating capacity fade with the formation and evolution of the cathode electrolyte interface with cycling. Our studies directly compare x-ray spectroscopy, electron spectromicroscopy, and high-resolution electrochemical characterization of the same NCA electrodes as a function of both initial charging and extended cycling.

9:30 AM

A-III-4: 2D TRANSITION METAL CARBIDES (MXENES) FOR ELECTROCHEMICAL CAPACITORS

[FIRST] Michael Naguib[1], Hsiu-Wen Wang[2], Yu Xie[3], Jeremy Come[3], Jennifer Black[3], Naresh C. Osti[4], Babak Anasori[5], Majid Beidaghi[5], Alireza Ostadhossein[6], Adri van Duin[6], Elayaraja Muthuswamy[7], Katharine Page[4], Gernot Rother[2], Eugene Mamontov[4], Nina Balke[3], Paul R. Kent[3], Alexandra Navrotsky[7], David J. Wesolowski[2], Yury Gogotsi[5]
[1]Materials Science and Technology Division, Oak Ridge National Laboratory; [2]Chemical Science Division, Oak Ridge National Laboratory; [3]Center for Nanophase Materials Sciences, Oak Ridge National Laboratory; [4]Spallation Neutron Source, Oak Ridge National Laboratory ; [5]A.J. Drexel Nanomaterials Institute, Drexel University ; [6]Department of Mechanical and Nuclear Engineering, The Pennsylvania State University; [7]Peter A. Rock Thermochemistry Laboratory & NEAT ORU, University of California Davis

MXenes are a recently discovered family of two-dimensional (2D) early transition metal carbides and carbonitrides, which have already shown many attractive properties and a great promise in energy storage applications. Many MXenes exhibit higher electronic conductivity than solution-processed graphene, and they offer compositional versatility. So far, more than a dozen MXenes with different compositions have been successfully synthesized, e.g. Ti_3C_2, Nb_2C, V_2C, Mo_2C, Ta_4C_3, and Ti_3CN. The surface of the as-synthesized MXene has a mixture of moieties, including O, OH, and F, which adds more versatility to this system. *Ab initio* calculations predict that tuning the surface composition of MXene leads to changes in the electronic structure, therefore changing their electrochemical behavior. In addition to being electrically conductive, MXenes' surfaces were found to be hydrophilic- a rare combination of properties. This suggests MXenes to be an excellent platform for investigating electrode/electrolyte interfaces for electrochemical energy storage with aqueous electrolytes. When tested as electrode material for supercapacitors, a stable volumetric capacitance of more than 900 F/cm^3 was achieved over 10,000 cycles for additives-free Ti_3C_2 electrode. Herein an overview of the synthesis, properties, and performance of MXenes in supercapacitors will be presented. The mechanisms of ion transport between MXene layers, and mechanisms of capacitive redox energy storage by MXenes will be discussed. In addition, the recent progress in resolving the structure of MXenes using neutron diffraction and scattering combined with atomistic modeling will be presented, as well as water dynamics on the surface of MXenes and between MXene layers.

9:50 AM

A-III-5: UNDERSTANDING THE SCIENCE AT COMPLEX INTERFACES FOR NANO-STRUCTURED BATTERY DESIGN

[NEES] Yue Qi[1], Kevin Leung[2], Gary W. Rubloff[3,4], A. Alec Talin[5]
[1] Chemical Engineering & Materials Science Department, Michigan State University; [2] Sandia National Laboratories, Albuquerque; [3] Dept. Materials Science and Engineering, University of Maryland; [4] Institute for Systems Research, University of Maryland; [5] Sandia National Laboratories, Livermore

One of the most significant challenges for current and future lithium ion batteries is the smart structure design at the nanoscale and the control of electron and ion transport at the electrode/electrolyte interface. This issue is further complicated by the existence of ultrathin interphase layers (IL) covering the electrode, forming a complex heterogeneous electrode/**IL**/electrolyte interface. Several computational methods have been developed by the Nanostructures for Electrical Energy Storage (NEES), a DOE Energy Frontier Research Center, to critically examine the different pathways of electrons and ions crossing this complex interface, that are critical to charge transfer, degradation mechanisms, nanostructured all-solid-state battery, and interphase design.

The electrochemical reactions responsible for electrolyte degradation are examined using both large-scale *ab initio* molecular dynamics simulations and complementary ultrahigh vacuum atomic layer deposition measurements. Other examples include rigorous voltage calibration in density functional theory calculations, prediction of electron transfer through interphase layers, estimation of irreversible capacity loss agreeing well with experimental measurements, and control of currents associated with single nanowires. In order to understand how to design interphase layers with higher ionic conductivity, the dominating diffusing carriers and their diffusion pathways are predicted, as a function of the voltage of the electrode. The chemical-mechanical degradation at the complex interface is further investigated by molecular dynamics simulations with ReaxFF approach in collaboration with FIRST EFRC. The insights gained from these simulations have enhanced our understanding on battery degradation mechanisms and inspired new designs across various length scales (nano to vehicle applications).

SESSION V: TUESDAY, OCTOBER 27, 2015; 1:30 – 3:10 PM; THURGOOD MARSHALL E/N

1:30 PM

A-V-1: SUPPRESSING MANGANESE DISSOLUTION FROM LITHIUM MANGANESE OXIDE CATHODES WITH SINGLE-LAYER GRAPHENE

[CEES] Laila Jaber-Ansari[1], Kanan P. Puntambekar[1], Soo Kim[1], Muratahan Aykol[1], Langli Luo[2], Jinsong Wu[1,2], Benjamin D. Myers[1,2], Hakim Iddir[3], John T. Russell[3], Spencer J. Saldaña[4], Rajan Kumar[1], Michael M. Thackeray[5], Larry A. Curtiss[3,6], Vinayak P. Dravid[1,2], Chris Wolverton[1], Mark C. Hersam[1,7]

[1]Department of Materials Science and Engineering, Northwestern University; [2]NUANCE Center, Northwestern University; [3]Materials Science Division, Argonne National Laboratory; [4]Department of Chemical and Biological Engineering, Northwestern University; [5]Chemical Sciences and Engineering Division, Argonne National Laboratory; [6]Center for Nanoscale Materials, Argonne National Laboratory; [7]Department of Chemistry, Northwestern University

Spinel-structured $LiMn_2O_4$ (LMO) is a desirable cathode material for Li-ion batteries due to its low cost, thermal stability, and high power capability. However, LMO suffers from a limited cycle life that is triggered by manganese dissolution into the electrolyte during electrochemical cycling. Here, we show that single-layer graphene grown by chemical vapor deposition and transferred onto the surface of LMO can significantly reduce the manganese dissolution process. Compared to uncoated LMO control cathodes that failed after 350 lithiation/delithiation cycles, graphene-coated LMO cathodes show no evidence of failure following 750 lithiation/delithiation cycles with less than 10% capacity loss. X-ray photoelectron spectroscopy depth profiling provides evidence that the graphene coating inhibits manganese depletion from the LMO surface. Furthermore, cross-sectional transmission electron microscopy demonstrates that a stable solid electrolyte interphase (SEI) layer is formed on graphene-coated LMO. Using density functional theory, two complementary mechanisms for the mitigation of manganese dissolution from graphene-coated LMO are proposed. First, graphene acts as a selective barrier for manganese diffusion while allowing the intercalation of lithium. Second, manganese disproportion reactions and the Jahn-Teller distortion at the spinel LMO surface are suppressed as the oxidation state of surface manganese changes from 3^+ to 4^+ with graphene stabilization.

1:50 PM

A-V-2: THE CHALLENGE OF 3D ALL SOLID STATE LI-ION BATTERY

[NEES] A. A. Talin[1], Dmitry Ruzmetov[2], Paul Haney[2], Andrei Kolmakov[2], Alexander C. Kozen[3], Alexander J. Pearse[3], Keith E. Gregorczyk[3], Tom Schmitt[3], Farid El Gabaly[1], Nicholas Ware[1,4], Kim M. McKelvey[5], Martin A. Edwards[5], Henry S. White[5], Bruce S. Dunn[4], Gary W. Rubloff[3,6]

[1] Sandia National Laboratories; [2] Center for Nanoscale Science and Technology, NIST; [3] Dept. Materials Science and Engineering, University of Maryland; [4] Dept. of Materials science and Engineering, University of California, Los Angeles; [5] Dept. of Chemistry, University of Utah; [6] Institute for Systems Research, University of Maryland

Demonstration of all-solid state 3-dimensional (3D) Li-ion batteries has been a long standing goal for numerous researchers in the battery community interested in developing high power and high areal energy density storage solutions for variety of applications. The basic idea is to use the 3D geometry to maximize the volume of active material per unit area, while keeping its thickness sufficiently small to allow for fast Li diffusion. The 3D approach also leads to high electrode/electrolyte interface area, which should prove beneficial by lowering the local current density and therefore the charge transfer resistance, assuming that the interface is stable against parasitic reactions and breakdown. While simple conceptually, realizing working all solid state Li ion batteries has proven to be a significant challenge. Specifically, the physical vapor deposition processes which have been successfully implemented for planar, thin film solid state Li ion batteries, fail miserably when applied to 3D substrates, particularly with high aspect ratio features. In our presentation, we will describe the structure and performance of all solid state 3D Li ion batteries fabricated by physical vapor deposition. Although these can be charged and discharged at low C-rates, their capacity decreases rapidly at higher C-rates. In our presentation we will discuss the underlying reasons for the poor performance, including dimensional non-uniformity and electrolyte scaling, and we will demonstrate how these problems can be addressed using atomic layer deposition, a thin film deposition method compatible with high aspect ratio geometries.

2:10 PM

A-V-3: STRUCTURE-FUNCTION RELATIONSHIPS OF ELECTROACTIVE MATERIALS MODULATED BY SYNTHETIC CONTROL

[m2M] Kenneth J. Takeuchi[1], Jessica L. Durham[1], Jianping Huang[1], Alexander B. Brady[1], David C. Bock[2], Altug S. Poyraz[1], Christopher C. Pelliccione[2], Yimei Zhu[2], Lijun Wu[2], Feng Xu[2], Feng Wang[2], Wei Zhang[2], Eric Dooryhee[2], Amy C. Marschilok[1], Esther S. Takeuchi[1,2]
[1]Stony Brook University; [2]Brookhaven National Laboratory

Fundamental studies involving the impact of physical and chemical properties of materials on their electrochemical properties are critical to the rational development of battery materials which may address the present and future requirements for stationary and portable power. Synthetic strategies utilizing low temperature methods described in this presentation provide new approaches for preparation of metal oxides and their composites. Several materials classes are under investigation including 1D, 2D and densely packed structures. The direct control of material composition and physical properties was demonstrated yielding significant impact on the electrochemical behavior. The impact of the active material size and morphology on electrochemical behavior is probed through preparation of samples with direct synthetic manipulation of the material properties. The detailed analysis regarding the roles of size, structure, and structural defects on electrochemical performance will be presented, providing key information for the rational design of next generation batteries.

2:30 PM

A-V-4: ELECTROCHEMICAL STIFFNESS IN LITHIUM-ION BATTERIES – A NEW CONCEPT FOR UNDERSTANDING ELECTRODE RESPONSE

[CEES] O. Ozgur Capraz[1], Hadi Tavassol[1], Elizabeth M. C. Jones[1], Scott R. White[1], Andrew A. Gewirth[1], Nancy R. Sottos[1]
[1]University of Illinois, Urbana-Champaign

The high-rate exchange of lithium ions required for more power and faster charging of Li-ion batteries generates significant stresses and strains in the electrodes that ultimately lead to performance degradation. To date, electrochemically-induced stresses and strains in battery electrodes have only been studied individually. We have developed a new technique to probe the chemo-mechanical response of electrodes by calculating the electrochemical stiffness via coordinated *in situ* stress and strain measurements. In graphitic composite anodes, dramatic changes in electrochemical stiffness occur due to the formation of different graphite-lithium intercalation compounds during cycling. Our analysis reveals that stress scales proportionally

with the lithiation/delithiation rate and strain scales proportionally with capacity (and inversely with rate). The technique is quite general and has potential to provide new insights into the origin of rate-dependent chemo-mechanical degradation and the evaluation of a wide range of advanced battery electrodes. Most recently, we have found that sharp changes in the electrochemical stiffness of $LiMn_2O_4$ (LMO) composite cathodes are associated with phase transformations that occur in the LMO structure during cycling.

2:50 PM

A-V-5: ADVANCING OPERANDO TOOLS TO PROBE MULTISCALE COMPLEXITY IN CHEMICAL ENERGY STORAGE

[NECCES] Karena W. Chapman[1], Peter J. Chupas[1], Philip Batson[2], Frederic Cosandey[2], Jordi Cabana[3], Y. Shirley Meng[4], Guangwen Zhou[5]

[1] Argonne National Laboratory; [2] Rutgers University; [3] University of Illinois at Chicago;
[4] University of California, San Diego; [5] Binghamton University

Electrochemical energy storage is a rapidly expanding area of study, driven by critical applications in alternative energy technologies (e.g. for grid storage coupled to intermittent solar/wind energy sources) and improved efficiency (e.g. in vehicle technology). Batteries, by their nature, do not operate under equilibrium conditions. Accordingly, there is a growing need for operando characterization tools to understand the dynamic mechanisms and kinetics of the electrochemical reactions which govern energy storage.

Within the NorthEast Center for Chemical Energy Storage (NECCES) EFRC, we are developing and applying a series of complementary operando tools to probe and decouple the structural, chemical, and electronic changes in operating batteries at the atomic-, particle- and electrode-levels. This will allow us to develop a comprehensive understanding of the fundamental processes that underlie performance limitations and failure. Methodologies span hard and soft X-ray scattering, spectroscopy and imaging, electron microscopies, and NMR-based spectroscopy and imaging.

B. Solar Energy Conversion

Session I: Monday, October 26, 2015; 1:10 – 2:50 PM; Thurgood Marshall S/W

1:10 PM – Graduate Student Finalist

B-I-1: Understanding and Improving the Chemistry of Lead Chalcogenide Quantum Dots for Photovoltaics

[CASP] Ashley R. Marshall[1,2], Arthur J. Nozik[2], Matthew C. Beard[1], Joseph M. Luther[1]
[1]National Renewable Energy Laboratory; [2]Dept. Chemistry and Biochemistry, University of Colorado

We are exploring the surface and defect chemistry of lead sulfide (PbS) and lead selenide (PbSe) quantum dots (QDs) to more effectively utilize multiple exciton generation (MEG) for next generation solar cells. Synthetic routes to PbS or PbSe QDs formerly involved PbO as a precursor, however new findings suggest that lead halide precursors produce "better" QDs. Diffusion-based syntheses *and* cation exchange syntheses using Pb-halides produce QDs with improved carrier transport, improved MEG efficiency, and better air stability due to halide incorporation from the precursor. Thus, understanding the role that the synthetic route plays in the photophysical properties of QD films is of timely interest.

To transition isolated, soluble QDs into a macroscopic semiconducting film (a "QD solid") for photovoltaic (PV) devices, for example, a solid-state surface ligand exchange replaces insulating long chain ligands with short molecular ligands and brings the QDs in close proximity for electronic transport. However, the treatment scheme can also add or exchange atoms on the surface or reassemble the surface configuration. Using these tools to control the surface, we are able to improve the photoluminescence characteristics and device performance of QD solids.

Photoluminescence (PL) studies on QDs synthesized from PbO have shown that temperature dependent PL quenching is a metric of the defect properties in a QD solid; PL is strong at low temperatures, but quenches as the film heats, due to free carriers moving to defect sites and recombining nonradiatively. Using halide syntheses, PbS QD solids show bimolecular, radiative recombination at room temperature (inset of Figure 1B). Persistent PL at room temperature suggests that these QDs have fewer trap states and can produce higher open circuit voltage in PV devices.

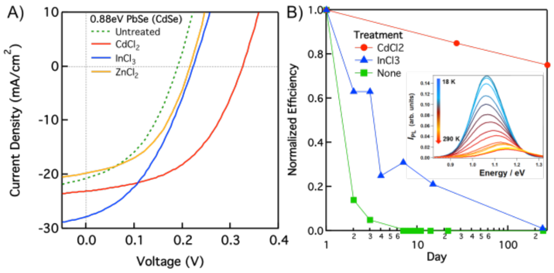


Figure 2: (A) *J-V* curves for PbSe QD solar cells with a selection of metal chloride treatments. (B) Plot of normalized efficiency over time; the CdCl2 treatment gives over 270 days of stability stored in air. Inset: temperature dependent PL for a PbS QD solid.

PV devices with remarkable efficiency were fabricated with these halide-synthesized PbS and PbSe QDs and show increased open circuit voltage (*Voc*). Furthermore these air-stable QDs give record efficiency devices (fabricated/stored in air) and were used for the first certified PbSe QD PV device. We explored how the uptake of metal chloride species into QD films influences device performance parameters (Figure 1A). We are able to tune either the short circuit current (J_{sc}) or V_{OC} in the device by choice of metal cation and devices treated with $CdCl_2$ show excellent resistance to degradation (Figure 1B).

While speculations on the surface of lead chalcogenide QDs is central to many of the papers proposing new ligands and treatments for QDs, very little work has been done to elucidate the chemistry at the QD surface. Using a combination of analytic and organic chemistry techniques, we probe the surface and composition of the QDs. We compare the QDs as a function of the synthesis route to determine why the new QDs show better properties. We also study the native ligands and ligand exchange processes using NMR, FTIR, and elemental analysis. Using all of these techniques in conjunction enables a comprehensive picture of the QD and the surface chemistry involved in making QD solids for optoelectronic devices.

1:30 PM

B-I-2: EXCITON FISSION AND FUSION

[CE] Dan Congreve, Mengfei Wu, Mark Wilson, Troy Van Voorhis, Moungi Bawendi, Vladimir Bulović, Marc Baldo
Center for Excitonics, Massachusetts Institute of Technology

Singlet exciton fission is the process in which a molecular excited state spontaneously splits into two 'child' excitons. In theory, singlet fission materials such as tetracene or rubrene could be integrated with silicon cells to double the photocurrent from high-energy solar photons ($\boxed{<}$550 nm), ultimately boosting the efficiency of the silicon cell to 30% or more. The outstanding challenge is how to get the energy from the triplet excitons (energy ~ 1.1eV) from tetracene into silicon (bandgap 1.1eV). We report direct excitonic energy transfer from 'dark' triplets in the organic semiconductor tetracene to colloidal PbS nanocrystals, thereby successfully harnessing molecular triplet excitons in the near infrared. Steady-state excitation spectra, supported by transient photoluminescence studies, demonstrate that the transfer efficiency is at least (90±13)%. The mechanism is a Dexter hopping process consisting of the simultaneous exchange of two electrons. Triplet exciton transfer to nanocrystals is expected to be broadly applicable in solar and near infrared light-emitting applications, where effective molecular phosphors are presently lacking. We conclude by also describing recent work on using colloidal PbS nanocrystals to sensitize the reverse process of exciton fusion, which may find application for harnessing infrared light in solar cells.

1:50 PM

B-I-3: IMPROVING THE UNDERSTANDING OF QUANTUM DOT SOLAR CELLS BY MODIFYING THE CHEMISTRY OF PBS AND PBSE QUANTUM DOTS

[CASP] Joseph M. Luther[1], Ashley R. Marshall[1,2], Ryan W. Crisp[1,3], Elisa M. Miller[1], Rachelle Ihly[4], Matt Law[4], Jianbing Zhang[1], Sungwoo Kim[1], Matthew C. Beard[1]
[1] National Renewable Energy Laboratory; [2] Department of Chemistry and Biochemistry, University of Colorado; [3] Department of Physics, Colorado School of Mines; [4] Departments of Chemistry and Chemical Engineering and Materials Science, University of California, Irvine

Although lead chalcogenide quantum dot solar cells (QDSCs) have achieved power conversion efficiencies of 10%, there is substantial room for improvement. Due to carrier transport limitations and very large V_{oc} deficits, the best devices are based on PbS QDs with band gaps >1.3 eV, and use films thicknesses <300 nm, well below that needed for complete absorption of sunlight. Moreover, as one of the most promising absorbers that can be readily tuned into the mid-infrared, a major interest for lead chalcogenides (especially PbSe and PbTe) lies in using QDs with band gaps <1.0 eV for multiple exciton generation or tandem solar cell applications. Recently, in CASP, we have investigated and modified the chemistry of PbSe QDs as a step toward addressing these issues, as well as toward enhancing QD stability. To date, we have developed PbSe QDs with photoluminescence efficiencies stable for *ca.* one year. We have also intensively studied QD surface passivation by halide ions, which we found to: 1) greatly enhance

transport such that cells are now optimized at 500-600 nm thicknesses; 2) substantially reduce the V_{oc} deficit for low-bandgap QDSCs; and 3) control the energy state positions of the QD films, greatly improving device stability and potentially enabling advanced device design. Finally, we will present and discuss cross-sectional potential measurements, which allow direct visualization of the fields within the device stack, leading to a deeper understanding of the current generation of QDSCs, and producing insights that can lead to further improvements.

2:10 PM

B-I-4: ELECTRON RATCHETS

[CBES] Bryan Lau[1], Ofer Kedem[1], Mario Tagliazucchi[2], Igal Szleifer[2], Mark Ratner[1], Emily Weiss[1]
[1]Department of Chemistry, Northwestern University; [2]Department of Biomedical Engineering, Northwestern University

This talk describes the design and fabrication of electron ratchets. The performance of third-generation "excitonic" solar energy conversion devices comprising solution-processable materials such as molecules, polymers, or nanoparticles is limited by random diffusion of electrons or weakly biased drift currents and an associated poor yield of charge collection. In these third-generation solar cells, energy from thermalization of electrons from above-band-edge excitations is lost as heat. We aim to transform random diffusive motion of electrons, powered by light and thermal energy, into vectorial charge transport through a phenomenon called "ratcheting". A ratchet is a non-equilibrium construct that induces unidirectional movement in otherwise randomly moving particles (classical or quantum) by continuously switching between a state that causes an asymmetric relaxation of the particle, and a state that allows random, uniform diffusion of the particle. The periodic modulation of the potential surface drives the system away from equilibrium. Additionally, a ratcheting potential surface must not be symmetric under inversion in the direction of transport. Classical Brownian ratchets are theoretically well-studied systems that are prominent in biology, where they convert chemical to mechanical energy. For example, linear motor proteins are ratchets responsible for muscle contraction, and ATP synthase is a rotary motor that enables ATP synthesis and hydrolysis. We use these motors as inspiration to design quantum ratchets, where the switching of the potential surface produces a net electrical current despite a zero source-drain bias and exerting a zero time-averaged force on the charge carriers.

2:30 PM

B-I-5: EXCITON DYNAMICS IN HYBRID 0D/2D SYSTEMS

[CE] Aaron J. Goodman, [1] Ferry Prins, [1] William A. Tisdale[1]
[1] Center for Excitonics, Massachusetts Institute of Technology

Hybrid structures that combine the superior charge carrier mobility of 2D transition metal dichalcogenides (TMDCs) and the remarkable absorption and emission properties of quantum dots (QDs) offer a tantalizing materials system for engineers designing novel optoelectronic devices. Both atomically-thin TMDCS and QDs support emissive excitons. When closely spaced, these excitonic states can interact on ultrafast time scales. Beyond potential device applications, studies have revealed interesting physics such as anomalous thickness dependence and low-dimensional dielectric screening phenomena in MoS_2 (Prins, Goodman, Tisdale; ***Nano Letters*** 14, 6087 [2014]). Here we report the use time-resolved photoluminescence and ultrafast second harmonic generation (SHG) spectroscopy performed in a microscope to monitor excitonic interactions in a model 0D/2D hybrid system featuring CdSe QDs and mono- and few-layer MoS_2.

SESSION II: MONDAY, OCTOBER 26, 2015; 3:20 – 5:00 PM; THURGOOD MARSHALL S/W

3:20 PM

B-II-1: LUMINESCENT SOLAR CONCENTRATORS USING ENGINEERED QUANTUM DOTS

[CASP] Thomas A. Baker[1], Kirill A. Velizhanin[2], Jaehoon Lim[1], Hunter McDaniel[1,3], Jeffrey M. Pietryga[1], Victor I. Klimov[1]
[1] *Chemistry Division, Los Alamos National Laboratory;* [2] *Theory Division, Los Alamos National Laboratory*
[3] *UbiQD, LLC*

Luminescent solar concentrators (LSCs) could become an important element of future net zero-energy-consumption buildings as semitransparent photovoltaic (PV) windows. Colloidal quantum dots (QDs) are promising materials for LSCs, as in addition to a tunable emission wavelength they can be engineered to provide a large spectral shift between the emission band and the onset of strong optical absorption, which can be interpreted in terms of a large "engineered" Stokes shift. This is important for suppressing re-absorption losses in large-area devices. We explore two different QD systems in this context. The first is based on II-VI core/shell heterostructures in which the absorption and emission functions are separated between a wider-gap shell and a narrower-gap core, leading to a large effective Stokes shift [1]. The second system, ternary I-III-VI_2 semiconductors ($CuInE_2$, where E = S or Se or their mixture), provides a heavy-metal-free alternative to Cd-based QDs [2]. In these materials, a large Stokes shift results from the involvement of an intra-gap hole state in the emission process. By incorporating these two types of QDs into polymeric matrices, we obtain freestanding, scattering-free slabs with negligible reabsorption losses over distances of a few tens of centimeters. Measurements under simulated solar illumination indicate high light-collection efficiencies of more than 3% with semi-transparent devices that transmit 80 to 90% of incident radiation. These studies demonstrate the large promise of engineered QDs for PV-window applications.

[1] Meinardi, F., *et al.*, *Nat. Photon.* **8**, 392 (2014).
[2] Meinardi, F., *et al.*, *Nat. Nano*. **10**, (*advanced online publication*).

3:40 PM

B-II-2: ARCHITECTING INFRARED ABSORPTION AND EMISSION – CONTROL OF BOTH AMPLITUDE AND PHASE

[LMI] Harry A. Atwater[1], Michelle Sherrott[1], Victor Brar[1], Howard Lee[1], Yao-Wei Huang[1], Ruzan Sokhoyan[1], Georgia Papadakis[1], Krishnan Thyagarajan[1]
[1]*California Institute of Technology*

Progress in understanding resonant subwavelength structures has fueled an explosion of interest in fundamental processes and nanophotonic devices. At infrared wavelengths, tailoring the photonic dispersion yields new approaches to energy conversion and tunable radiative emission. We will discuss electronic control of blackbody emission frequency and intensity in graphene metasurfaces and also describe designs for metasurfaces based on patch antenna arrays that allow general control of the reflection and scattering amplitude and phase distributions.

4:00 PM

B-II-3: NANOPHOTONICS IN MATERIAL-SYSTEMS OF LARGE SIZES

[S^3TEC] Marin Soljacic[1], Yichen Shen[1], Veronika Stelmakh[1], Veronika Rinnerbauer[1], Bo Zhen[1], Ling Lu[1], Chia Wei Hsu[1], John Joannopoulos[1], Evelyn N. Wang[1], Ivan Celanovic[1]
[1]Massachusetts Institute of Technology

Nanophotonics provides superb opportunities for tailoring the flow of light. This way, many novel physical phenomena can be enabled, as well as many important functionalities for novel energy applications (e.g. energy conversion, lighting). In order to make these phenomena useful for large systems, large-area nano-fabrication techniques have to be successfully implemented. In this talk, I will present some of our recent theoretical and experimental progress in exploring these opportunities

4:20 PM

B-II-4: OPTICAL MATERIALS AND ARCHITECTURES FOR ULTRAHIGH-EFFICIENCY PHOTOVOLTAICS

[LMI] Ralph G. Nuzzo[1,2], John A. Rogers[1], Yuan Yao[1], Junwen He[1], Lu Xu[1], Mikayla Anderson[1]
[1]University of Illinois at Urbana-Champaign, [2]California Institute of Technology

The production of integrated electronic circuits provides examples of the most advanced fabrication and assembly approaches that are generally characterized by large-scale integration of high-performance compact semiconductor elements that rely on rigid and essentially planar form factors. New methods of fabricating semiconductor devices provide a set of enabling means to lift these constraints by engendering approaches to device configurations that would be impossible to realize with bulk, wafer-scale materials while retaining capacities for high (or altogether new forms of) electronic and/or optoelectronic performance. An exemplary case of interest in our work includes large-area integrated electro-optical systems for photovoltaic energy conversion that can provide a potentially transformational approach to supplant current technologies with high performance, low cost alternatives. The current talk will highlight progress made in the collaborative research efforts of the LMI EFRC that illustrates important opportunities for exploiting advances in advanced optical and electronic materials in synergy with physical means of patterning, fabrication, and assembly to advance capabilities for photovoltaic energy conversion. Of particular interest are the materials, and new understandings of science, that will allow a full and facile utilization of the full solar resource.

4:40 PM

B-II-5: ENERGY HARVESTING USING RANDOM ASSEMBLIES OF CHROMOPHORES

[PARC] Andrew P. Shreve[1], Nesia A. Zurek[1], Peter G. Adams[2], Aaron M. Collins[2], Tuba Sahin[3], Vijaya Subramanian[1], Volker S. Urban[4], Pothiappan Vairaprakash[4], Michelle A. Harris[5], Dariusz M. Niedzwiedzki[5], Deborah G. Evans[1], Gabriel A. Montaño[2], David F. Bocian[6], Dewey Holten[5], Jonathan S. Lindsey[3]

[1]Center for Biomedical Engineering and Department of Chemical and Biological Engineering, University of New Mexico; [2]Center for Integrated Nanotechnologies, Los Alamos National Laboratory ; [3]Department of Chemistry, North Carolina State University; [4]Biology and Soft Matter Division, Oak Ridge National Laboratory; [5]Department of Chemistry, Washington University, St. Louis; [6]Department of Chemistry, University of California, Riverside

We demonstrate high energy transfer efficiencies achieved by incorporating chromophores into modular assemblies of amphiphilic polymers and molecules. An integrated approach that brings together steady-state and time-resolved spectroscopic studies, structural characterization, and theoretical modeling of energy transfer between randomly distributed chromophores provides insight into the performance of these systems. Overall, we find that a high degree of predictability is possible, so that the design of systems with energy harvesting performance across wide spectral ranges is straightforward. This approach to producing light-harvesting materials has many attractive features, including ease of preparation, scalability, tunable performance, simple adaptation to surfaces, straightforward integration of biological and non-biological components, and quantitatively predictable performance. Systems investigated include chromophores distributed in lipid bilayer systems and chromophores distributed in polymer micelle systems, and each of these constructs is shown to produce excellent light-harvesting efficiency across broad wavelength ranges.

SESSION III: TUESDAY, OCTOBER 27, 2015; 8:30 – 10:10 AM; THURGOOD MARSHALL S/W

8:30 AM

B-III-1: WATER-OXIDATION CATALYSTS FOR SOLAR FUEL PRODUCTION

[ANSER] Gary W. Brudvig[1], Stafford W. Sheehan[1], Julianne M. Thomsen[1], Benjamin Rudshteyn[1], Ke R. Yang[1], David M. Tiede[2], Robert H. Crabtree[1], Victor S. Batista[1]

[1] Department of Chemistry, Yale University; [2] Chemical Sciences and Engineering Division, Argonne National Laboratory

Molecular catalysts are known for their high activity and tunability, but their solubility and limited stability often restrict their use in practical applications. We have characterized a molecular iridium catalyst for water oxidation that binds directly and robustly to oxide surfaces without the need for any external stimulus or additional linking groups. On conductive electrode surfaces, this heterogenized molecular catalyst oxidizes water with low overpotential, high turnover frequency, and minimal degradation. Spectroscopic and electrochemical studies show that it does not decompose into iridium oxide, thus preserving its molecular identity, and that it is capable of sustaining high activity toward water oxidation with stability comparable to state-of-the-art bulk metal oxide catalysts.

8:50 AM

B-III-2: TO THE MOLECULAR DYNAMICS AT THE CATHODE/ELECTROLYTE INTERFACE OF ELECTROCATALYST MATERIALS FOR CO_2 REDUCTION IN THE PRESENCE OF IMIDAZOLIUM BASED IONIC LIQUIDS

[FIRST] John L. Dimeglio[1], Jonnathan Medina-Ramos[2], David Mullins[3], Robert Sacci[3], Raymond Unocic[3], Daniel Lutterman[3], Sheng Dai[3], Matthew Neurock[4], Joel Rosenthal[1]
[1]University of Delaware, [2]Argonne National Laboratory, [3]Oak Ridge National Laboratory, [4]University of Minnesota

The electrochemical reduction of CO_2 to CO generates an energy rich commodity chemical that can be coupled to liquid fuel production. The limited number of affordable platforms that can efficiently promote this transformation spur our efforts to understand how catalyst systems that promote CO evolution function. To this end, we have undertaken a multipronged study aimed at understanding how post-transition metal derived cathode materials promote the electrocatalytic conversion of CO_2 to CO in the presence of weakly acidic room temperature ionic liquids (RTILs). A major focus of this work has centered on elucidation of the molecular design principles that are attendant to the energy efficient activation of CO_2. A combination of spectroscopic, electroanalytical and computational methods has been used to interrogate the dynamics between electrocatalyst, RTIL and CO_2 at the cathode/electrolyte interface. These experiments have provided insight into the pathway by which these catalyst systems activate CO_2 and have revealed the primary factors that drive fuel generation at the cathode/electrolyte interface. Implications for the future development of systems and electrolytes that can efficiently promote CO_2 reduction with high selectivity and efficiency will be discussed.

9:10 AM – Graduate Student Finalist

B-III-3: Incorporation of Perylene-3,4-dicarboximides into Photoanodes and Photocathodes for Solar Fuels

[ANSER] Rebecca J. Lindquist[1], Marek B. Majewski[1], Julianne M. Thomsen[2], William L. Hoffeditz[1], Brian T. Phelan[1], Kelly L. Materna[2], Joseph T. Hupp[1], Gary W. Brudvig[2], Michael R. Wasielewski[1]
[1] Department of Chemistry, Northwestern University; [2] Department of Chemistry, Yale University

The rational design of efficient photoelectrochemical cells (PECs) for the production of fuels using solar energy will require an understanding of the catalytic mechanisms and rate-limiting steps of photodriven water oxidation and fuel-forming reactions. Perylene-3,4-dicarboximide (PMI) chromophores are promising candidates for incorporation into PECs and for the mechanistic investigation of these processes by ultrafast spectroscopic techniques due to their synthetic tunability, strong absorptivity in the midvisible spectral region, and distinctive spectral features. We have previously used femtosecond to millisecond transient absorption spectroscopies to identify a PMI derivative capable of injecting electrons into nanostructured TiO_2 films and oxidizing a covalently attached homogeneous water oxidation catalyst (WOC) precursor $Cp^*Ir^{III}(ppy)Cl$, where ppy = 2-phenylpyridine,[1,2] following photoexcitation.[3] We now incorporate PMI into several photoelectrodes for the photodriven oxidation and reduction of solar fuels catalysts. The TiO_2-based photoanodes contain a coadsorbed WOC $[(Ir^{IV}(pyalc)(H_2O)R)_2(\mu\text{-}O)]^{+2}$, where pyalc = 2-(2′pyridyl)-2-propanolate,[4] or a heterogeneous cobalt oxide (Co-Pi) WOC.[5] Photocathodes include molecular $[Ni(P^2N^2)_2]^{2+}$-based proton reduction catalysts[6] on nanostructured NiO. Atomic layer deposition of Al_2O_3 following chromophore adsorption[7] was employed to improve the chemical stability of the chromophores and to prevent rapid electron-hole recombination. Photoelectrochemical experiments and ultrafast optical spectroscopies were used to probe the photocatalytic activities and photodriven electron transfer events of the photoelectrodes.

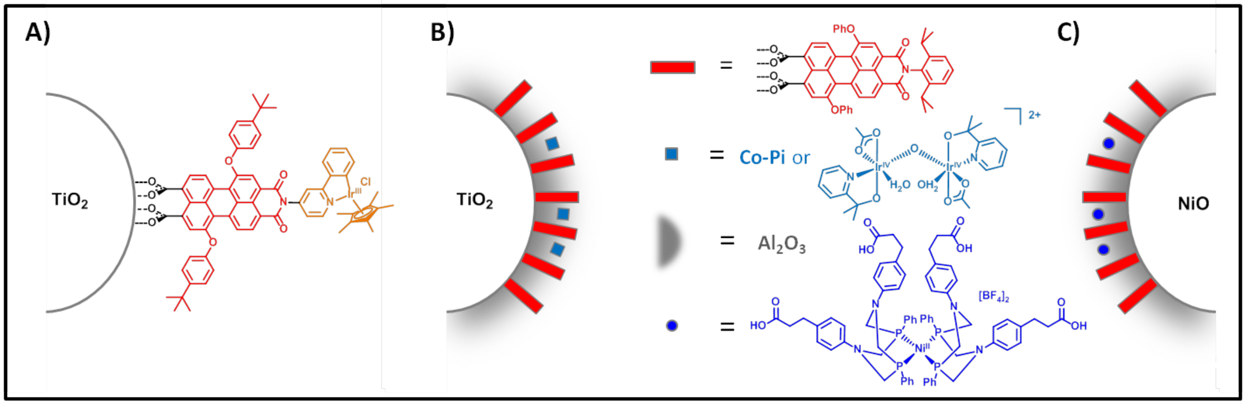


Fig.1 – Designs of model TiO_2/PMI-Cp*Ir^{III}(ppy)Cl (**A**) and TiO_2/PMI/Al_2O_3/Co-Pi or $[(Ir^{IV}(pyalc)(H_2O)R)_2(\mu\text{-}O)]^{+2}$ (**B**) photoanodes and NiO/PMI/Al_2O_3/$[Ni(P^2N^2)_2]^{2+}$ photocathodes (**C**).

[1] J. D. Blakemore, G. W. Brudvig, R. H. Crabtree, *et al. J. Am. Chem. Soc.* **132**, 16017-16029 (2010).
[2] M. T. Vagnini, L. X. Chen, M. R. Wasielewski, *et al. Chem. Sci.* **4**, 3863-3873 (2013). [3] R. J. Lindquist, B. T. Phelan, J. R. Durrant, M. R. Wasielewski, *et al. Submitted.* [4] S. W. Sheehan, J. M. Thomsen, R. H. Crabtree, G. W. Brudvig, C. A. Schmuttenmaer, *et al. Nat. Commun.* **6**, 6469 (2015). [5] M. W. Kanan, D. G. Nocera, *Science* **321**, 1072-1075 (2008). [6] U. J. Kilgore, R. M. Bullock, D. L. DuBois, *et al. J. Am. Chem. Soc.* **133**, 5861-5872 (2011). [7] H.-J. Son, O. K. Farha, J. T. Hupp, *J. Am. Chem. Soc.* **135**, 11529-11532 (2013).

9:30 AM

B-III-4: DESIGN OF MULTIFUNCTIONAL TWO-DIMENSIONAL MATERIALS: TOWARD IDEAL PHOTOCATALYSTS FOR SOLAR WATER SPLITTING

[CCDM] Linyou Cao[1], Guoqing Li[1], Du Zhang[2], Weitao Yang2[2] Qiao Qiao[3], Yimei Zhu[3], Ian G. McKendry[4], Akila C. Thenuwara[4], Michael Zdilla[4], Daniel R. Strongin[4]
[1]MSE, NC State U., [2]Chemistry, Duke U., [3] BNL, [4]Chemistry, Temple U.

The overarching goal of this effort is to explore synergistic efforts on both experimental and theoretical grounds to rationally design multifunctional two-dimensional (2D) transition metal dichalcogenide (TMDC) and transition metal oxide (TMO) materials as ideal photocatalysts for solar-driven water splitting. Solar-driven water splitting is considered as the ultimate solution for the current grand challenge of energy and environment. But its implementation has been delayed by the lack of ideal photocatalysts. Our recent studies on the catalytic activities, light absorption, and exciton dynamics of the 2D materials have indicated that multifunctional 2D TMDC and TMO materials have the potential to make low-cost and high-performance photocatalysts. We have discovered that sulfur vacancies of MoS_2 may be catalytic active sites for the hydrogen evolution reaction (HER), and continuous monolayer MoS_2 films with no edge sites can be made to show excellent catalytic activities (20mA/cm^2 at -0.2 V vs. RHE) and stability (> 10000 cycles) by proper defect engineering. This is in stark contrast with the conventional wisdom, which believes only the edge sites of MoS_2 may be catalytically active for the HER. Besides HER catalysts, we have also developed highly efficient catalysts for the oxygen evolution reaction (OER) by engineering the structures and composition of layered TMDC and TMO materials. Additionally, we have made significant progress in the studies of exciton dynamics and solar light superabsorption of 2D materials. With all the new fundamental understanding, we are now proceeding to designing prototype 2D materials photocatalysts for low-cost high-performance solar-driven water splitting.

9:50 AM

B-III-5: DYE-SENSITIZED WATER OXIDATION IN PHOTOELECTROSYNTHESIS CELLS

[UNC] Ke Hu, Leila Alibabaei, M. Kyle Brennaman, Gerald J. Meyer
Department of Chemistry, University of North Carolina at Chapel Hill

The University of North Carolina at Chapel Hill Energy Frontier Research Center (UNC) for Solar Fuels has demonstrated light driven water oxidation with molecular dyes and catalysts in what have been termed Dye-Sensitized Photoelectrosynthesis Cells (DSPECs). Photoelectrochemical measurements coupled with O_2 gas quantification have enabled the solar conversion efficiencies to be calculated. These results show that single photon absorption events can be coupled to multi-electron transfer water oxidation catalysis at a sensitized mesoporous thin film electrode with a core/shell structure. Efficient water oxidation to yield $O_2(g)$ in DSPECs requires that four photons be absorbed and that the catalyst be oxidized four times without competitive recombination of the injected electrons with the oxidized dye or catalyst. Catalyst oxidation also involves proton transfer reactivity. The yields and dynamics of the first two oxidations have been quantified and were shown to occur quantitatively. The data implicate recombination of injected electrons with catalysts present as metal oxo species as the dominant loss pathway in DSPECs.

SESSION IV: TUESDAY, OCTOBER 27, 2015; 10:40 – 12:00 PM; THURGOOD MARSHALL S/W

10:40 AM

B-IV-1: LEAD FREE INORGANIC-ORGANIC HYBRID PEROVSKITES: CHEMISTRY AND SOLAR CELLS

[ANSER] Feng Hao[1], Duyen H. Cao[1], Constantinos C. Stoumpos[1], Byunghong Lee[2], Joseph T. Hupp[1], Chan Myae Myae Soe[2], Michael. R. Wasielewski[1], Tobin J. Marks [1], Robert P. H. Chang[2], Mercouri G. Kanatzidis[1]
[1] Dept. Chemistry, Northwestern University; [2] Dept. Materials Science and Engineering, Northwestern University; [3] Chemical Sciences and Engineering Division, Argonne National Laboratory

This collaborative effort within our ANSER Center focuses on fundamental studies on perovskite based interfaces and solar cells as well as the development of lead free materials. The perovskites afford several important features including excellent optical properties that are tunable by controlling the chemical compositions, ambipolar charge transport, and long electron and hole diffusion lengths. We will present our results in devising effective ways and solution-based methods to process lead and tin based perovskites into layers deposited over other materials such as electron or acceptor layers. The solution processing of perovskites for solar cells is a challenge. The deposition of continuous and homogeneous films in a multilayer system, which contains other layers below and above is a huge issue that needs to be understood and tackled. This is because electron transport happens across the diverse interfaces of the layers. We are tackling important questions such as what electron donor structural and organizational features in a solar cell maximize light capture and energy harvesting with minimal geminate recombination? Which perovskite material and film processing strategies enhance these characteristics? Solar cells based on $MeNH_3PbI_3$ perovskites have progressed significantly and reached power conversion efficiencies of ~20%, approaching the efficiency of commercialized c-Si solar cells. Because of the toxicity of Pb however the search is on for lead free alternatives. In this talk we will report on the chemistry of tin-based perovskite compounds their chemical and physical properties as well as phase transitions. The challenges for controlling the carrier concentrations, chemical stability and various interfaces between different materials and several promising and exciting directions will be presented.

11:00 AM

B-IV-2: PEROVSKITE INSPIRED SEARCH FOR NEW PV MATERIALS

[CNGMD] Riley Brandt[1], Vladan Stevanović[2,3], Tonio Buonassisi[1], Robert Hoye[1], Rachel Kurchin[1], Prashun Gorai[2], John Perkins[3], David Ginley[3], William Tumas[3]
[1]Massachusetts Institute of Technology, [2]Colorado School of Mines, [3]National Renewable Energy Laboratory

The recent success of methylammonium lead halide perovskites suggests that the existing approach for identifying promising semiconductors for PV absorbers, using the band gap value and strength of absorption, may be inadequate. PV materials search must also consider the minority carrier lifetime and mobility, but these remain difficult to assess both from theory and experiment. However, we can consider potential electronic structure criteria that could lead to high lifetimes in the presence of defects. We propose that this "defect-tolerance" may be enabled by the electronic structure properties such as a high dielectric constant, disperse band edges due to spin-orbit interactions, and antibonding character to the valence band maximum. Motivated by the success of lead halide perovskites that satisfy these criteria, we identify several classes of semiconductors that include partially-oxidized *p*-block cations, and which share a similar electronic structure to the lead halide perovskites. These are identified through a broad search of the MaterialsProject.org database based on the developed design rules. We then experimentally screen materials informed by the first principles calculations, starting with bismuth triiodide (BiI_3) and methylammonium bismuth iodide ($MA_3Bi_2I_9$). First, we optimize the growth and verify the phase, purity, and morphology of the desired semiconductor; second, we use minority carrier lifetime as the response variable to evaluate each candidate semiconductor. In doing so, we combine more targeted computational screening with subsequent experimental screening to leverage the best of both approaches. We discuss the challenges identified in exploring the first few materials, and how this informs our future search.

11:20 AM

B-IV-3: INTERFACE SCIENCE OF SOFT MATERIAL SOLAR CELLS

[ANSER] Brett Savoie[1], Nanjia Zhou[1], Xugang Guo[1], Antonio Facchetti[2], Li Zheng[1], Eric Manley[1], Sylvia Lou[1], Patrick Hartnett[1], Kyle Luck[1], Nicholas Eastman[1], Alex Dudnik[1], Stephen Loser[1], Charles Song[1], Nicholas Jackson[1], Lin X. Chen[1], Mark Ratner[1], Michael Bedzyk[3], Mark Hersam[3], Robert P. H. Chang[3], Michael R. Wasielewski[1], Tobin Marks[1]
[1] Department of Chemistry, Northwestern University; [2] Polyera Corporation; [3] Department of Materials Science and Engineering, Northwestern University

The ability to fabricate molecularly tailored interfaces with nanoscale precision offers means to selectively modulate charge transport, molecular assembly, and exciton dynamics at hard matter-soft matter and soft-soft matter interfaces. Such interfaces can facilitate transport of the "correct charges" while blocking transport of the "incorrect charges" at the electrode-active layer interfaces of organic photovoltaic cells. This interfacial tailoring can also suppress carrier-trapping defect densities at interfaces and stabilize them with respect to physical/thermal de-cohesion. For soft matter-soft matter interfaces, interfacial tailoring can also facilitate exciton

scission and photocurrent generation in such cells. In this lecture, challenges and opportunities in organic photovoltaic interface science are illustrated for four specific and interrelated areas of research: 1) controlling charge transport across hard matter(electrode)-soft matter interfaces in organic photovoltaic cells, 2) controlling charge transport by specific active layer nano/microstructural organization in the bulk active material and at the electrodes, 3) controlling exciton dynamics and carrier generation at donor-acceptor interfaces in the active layer, 4) designing transparent conducting electrodes with improved properties. It will be seen that such rational interface engineering along with improved bulk-heterojunction polymer structures guided by theoretical/computational analysis affords exceptional fill factors, solar power conversion efficiencies as high as 10%, and enhanced cell durability.

11:40 AM

B-IV-4: MATERIALS FOR SOLAR ENERGY CONVERSION USING EXTREME CONDITIONS: AN OVERVIEW

[EFree] Timothy A. Strobel[1], Haidong Zhang[1], Anne M. Davis[1], Venkata Bhadram[1], Lakshmi Krishna[2]
[1] Geophysical Laboratory, Carnegie Institution of Washington; [2] Department of Physics, Colorado School of Mines

Novel materials are required in order to make both fundamental and applied advances in a vast range of areas. While traditional materials synthesis relies on thermochemical methodologies, i.e., using temperature to overcome activation energy barriers and stimulate chemical bond rearrangement at ambient pressure, synthesis methods utilizing extreme conditions of pressure show promise to create novel materials with superlative properties and give access to an entirely new materials space. We provide an overview of how high pressure (one thousand to one million times atmospheric pressure) is used to create new solar materials and provide insights into novel phenomena within EFree. We present results on the synthesis of a new, low-density allotrope of silicon, Si_{24}, formed by thermal "degassing" of sodium from a Na_4Si_{24} precursor that was formed at high pressure. Si_{24} contains atom-sized channels along the crystallographic a-axis that are formed from six- and eight-membered sp^3 silicon rings, which facilitates the sodium removal when the material is subjected to thermal degassing. X-ray diffraction and energy-dispersive spectroscopy confirm the high purity of this new phase. Si_{24} is mechanically stable at ambient pressure and is energetically more favorable than known metastable silicon allotropes. Density functional and quasiparticle calculations give a direct band gap of 1.34 eV and an indirect gap of 1.30 eV, and are corroborated by electrical resistivity and optical absorption measurements. The quasidirect band gap near 1.3 eV is close to the theoretically suggested optimal value for solar energy conversion, and provides improved visible light absorption properties compared with diamond-structured silicon.

SESSION V: TUESDAY, OCTOBER 27, 2015; 1:30 – 3:10 PM; THURGOOD MARSHALL S/W

1:30 PM

B-V-1: MODELING OF THE ELECTRONIC STRUCTURE OF SEMICONDUCTOR NANOCRYSTALS, AND CARRIER TRANSPORT IN NANOCRYSTAL ARRAYS

[CASP] Andrew Shabaev[1], Cherie Kagan[2], Barbara K. Hughes[3,4], Giulia Galli[5], Kirill A. Velizhanin[6], Joseph M. Luther[4], Matthew C. Beard[4], Alexander L. Efros[1,7]
[1] Department of Computational and Data Sciences, George Mason University; [2] Departments of Chemistry, Electrical and Systems Engineering, and Materials Science and Engineering, University of Pennsylvania; [3] Department of Chemistry and Biochemistry, University of Colorado; [4] National Renewable

Energy Laborator; [5] Institute for Molecular Engineering, University of Chicago; [6] Theory Division, Los Alamos National Laboratory; [7] Naval Research Laboratory

Design of nanocrystal (NC) solar cells requires a detailed understanding of the electronic structure and processes of single NCs and coupled NC arrays. CASP applies a range of complementary theoretical and computational methods to provide key insights in these areas at multiple scales. For instance, we have developed a computational platform to analyze the electronic structure of arbitrary-shaped and heterostructured NCs based on Wannier-like spatially localized wavefunctions. To better understand surface structure and electronic states of quantum dots toward optimizing charge extraction, we have applied ab-initio calculations with a focus on interfaces with ligands. Finally, to approach the device-relevant mesoscale, we have developed a theory of dark and photo-conductivity in arrays of NCs[1], which will be the main focus of this talk. We suggest a new mechanism of photoconductivity in an ensemble of charged NCs based on a large difference in mobility between quasi-localized and quasi-free carriers. Through Auger ionization, optical excitation of a charged NC boosts an electron into the quasi-free state, resulting in a large increase of mobility consistent with available experimental data.[2,3] We will conclude by examining how electron band width and carrier mobility can be increased in arrays of NCs fused into each other to form so-called “dimers.”[4]

[1] Shabaev, A.; Efros, Al. L.; Efros, A. L., *Nano Lett.* **13**, 5454 (2013).
[2] Choi, J.-H., *et al., Nano Lett.* **12**, 2631 (2012).
[3] Turk, M. E., *et al.*, *Nano Lett.* **14**, 5948 (2014).
[4] Hughes, B. K., *et al., J. Am Chem. Soc.* **136**, 4670 (2014).

1:50 PM

B-V-2: SYSTEMS AND ASSEMBLIES FOR APPLICATIONS IN DYE-SENSITIZED PHOTOELECTROSYNTHESIS CELLS

[UNC] Melissa K. Gish[1], Junlin Jiang[1], Alexander M. Lapides[1], Gyu Leem[2], Zachary A. Morseth[1], Animesh Nayak[1], Benjamin D. Sherman[1], Kyung-Ryang Wee[1], John R. Reynolds[3], Joseph L. Templeton[1], Kirk S. Schanze[2], John M. Papanikolas[1], Thomas J. Meyer[1]
[1]Department of Chemistry, University of North Carolina at Chapel Hill; [2]Department of Chemistry, Center for Macromolecular Science and Engineering, University of Florida: [3]School of Chemistry and Biochemistry, School of Materials Science and Engineering, Center for Organic Photonics and Electronics, Georgia Institute of Technology

The Dye-Sensitized Photoelectrosynthesis Cell (DSPEC) has been pioneered by the UNC EFRC. Inspired by natural photosynthesis, the goal of the UNC EFRC is to develop the concept of the DSPEC for applications in water splitting and reduction of CO_2 to reduced carbon fuels. The DSPEC functions as an artificial leaf utilizing molecular assemblies that both absorb light and catalyze water oxidation at an anode, or proton/CO_2 reduction at a cathode or photocathode, in tandem cell configurations. It integrates molecular light absorption and catalysis with the band gap properties of nanoparticle oxide semiconductors.

A key advantage of the DSPEC is the flexibility provided by the use of chemical synthesis to vary the light absorbing/reactivity/stability properties of the assembly. The challenges are understood: for example, for the **chromophore** in water splitting: maximized visible/near IR light absorption, excited state injection into oxide electrodes, an oxidized chromophore capable of driving water oxidation catalysis; for the **catalyst** sustained water oxidation catalysis at oxide interfaces on timescales rapid compared to the rate of solar insolation, 1-2 s^{-1}.

An extensive research effort has led to a variety of chemically linked chromophore-catalyst assemblies based on covalent bonding, oligoprolines, polymers, and electro-assembly formation with a covalently linked assembly providing the first example of a working DSPEC for solar water splitting. Recent extensions have been to porphyrin and organic dyes to cover more of the solar spectrum and to dyes and catalysts for photocathode applications.

2:10 PM

B-V-3: CHARGE TRANSPORT IN MESOSCALE ASSEMBLIES OF QUANTUM DOTS

[CASP] Matt Law[1], Cherie Kagan[2], Jason Tolentino[1], Daniel Straus[3], Andrew Fidler[4], Justin C. Johnson[5], Andrew Shabaev[6], Samuel Keene[1], Alexander L. Efros[6], Uwe Kortshagen[7], Matthew C. Beard[5], Victor I.Klimov[4]

[1] Departments of Chemistry and Chemical Engineering and Materials Science, University of California, Irvine: [2] Departments of Electrical and Systems Engineering, Materials Science and Engineering, and Chemistry, University of Pennsylvania; [3] Department of Chemistry, University of Pennsylvania; [4]Chemistry Division, Los Alamos National Laboratory; [5] National Renewable Energy Laboratory; [6]Department of Computational and Data Sciences, George Mason University; [7] Department of Mechanical Engineering, University of Minnesota

Colloidal semiconductor quantum dots (QDs) are attractive building blocks for next-generation solar photovoltaics (PV). In this talk, we describe recent progress by the Center for Advanced Solar Photophysics (CASP) in understanding, improving, and controlling charge transport within mesoscale assemblies of IV-VI and IV QDs, with the aim of achieving simultaneously efficient carrier multiplication (CM) and charge extraction to produce record-efficiency single-junction PV. We begin by discussing QD film fabrication, charge transport physics, insights from theory, and evidence that the carrier diffusion length is short and limited by electronic states in the QD band gap. Coordinated CASP studies of the mechanism and dynamics of charge transport using transistor, photoluminescence, ultrafast transient photocurrent, time-resolved microwave conductivity, and terahertz time-domain spectroscopies will be presented. We highlight achievements in improving carrier mobility by enhancing inter-dot electronic coupling, passivating surface states, and implementing surface doping to control the Fermi level. Engineering the inter-QD matrix to produce QD/inorganic or QD/organic nanocomposites is presented as a powerful way to optimize coupling, remove surface states, eliminate hysteretic charge trapping and ion motion, and achieve long-term environmental stability for high-performance, robust QD films that feature good CM efficiency. Prospects for overcoming the diffusion-limited recombination that seems to constrain diffusion length are discussed, as well as the possibility of band-like transport through extended electronic states and the status/importance of utilizing superlattice QD arrays for this purpose. CASP's ongoing work includes fabricating record-performance PV from the improved QD films, studying QD surface states, and evaluating transport in novel, more CM-efficient materials.

2:30 PM

B-V-4: ULTRAFAST DYNAMICS IN MOLECULAR ASSEMBLIES FOR SOLAR ENERGY CONVERSION

[UNC] Zachary A. Morseth[1], Gyu Leem[2], Egle Puodziukynaite[2], Junlin Jiang[2], Zhen Fang[1], Alexander T. Gilligan[1], John R. Reynolds[3], Kirk S. Schanze[2], John M. Papanikolas[1]

[1]Department of Chemistry, University of North Carolina at Chapel Hill; [2]Department of Chemistry, Center for Macromolecular Science and Engineering, University of Florida; [3]School of Chemistry and Biochemistry, School of Materials Science and Engineering, Center for Organic Photonics and Electronics, Georgia Institute of Technology

One of the great challenges in the development of light-driven solar fuels production is the coupling of molecular components that harvest visible light, separate charge, and transfer redox equivalents to drive catalytic water oxidation. Interfacial molecular assemblies offer one design approach for arranging chromophores and catalysts in close proximity. We have used a combination of time-resolved absorption and emission methods, on time scales ranging from femtoseconds to microseconds, to follow the excited state dynamics in molecular assemblies based on polymer scaffolds, both in solution and on TiO_2 electrodes. Competitive energy transfer and charge separation are observed in assemblies combining conjugated polymers with Ru(II) complexes. Ultrafast transient absorption studies across 9 decades of time of polymer assemblies anchored to TiO_2 show evidence of ultrafast electron injection in chromophores attached to the metal oxide, which is then followed by rapid transfer of the oxidative equivalent to the conjugated polymer. On longer time scales light-harvesting and energy transport from remote chromophore sites are also observed. We have combined spectroscopic observations with large-scale computer simulation to gain a detailed picture of the photoexcited dynamics.

2:50 PM

B-V-5: BIOHYBRID LIGHT-HARVESTING ARCHITECTURES-BLENDING CHEMISTRY AND BIOLOGY

[PARC] Jonathan S. Lindsey[1], Michelle A. Harris[2], Joseph W. Springer[2], Jianbing Jiang[1], Kanumuri Ramesh Reddy[1], Tuba Sahin[1],_Pothiappan Vairaprakash[1], M. Phani Pavan[1], Elisa Lubian[1], Michael Krayer[1], Masahiko Taniguchi[1], Jieying Jiao[3], Elizabeth C. Martin[4], Pu Qian[4], Dariusz M. Niedzwiedzki[5], Gregory M. Lee[6], Pamela S. Parkes-Loach[6], Paul A. Loach[6], Christine Kirmaier[2] , C. Neil Hunter[4], David F. Bocian[3], Dewey Holten[2]

[1]Department of Chemistry, North Carolina State University; [2]Department of Chemistry, Washington University, St. Louis; [3]Department of Chemistry, University of California, Riverside; [4]Department of Molecular Biology and Biotechnology, University of Sheffield, UK; [5]Photosynthetic Antenna Research Center, Washington University, St. Louis; [6]Department of Molecular Biosciences, Northwestern University

Biohybrid light-harvesting antennas are an emerging platform technology with versatile tailorability for solar-energy conversion. These systems combine the proven peptide scaffold unit utilized for light harvesting by purple photosynthetic bacteria with attached tunable bioconjugatable synthetic chromophores to extend solar coverage beyond that of the natural systems. The biohybrid LH1-type constructs are formed by a two-tier self-assembly process that produces cyclic oligomers in which the synthetic components are piggy-backed on the native-like scaffold. The key design features of such architectures are as follows: (1) complementarity of spectral features of synthetic (appended) and natural (integral) chromophores to achieve panchromatic absorption throughout the visible and into the near-infrared region, (2) as many synthetic chromophores as possible to provide a large density (optical cross-section) for absorption, and (3) appropriate energy levels to funnel the captured light energy in a directional and efficient manner to sites for chemical processing for fuels production or photocurrent generation. The approach is highly disciplinary and collaborative in combining organic synthesis, protein biochemistry, molecular biology, electron microscopy, infrared spectroscopy, and static/ time-resolved optical absorption/emission spectroscopies. The presentation will describe various strategies for the biohybrid light-harvesting assemblies that have been implemented and the outlook for future directions.

C. CONTROL AT THE LEVEL OF ELECTRONS

SESSION I: MONDAY, OCTOBER 26, 2015; 1:10 – 2:50 PM; LINCOLN 2

1:10 PM

C-I-1: RAPID ENHANCEMENT OF THE CRITICAL CURRENT OF HIGH-PERFORMANCE SUPERCONDUCTING WIRES

[CES] Ulrich Welp[1], M. Leroux[1], K. J. Kihlstrom[1,4], S. Holleis[1,5], M. W. Rupich[3], S. Sathyamurthy[3], S. Fleshler[3], H. P. Sheng[2], D. J. Miller[2], S. Eley[6], L. Civale[6], A. Kayani[7], P. M. Niraula[7], Q. Li[8], J. M. Zuo[9], W.-K. Kwok[1]
[1]Materials Science Division, Argonne National Laboratory; [2]Electron Microscopy Center-CNM, Argonne National Laboratory, Argonne; [3]American Superconductor Corp.; [4]Department of Physics, University of Illinois at Chicago; [5]Atominstitut, TU Wine ; [6]*MPA & CMMS, Los Alamos National Laboratory*; [7]*Department of Physics, Western Michigan University*; [8]*Condensed Matter Physics & Materials Science Department, Brookhaven National Laboratory;* [9]*Materials Research Laboratory, University of Illinois-Urbana Champaign*

Tremendous improvements have been made during the past decade in the performance of high temperature superconducting cables based on $YBa_2Cu_3O_{7-\delta}$ (YBCO). Superconducting wires are becoming competitive for space-limited and weight-limited applications: several projects involving urban grid, transformers, compact engines or offshore windmill turbines are being developed or deployed worldwide. Yet, widespread electric power grid penetration of superconducting cables has been hindered by the high cost of the fabrication process, while in-field applications struggle with the rapid fall of the critical current in an external magnetic field. We demonstrate that 4.6-MeV oxygen irradiation can markedly enhance the in-field critical current density, J_c, of commercial 2nd generation superconducting tapes with an exposure time of just one second per 0.8 cm^2. We achieve doubling of the critical current in fields of several Tesla and temperatures up to 45 K thereby alleviating the limitations in applications caused by the field suppression of J_c. The irradiation times demonstrated here are now at the level suitable for a viable reel-to-reel manufacturing process, and this enhancement can be applied to industrial production tapes over long lengths without any modification of the growth process. From TEM imaging, we identify small clusters as the main source of increased vortex pinning.

1:30 PM

C-I-2: TRANSITIONS BETWEEN INSULATING, METALLIC AND SUPERCONDUCTING STATES IN LOW-Z MATERIALS

[EFree] Ivan Naumov, Russell J. Hemley
Geophysical Laboratory, Carnegie Institution of Washington

Phonon-mediated superconductivity with high T_c is expected in materials with (i) high frequency phonons, (ii) strong electron-phonon coupling, and (iii) high density of states at the Fermi level, which can be met in low-Z dominant systems. Superconductivity in B-doped diamond, MgB_2, intercalated graphite compounds, and H_2S supports this conjecture. Hydrogen and hydrogen-rich materials are special in this regard, as they are expected have T_c about room temperature or higher. Since superconductivity often exists in close proximity to metal-insulator transitions, the latter require further understanding, especially in hydrogen and other simple elemental systems.

We have performed *ab-initio* comparative studies of transitions between insulating and metallic states in hydrogen and a number of other simple systems. All the elements undergo continuous pressure-induced *s*-*p*(-*d*)electronic transitions, though at a much earlier stage for H than for Li and Na. The character of insulating states is in H is drastically different those of Li and Na. In alkali metals, the character of the Wannier functions is closely related to the degree of *s*-*p*(-*d*) hybridization and reflects multi-center bonding.

Near insulator-to-metal transitions, many simple elements are prone to develop *topological surface states* characterized by extremely high densities of states at the Fermi level, which can lead to enhanced electron transport along the surface and even induce an unusual form of surface superconductivity with high T_c. Experimental identification of these and other predicted novel superconductivity states under pressure may lead to new classes of very high T_c superconductors that may ultimately be recovered for technological applications.

1:50 PM

C-I-3: DIRECTED SYNTHESIS AND FAST CHARACTERIZATION OF CORRELATED-ELECTRON MATERIALS FOR THE CENTER FOR EMERGENT SUPERCONDUCTIVITY

[CES] Daniel Shoemaker
Fredrick Seitz Materials Research Laboratory, University of Illinois

Experimental synthesis and doping of superconducting compounds has long been the realm of chemical intuition and a huge number of trial reactions. We seek a genomic approach to accelerate this process. In the absence of a fully defined genome, as is the case for superconductivity, computational approaches to materials discovery can dramatically increase the experimental load by identifying many possible candidates rather than a few definite hits. We will discuss how a flexible platform for in-situ X-ray diffraction under air-free conditions allows us to search for formation of new phases on the fly, instead of many days of traditional concurrent reactions. Aside from the discovery of new compounds, the doping limits of prospective compounds can also be quantified quickly. These two thrusts, stability and doping, seem to be equally necessary to effectively search for unconventional superconductors.

2:10 PM

C-I-4: OBSERVATION OF P-WAVE SUPERCONDUCTIVITY IN EPITAXIAL BI/NI BILAYERS

[SHINES] G. J. Zhao[1], X. X. Gong[2], J. A. Gifford[1], H. X. Zhou[2], X. F. Jin[2], C. L. Chien[3], T. Y. Chen[1]
[1]*Arizona State University;* [2]*Fudan University, China;* [3]*Johns Hopkins University*

Most superconductors to date are singlet superconductors with an s-wave (e.g., Pb, Nb) isotropic gap, except the high TC cuprates with a d-wave gap with nodes. We report observation of p-wave triplet superconductivity in epitaxial Bi/Ni bilayers with TC up to 4 K in multiple thickness ranges. Using ballistic injection of unpolarized and especially highly spin-polarized electrons with energies within the superconducting gap, Andreev reflection spectroscopy directly and conclusively demonstrates p-wave superconductivity in epitaxial Bi/Ni.

2:30 PM – Graduate Student Finalist

C-I-5: CHARACTERIZATION OF THE LOW-ENERGY BOSONIC MODES IN $Bi_2Sr_2CaCu_2O_{8+x}$ WITH INCIPIENT CHARGE ORDER

[CES] Sean Vig[1], Anshul Kogar[1], Vivek Mishra[2], Luke Venema[1], Melinda S. Rak[1], Ali A. Husain[1], Genda D. Gu[3], Eduardo Fradkin[1], Mike R. Norman[2], Peter Abbamonte[1,2]
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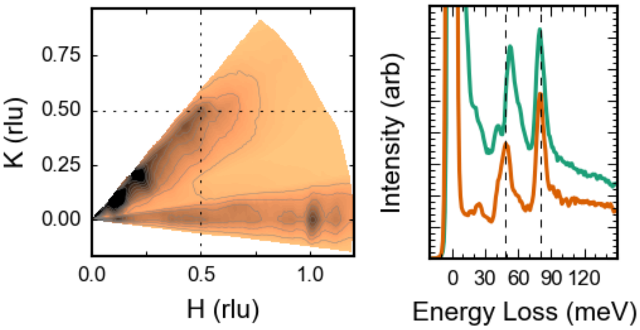
[2] *Materials Science Division, Argonne National Laboratory*
[3] *Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory*

Efficiently engineering novel and useful superconducting materials requires an understanding of the mechanism responsible for high-temperature superconductivity and its relation to other emergent phenomena. Though cuprate high-temperature superconductors have been studied intensely for the past 30 years, understanding the mechanism responsible for superconductivity remains a significant challenge in condensed matter physics. Developing this understanding requires knowledge of both the fermionic charge excitations and many-body bosonic interactions that drive the associated emergent phenomena. Much of our current understanding of cuprate superconductors has come from probing fermionic charge degrees of freedom at meV energy scales, which is the energy scale relevant to understanding high-temperature superconductivity and the various collective phases, such as charge order, that compete with it. This mapping has been done both in reciprocal space, with angle-resolved photoemission spectroscopy (ARPES), and in real space, with scanning tunneling spectroscopy (STS). Both of these techniques are able to measure the single particle spectra over several Brillouin zones. However, there is no comparable probe of the bosonic charge degrees of freedom, parameterized by the dynamic susceptibility, $\chi(\mathbf{q},\omega)$. Through work done in the Center for Emergent Superconductivity (CES), we have developed the technique of momentum-resolved electron energy-loss spectroscopy (M-EELS). M-EELS is capable of performing a full momentum-space mapping of the low-energy bosonic degrees of freedom over the first Brillouin zone with meV energy resolution, allowing us to characterize the interactions that give rise to collective electron dynamics. We present a study of the high-temperature superconductor material $Bi_2Sr_2CaCu_2O_{8+x}$ (Bi2212) using M-EELS to measure low-energy electron dynamics. In optimally doped Bi2212, we find the emergence of static, short-range charge order at low temperature. The full measurement of $\chi''(\mathbf{q},\omega)$ shows low-energy charge excitations, and resolving these excitations in momentum space, we see these excitations carry a similar structure to the charge order, suggesting that the static electronic order modulates the many-body interaction. We show that this observation is qualitatively consistent with features observed in the single particle spectral function by ARPES, namely the nodal dispersion anomaly, or "kink". We performed a one-loop self-energy calculation to compute the dispersion and showed the interactions measured by M-EELS recovers the kink feature. This study leverages all three CES institutions, with Bi2212 crystals grown at Brookhaven National Lab, the M-EELS measurements acquired at University of Illinois, and the self-energy calculation performed at Argonne National Lab. Through this work, M-EELS provides insight into collective dynamics that drive high-temperature superconductivity and is a promising technique to advance our understanding of the high-T_c problem.



SESSION IV: TUESDAY, OCTOBER 27, 2015; 10:40 – 12:00 PM; LINCOLN 2

10:40 AM

C-IV-1: PRECISION PLUTONIUM THERMODYNAMICS-EQUILIBRIA, KINETICS, AND COMPLICATIONS

[MSA] Albert Migliori[1], Boris Maiorov[1], Franz Freibert[1], Jon B. Betts[1], Xiaofeng Guo[1], Alexandra Navrotsky[2], Hongwu Xu[1]
[1] Los Alamos National Laboratory; [2] University of California, Davis

The exceptionally delicate electronics structure of plutonium metal, a subject of decades of intense study, drives properties that are not captured by even the very best modern theories. Magnetism, valence fluctuations, thermodynamic stability and more, have all been tried. But radiation-induced complications, the need for gallium to stabilize the most important phase to ambient temperatures, and the safety and security issues surrounding the most available isotope, ^{239}Pu, cloak the route to a fundamental understanding, something increasingly important for nuclear energy as well as nuclear weapons. Recent advances in precision thermodynamic measurements, including elastic moduli and heat capacity, have quantified essential properties that are not captured by today's theories of the metal but must be for those theories to be valid. We describe this ongoing work and its implications.

11:00 AM

C-IV-2: UNDERSTANDING ELECTRON TRANSPORT IN THERMOELECTRICS FROM FIRST-PRINCIPLES

[S^{3}TEC] Bolin Liao[1], Bo Qiu[1], Jiawei Zhou[1], Mildred S. Dresselhaus[2,3], Gang Chen[1]
[1]Department of Mechanical Engineering, Massachusetts Institute of Technology; [2]Department of Electrical Engineering and Computer Science, Massachusetts Institute of Technology; [3]Department of Physics, Massachusetts Institute of Technology

Electrons and phonons are major participants in thermoelectric transport, and the development of high-performance thermoelectrics entails optimization of both electron and phonon transport properties. Whereas remarkable progress has been made in both simulation and experimental techniques for mapping out the phonon mean free path distributions in solids, a detailed understanding of electron transport in real materials has lagged behind. Thanks to the recent development of a Wannier-function-based interpolation scheme, we are now able to accurately calculate the electron scattering rate due to electron-phonon interactions, the limiting factor of intrinsic electron transport in semiconductors. Applying this technique to real materials, we have quantitatively verified the length scale separation of electron and phonon mean free paths in silicon, predicted all thermoelectric properties of the newly-discovered 2D semiconductor phosphorene, and revealed that electron scatterings of phonons can significantly reduce the thermal conductivity of heavily-doped semiconductors. Furthermore, this technique has enabled us to quantitatively study higher-order non-equilibrium thermoelectric effects, such as the phonon drag effect that in the past has only been understood within simplified analytic models. The simulation suggests that properly designed "phonon filtering" mechanisms can be introduced to reduce the thermal conductivity while preserving the phonon drag effect, in contrast to previous beliefs. This new ability of simulating electron transport has opened up the venue towards fully *ab initio* understanding of thermoelectric materials, and we envision that it will serve as a necessary cornerstone for further optimization of realistic thermoelectric materials by providing quantitative guidelines.

11:20 AM

C-IV-3: PRODUCING NANOCRYSTALLINE MAGNETIC INSULATORS FOR SPIN AND THERMAL CONDUCTIVITY STUDIES

[SHINES] A. A. Balandin, J. Shi, J. E. Garay
University of California, Riverside

I will introduce two ongoing collaborative projects based on producing nanocrystalline magnetic insulators. The motivation for the first is increasing the understanding phonon behavior in magnetic materials by investigating thermal transport in nanostructured $SrFe_{12}O_{19}$ ferrimagnets. We vary the porosity and grain size to determine their relative effects on heat conduction. It was established that the heat conduction is dominated by phonons near room temperature. Clear trends relating the in-plane thermal conductivity to grain size and porosity were found. The observed anisotropy of thermal conductivity was attributed to the brick-like alignment of grains with the longer grain direction in-plane with the sample. In the second project we are looking to increase the perpendicular magnetization of yttrium iron garnet (YIG) based materials. The motivation is that although YIG is currently one of the most used magnetic insulators in spin based devices, it has a relatively large magnetic anisotropy, causing low magnetization in the perpendicular direction. We use both doping (with Bi ions) and lattice matching based strain strategies to increase the perpendicular magnetization. Doped nanocrystalline bulk Bi:YIG targets were first fabricated using a new chemical based synthesis and densification approach. Magnetic measurements clearly show that comparable magnetization in the in-plane and out of plane direction. Furthermore, we demonstrate successful tuning of the squareness (Mr/Ms ratio) of the B:YIG films.

11:40 AM

C-IV-4: INTERPLAY OF D-SYMMETRY COOPER PAIRS AND D-SYMMETRY DENSITY WAVES WITHIN THE CUPRATE PSEUDOGAP PHASE

[CES] K. Fujita[1,2,3,†], M. H. Hamidian[1,2,†], S.D. Edkins[2,4], Chung Koo Kim[1], Y. Kohsaka[5], M. Azuma[6], M. Takano[7], H. Takagi[3,8,9], H. Eisaki[10], S. Uchida[3], M. J. Lawler[2,12], E. -A. Kim[2], A.P. Mackenzie[4,9] S. Sachdev[11,13] & J. C. Séamus Davis[1,2,4]
[1] CMPMS Department, Brookhaven National Laboratory; [2]LASSP, Department of Physics, Cornell University; [3]Department of Physics, University of Tokyo; [4]School of Physics and Astronomy, University of St. Andrews; [5]RIKEN Center for Emergent Matter Science, Japan; [6]Materials and Structures Lab., Tokyo Institute of Technology; [7]Institute for Integrated Cell-Material Sciences, Kyoto University; [8]RIKEN Advanced Science Institute, Japan; [9]Max-Planck-Institut für Festkörperforschung; [10]Institute of Advanced Industrial Science and Technology, Japan; [11]Department of Physics, Harvard University; [12]Dept. of Physics and Astronomy, Binghamton University; [13]Perimeter Institute for Theoretical Physics Canada

A central issue of copper-oxide high temperature superconductivity research is to understand the nature of the pseudogap phase and its relationship to the *d*-symmetry superconductivity. Using our recently developed technique of sub-lattice phase-resolved electronic structure visualization within each CuO_2 unit-cell, we found that the density wave that is now widely observed in the cuprate pseudogap regime, itself exhibits *d*-symmetry. Although long predicted, such an unconventional density-wave state has not previously been observed in any condensed matter system. Our simultaneous visualizations of both real-space and momentum-space electronic structure across the cuprate phase diagram then revealed that the transition of Fermi surface topology from “Fermi arc” to conventional Fermi surface occurs simultaneously with the disappearance of the d-symmetry form factor density wave.

Now we report that the cuprate density wave state maintains its predominantly *d*-symmetry form factor (dFF) throughout the whole pseudogap region of the phase diagram, and that the characteristic energy of this DW state is actually the pseudogap energy. Moreover, we find robust dFF DW states induced at each vortex core. They are predominantly unidirectional and co-oriented (nematic), exhibiting strong spatial-phase coherence. At each vortex, we also detect the field-induced conversion of the SC to DW components, and demonstrate that this occurs at precisely the eight momentum-space locations predicted in many composite order theories. These data provide direct microscopic evidence for the existence of composite order in the cuprates, and new indications of how the DW state becomes long-range ordered in high magnetic fields.

D. CARBON SEQUESTRATION

SESSION I: MONDAY, OCTOBER 26, 2015; 1:10 – 2:50 PM; LINCOLN 6

1:10 PM

D-I-1: MICROSTRUCTURAL CONSTRAINTS ON THE ENERGY TECHNOLOGY USES OF FINE-GRAINED SEDIMENTARY ROCKS

[NCGC] Ian C. Bourg[1]
[1]*Princeton University*

Fine-grained sedimentary rocks (shale, mudstone) play important roles in global CO_2 abatement efforts through their importance in carbon capture and storage (CCS), radioactive waste storage, and shale gas extraction. These different technologies, however, rely on seemingly conflicting premises regarding the sealing properties of shale and mudstone, suggesting that fine-grained rocks that lend themselves to hydrocarbon extraction may not be optimal seals for CCS or radioactive waste storage, and vice versa. Here, experimental data on the properties of well-characterized shale and mudstone formations are used to demonstrate that clay mineral mass fraction, X_{clay}, controls key material properties of these formations. A remarkably sharp threshold at X_{clay} ~ 1/3 separates fine-grained rocks that are brittle (hence amenable to hydrocarbon extraction) from those that are ductile (hence suitable for use in CCS and radioactive waste storage). This threshold coincides with the predictions of a very simple conceptual model of the microstructure of sedimentary rocks and is reflected in the current uses of shale and mudstone formations.

1:30 PM

D-I-2: MANCOS SHALE-BRINE-CO_2 INTERACTIONS AND THE LONG-TERM STABILITY OF SHALE CAPROCK

[CFSES] Anastasia G. Ilgen[1], Thomas A. Stewart[1], Michael Aman[2], Randall T. Cygan[3], Thomas Dewers[4], Nicolas Espinoza[2]
[1]*Geochemistry Department, Sandia National Laboratories;* [2]*Center for Petroleum and Geosystems Engineering, The University of Texas at Austin;* [3]*Geoscience Research and Applications Group, Sandia National Laboratories;* [4]*Geomechanics Department, Sandia National Laboratories*

The successful geological storage of carbon dioxide (GCS) relies on the sealing properties of shale caprock. This study examines mineralogical changes in shale triggered by the introduction of carbon dioxide (CO_2). This project addresses the long-term stability of shale caprock, in particular the link between geochemical and geomechanical response of caprock to injection of CO_2. We examine representative shales: Mancos (Cretaceous), Woodford (Devonian), and Eau Claire (Cambrian). Shale samples are exposed to CO_2-brine mixtures at pressure and temperature conditions typical for GCS. Following the chemical evolution of the systems, we measure the apparent mineral dissolution rates, and characterize secondary mineral and amorphous precipitates. The link between mineral alteration and fracture toughness is assessed using nano-mechanical methods. This talk will describe the mineralogical changes observed for Mancos shale during exposure to CO_2-brine mixture. The dissolution of calcite and kaolinite and the precipitation of gypsum and gibbsite are documented based on the aqueous chemistry, characterization of the solid samples and geochemical modeling. The implications for the long-term stability of shale caprock will be discussed.

1:50 PM

D-I-3: SELF-SEALING OR SELF-ENHANCING? OBSERVATIONS OF FRACTURE EVOLUTION DURING CO_2 INDUCED DISSOLUTION AT IN-SITU CONDITIONS USING SYNCHROTRON MICROTOMOGRAPHY

[NCGC] Jonathan Ajo-Franklin[1], Marco Voltolini[1], Li Yang[1], Carl Steefel[1]
[1]*Lawrence Berkeley National Laboratory*

The long-term security of sequestered CO_2 is dictated partially by the integrity of sealing formations, typically shales, tight carbonates, or anhydrites. At present, the permeability evolution of flaws in such seals (e.g. fractures and faults) when exposed to streams of either scCO_2 or carbonated brines is not well understood; this is due to the complex coupling between reactions, flow, and in-situ stress conditions. A key open problem is the long-term evolution of fracture aperture (and therefore permeability) for induced fractures in low permeability carbonates, a process which can control seal integrity at sites being utilized for CO_2 storage. Examples from laboratory studies with analog samples have shown both self-enhancing and self-sealing behaviors during flow of carbonated brines depending on experimental parameters and chosen formation samples.

We present results from a series of dynamic synchrotron X-ray microtomography (SXR-µCT) experiment investigating changes in fracture aperture during dissolution induced by CO_2 saturated water. The samples explored include a low-permeability dolomite from the Duperow formation and a carbonate rich shale from the Niobrara unit. Both experiments were conducted near *in-situ* conditions using an x-ray compatible triaxial pressure vessel. Results show distinct fracture evolutions pathways for the two samples due to the microstructure of the non-reactive phase in both cases. Both experiments also revealed a strong feedback between reaction rates in the reactive and non-reactive mineral phases during dissolution and the development of a pronounced high-porosity weathered zone in the near-fracture region. On-going modeling studies should assist generalization of these observations to assist in selection of seals with higher likelihood of resilience after fracturing or fault reactivation.

2:10 PM

D-I-4: MASS TRANSFER AND SORPTION IN THE CONTEXT OF CO_2 STORAGE IN SALINE FORMATIONS

[GSCO2] Kristian Jessen, Muhammad Sahimi[1], Theodore T. Tsotsis[1]
[1]*Mork Family Department of Chemical Engineering and Materials Science, University of Southern California*

We combine characterization, flow/sorption experiments and MD/continuum-scale simulation to delineate modes and impact of sorption and mass transfer in core samples from Mt. Simon. Our characterization activities include sorption studies with Nitrogen and CO_2 to probe the pore structures and to determine specific surface areas of relevant Mt. Simon core material. The experimental observations indicate that the combined micro- and meso-porous range of the pore-size-distribution is attributed to clays and cementation materials while the bulk of the pore volume exists in larger pores. A high-pressure flow and sorption experimental apparatus has been designed for application to CO_2 storage in the Mt. Simon formation. The high-pressure facilities will assist our fundamental study of sorption and mass transfer at relevant storage conditions, including the potential impact of clay swelling on storage capacity and displacement dynamics. In our attempt to understand the clay swelling process due to shear, as well as setting up the proper molecular model for adsorption of CO_2 in rock in the presence of brine, we use MD simulation to study the swelling and shrinkage of clay particles. In order to show the

coupling between swelling and shear in liquid-saturated clay pores, we use Montmorillonite structure and the SPC/E model of water molecules. Our results indicate that shear can induce swelling and vice versa, due to the confined fluid phase structure. It implies that the response to a variation in the external load can be a combination of volumetric and shear deformations, because of the presence of the fluid.

2:30 PM – Postdoctoral Researcher Finalist

D-I-5: THE ROLE OF ADVANCED REACTIVE SURFACE AREA CHARACTERIZATION IN IMPROVING PREDICTIONS OF MINERAL REACTION RATES IN SUBSURFACE POROUS MEDIA

[NCGC] Lauren E. Beckingham[1], Elizabeth Mitnick[2], Carl I. Steefel[1], Shuo Zhang[2], Li Yang[1], Marco Voltolini[1], Alexander M. Swift[3], David R. Cole[3], Julie M. Sheets[3], Timothy Kneafsey[1], Gautier Landrot[4], Lawrence Anovitz[5], Saeko Mito[6], Ziqiu Xue[6], Donald DePaolo[1,2], Jonathan Ajo-Franklin[1]

[1]Lawrence Berkeley National Laboratory; [2]University of California, Berkeley; [3]Ohio State University; [4]Synchrotron SOLEIL; [5]Oak Ridge National Laboratory; [6]Research Institute of Innovative Technology for the Earth (RITE)

Mineral reaction rates remain difficult to predict as numerous uncertainties and imprecisions exist in current mineral dissolution and precipitation modeling capabilities. One of the major uncertainties arises from a lack of understanding of mineral reactive surface area. Common estimates of mineral reactive surface area are ad hoc and typically based on grain size, adjusted several orders of magnitude to account for surface roughness and reactivity. This results in orders of magnitude discrepancies in estimated mineral reactive surface area that directly translate into orders of magnitude discrepancies in model predictions. Additionally, natural systems can be highly heterogeneous and contain abundant nano- and micro-porosity, which can limit connected porosity and access to mineral surfaces. In this study, mineral-specific accessible surface areas are computed for a sample from the reservoir formation at the Nagaoka pilot CO_2 injection site (Japan). Accessible mineral surface areas are determined from a multi-scale image analysis including X-ray microCT, SEM QEMSCAN, XRD, SANS, and SEM-FIB. These estimates not only account for accessibility of mineral surfaces to macro-pores, but accessibility through nano-pores, especially important given the abundance of mineral surfaces coated by porous smectite in this sample. Powder and flow-through column laboratory experiments are performed and the evolution of solutes in the aqueous phase is tracked. Continuum-scale reactive transport models are used to evaluate the impact of reactive surface area on predictions of experimental reaction rates. Evaluated reactive surface areas include geometric and specific surface areas (eg. BET) in addition to their reactive-site weighted counterparts. The most accurate predictions of observed powder mineral dissolution rates were obtained through use of grain-size specific surface areas computed from a BET-based correlation. Effectively, this surface area reflects the grain-fluid contact area, or accessible surface area, in the powder dissolution experiment. In the model of the flow-through column experiment, the accessible mineral surface area, computed from the multi-scale image analysis, is evaluated in addition to the traditional surface area estimates.

SESSION IV: TUESDAY, OCTOBER 27, 2015; 10:40 – 12:00 PM; LINCOLN 6

10:40 AM

D-IV-1: PORE-SIZE DEPENDENT MINERAL REACTIONS IN POROUS MEDIA

[NCGC] Andrew G. Stack[1], Michael C. Cheshire[1], Timothy R. Prisk[1], J. William Carey[2], Lawrence M. Anovitz[1]
[1]Oak Ridge National Laboratory; [2]Los Alamos National Laboratory

Mineral precipitation and dissolution in the subsurface, particularly any pore-size dependence for the reactions, will determine how porosity and permeability evolve in response to system perturbations such as mineralization during carbon sequestration. This in turn will affect storage security of the site and fluid transport. In this talk I will review the competing theories for the pore size distribution in which precipitation preferentially prefers (Stack, 2015). Factors such as precipitate-substrate interaction and nucleation density have been found to correlate with whether precipitation occurs preferentially in large or small pores, with no pore-size dependence at all. The implications of different pore-size dependent behaviors on these systems will be discussed in light of these competing theories, with particular attention to permeability evolution in the subsurface. Examples from our recent research to observe mineral reactions in nano- and microporous systems using X-ray scattering will be presented to illustrate these. Of special focus will be our work on a cement well casing sample that was exposed to carbon dioxide for the purposes of enhanced oil recovery for 30 years. This sample forms an important analogue for the types of geochemical reactions that take place during long term carbon sequestration. In this sample, we find that often distributions of smaller pores are unaffected and the largest changes in porosity in the reacted zone are in larger pores, but a clear reaction front is observed at the boundary of the alteration layer.

11:00 AM

D-IV-2: PORE-SCALE PHENOMENA AFFECTING TRANSPORT AND FATE OF SUPERCRITICAL CO_2 IN GEOLOGICAL RESERVOIRS: FLOW DYNAMICS, WETTABILITY AND MODELING IMPLICATIONS

[GSCO2] Yaofa Li[1], Farzan Kazemifar[1,2], Gianluca Blois[1,2], Julien Botto[3], Yu Chen[4], Amir H. Kohanpur[2,4], Charles Werth[3], Albert Valocchi [2,4], Kenneth T. Christensen[1,2]
[1]University of Notre Dame; [2]International Institute for Carbon-Neutral Energy Research (I^{2}CNER), Kyushu University, Japan; [3]University of Texas at Austin; [4]University of Illinois at Urbana-Champaign

One of the primary factors limiting widespread application of geological carbon sequestration is uncertainty regarding the fate of CO_2 in a formation during and post-injection. There is concern that CO_2 will remain buoyant, and escape to overlying groundwater or the ground surface through fractures/faults in the cap rock, and leaky well bores. To this end, we are exploring a range of pore-scale phenomena that affect CO_2 migration and fate, particularly the pore-scale flow dynamics of water and liquid/supercritical CO_2 and the impact of wettability on flow and trapping at the pore scale. Measurements of flow are being conducted in 2D homogeneous and heterogeneous porous micromodels *at reservoir-relevant* conditions. The micromodels are fabricated from silicon, with the porous matrix formed from regularly arranged cylindrical/elliptic pillars and the reprint of the pore structure of real sandstone for the homogeneous and heterogeneous models, respectively. Fluorescent microscopy and the micro-PIV technique are employed to simultaneously measure the spatially-resolved instantaneous velocity field in the water and quantify the instantaneous spatial configuration of both phases. We are also determining pore-scale wettability by measuring contact angles on reservoir rock

samples under reservoir conditions. The flow and wettability results are being used to calibrate pore-scale models, with the goal of accurately simulating CO_2 migration in the experiments, and to develop upscaled relationships to inform continuum-scale models for more accurate field scale simulation.

11:20 AM

D-IV-3: CONSTRAINING THE INFLUENCE OF MESO-SCALE HETEROGENEITY ON CO_2 SATURATION RESULTING FROM BUOYANT FLOW USING INVASION PERCOLATION SIMULATIONS

[CFSES] Tip Meckel[1], Luca Trevisan[1], Prasanna Krishnamurthy[2], Hongkyu Yoon[3], Mario Martinez[4]

[1]Gulf Coast Carbon Center, Bureau of Economic Geology, The University of Texas at Austin; [2]Center for Petroleum and Geosystems Engineering, The University of Texas at Austin; [3]Geoscience Research and Applications, Sandia National Laboratories; [4]Engineering Sciences Center, Sandia National Laboratories

Estimating the pore saturation of CO_2 injected into heterogeneous rocks for permanent storage is a key challenge for sustaining large storage rates and utilizing pore space with unprecedented efficiency. We investigate CO_2 saturations resulting from buoyancy-driven capillary flow, where buoyancy forces dominate viscous forces. These low capillary number flow regimes ($Ca < 10^{-4}$) exist some distance from injection wells, potentially representing the majority of the storage domain during and after injection. We simulate CO_2-brine buoyant displacement patterns using invasion percolation methods in various decimeter-scale, highly resolved heterogeneous clastic 3-D models exhibiting realistic depositional fabrics. We seek a generalized predictive model that allows CO_2 saturation resulting from buoyant flow to be estimated reasonably from fundamental geologic rock descriptions (grain size distribution and fabric length scales) and fluid properties (density contrast, interfacial tension).

11:40 AM

D-IV-4: NEUTRON SCATTERING LINKS CO_2 ADSORPTION PERFORMANCE TO POLYMER MORPHOLOGY IN SILICA/PEI COMPOSITE ADSORBENTS

[UNCAGE-ME] Adam Holewinski[1], Miles A. Sakwa-Novak[1], Songhai Chai[2], Sheng Dai[2,3], Gernot Rother[3], Christopher W. Jones[1]

[1]School of Chemical & Biomolecular Engineering, Georgia Institute of Technology; [2]Department of Chemistry, University of Tennessee; [3]Chemical Science Division, Oak Ridge National Laboratory

Composites of poly(ethyleneimine) (PEI) and mesoporous silica are effective, reversible adsorbents for CO_2, both from flue gas and in direct air-capture applications. The morphology of the PEI within the silica pores can strongly impact the overall carbon capture efficiency and rate of saturation. However, to date, there is very limited knowledge of the morphology of PEI domains within the pores. Here, the spatial distribution of the supported polymer is directly probed using small-angle neutron scattering (SANS). Combined with textural characterization from physisorption analysis, the data indicate that PEI first forms a thin conformal coating on the pore walls, but all additional polymer aggregates into plug(s) that grow along the pore axis. This model is consistent with observed trends in amine-efficiency (CO_2/N binding ratio) and pore size distributions, and points to a tradeoff between achieving high chemical accessibility of the amine binding sites, which are inaccessible when they strongly interact with the silica, and high accessibility for mass transport, which can be hampered by diffusion through PEI plugs. This design principle is illustrated by demonstrating higher CO_2 capacity and uptake rate for PEI supported in a hydrophobically-modified silica, which exhibits repulsive interactions with the PEI, freeing acid gas binding sites.

SESSION V: TUESDAY, OCTOBER 27, 2015; 1:30 – 3:10 PM; THURGOOD MARSHALL E/N

1:30 PM

D-V-1: GEOMECHANICS AND RESEARCH CHALLENGES FOR GEOLOGIC CARBON STORAGE

[CFSES] Thomas Dewers[1], Alex Rinehart[2], Jon Major[3,4], Sanghyun Lee[5], Jacqueline Reber[6], Peter Eichhubl[4], Mary Wheeler[5], Nick Hayman[6], Anastasia Ilgen[1], Joseph Bishop[1], Matt Balhoff[7], Nicolas Espinoza[7], Mario Martinez[8], Hongkyu Yoon[1]

[1]Geomechanics Department, Sandia National Laboratories; [2]Department of Earth and Environmental Science, New Mexico Tech; [3]Department of Geological Sciences, The University of Texas at Austin; [4]Bureau of Economic Geology, The University of Texas at Austin; [5]The Institute for Computational Engineering and Sciences, The University of Texas at Austin; [6]Institute for Geophysics, The University of Texas at Austin; [7]Center for Petroleum and Geosystems Engineering, The University of Texas at Austin; [8]Engineering Sciences Center, Sandia National Laboratories

Growing evidence points to hydromechanical and hydromechanical-chemical coupling as important classes of time dependent deformation in the subsurface that have several engineering implications for intentional or unintentional stimulation of reservoirs and caprock during geologic carbon storage (GCS). The range of observed geomechanical responses to current and historical large scale GCS efforts (and underground injection in general) requires a greater geomechanical understanding for potential hazard mitigation. The Center for Frontiers of Subsurface Energy Security (CFSES) focuses on three research challenges for GCS: 1. using pore space with unprecedented efficiency; 2. preserving injectivity throughout a storage program; and 3. predicting emergent behavior and avoiding unintended consequences. This talk describes a linked CFSES experimental and modeling program aimed at advancing solutions to these challenges, and places each in the context of field injection examples and natural analog sites for GCS. Focus is placed on the coupling between geomechanics and subsurface chemical perturbations associated with injection and long-term storage and the impact on caprock leakage, wellbore integrity, and reservoir properties.

1:50 PM

D-V-2: PORE-SCALE AND CONTINUUM MODELING OF FRACTURE EVOLUTION AND MINERAL TRAPPING DURING CO_2 SEQUESTRATION

[NCGC] Carl I. Steefel[1], Hang Deng[1], Sergi Molins[1], David Trebotich[1]

[1]Lawrence Berkeley National Laboratory

During subsurface CO_2 injection and sequestration, the evolution of fractures in caprocks as well as mineral trapping in reservoir rocks may be controlled by coupled flow, transport, and mineral precipitation/dissolution processes. Fractures may open and “wormhole” due to mineral dissolution, or they may seal due to mineral precipitation or as a result of mechanical effects on fracture asperities. Interaction with rock matrix may modify chemical and fluid fluxes to and from fractures. Mineral composition and spatial distribution play an important role in controlling fracture surface alteration and the extent of mineral trapping in. Fracture surfaces may simply retreat as the rock matrix dissolves such as in limestone fractures, or an altered layer, which will affect subsequent fracture alterations, may develop on the fracture surfaces in presence of mineral heterogeneity. Some of these effects can be investigated experimentally, but modeling has an important role to play in this analysis because of its ability to consider multiple length and time scales. These effects are investigated in this study with a combination of pore-scale and continuum reactive transport modeling.

In the case of pore-scale modeling, the modeling domain was constructed from x-ray microtomographic images of a carbonate core experiment in which CO_2-saturated brine was injected into a fracture. The ability to accurately image the fracture geometry made it possible to distinguish between fast and slow flow paths in the simulations. Mineralogical composition in the form of dolomite and calcite was incorporated in the model based on the differing micro-tomographic attenuation values for these two phases. Faster dissolution of calcite contributes to the channeling of flow in the dissolution simulations. A 2-D continuum model was developed to explore different scenarios of fracture surface alteration under a variety of mineral compositions (including both carbonate and clay phases), as well as the resulting changes in fracture permeability and geochemical reactions.

2:10 PM

D-V-3: IMPROVED QUANTIFICATION OF RESERVOIR PARAMETERS FROM SEISMIC DATA

[GSCO2] Michael Jordan[1], Bob Hardage[2], Alexander Klokov[2], Bastian Dupuy[1], Erling Fjær[1], Pierre Cerasi[1], Srutarshi Pradhan[1], Anna M. Stroiz[1]
[1]SINTEF, Trondheim, Norway; [2]Bureau of Economic Geology, The University of Texas at Austin

One of the questions addressed by geophysics research within the Center for Geologic Storage of CO_2 (GSCO2) is the monitoring of the pressure plume, as required by US EPA Class 6 regulations, and how to distinguish between pressure and saturation effects using seismic data. Previous laboratory studies indicate that stress, pore pressure, and saturation may have a strong effect on seismic P- and S-wave velocities, attenuation, and anisotropy. We investigate how these quantities can be used to identify pressure plumes and quantify saturation effects for large-scale carbon dioxide (CO_2) storage projects, particularly postinjection monitoring, using a CO_2 storage project in the Illinois Basin, USA, as an example. The work presented here includes ultrasonic and low-frequency laboratory tests on cores from the storage reservoir; the upscaling of results from the core to seismic scale; modeling of synthetic seismic data, including the expected effects; and verification of whether the predicted effects can be observed in and extracted from data acquired from the storage reservoir. In this work, upscaling is an important topic that has to be addressed when transferring knowledge and data between the lab and field, and for establishing the connection between the microscale and macroscale during modeling. Elastic waves are characterized by frequency, wavelength, and amplitude, and there are upscaling issues associated with each of these quantities. There are also upscaling issues for stress and pore pressure, which describe the condition of the rock, that may need attention. We present the results of ultrasonic wave transmission laboratory experiments for varying pressure and saturation, the initial data analysis, and our upscaling approach. The seismic data that will be used in our upscaling comparisons will include images made from both P- and S-wave modes.

2:30 PM

D-V-4: CONSTRAINTS ON LONG-TERM SAFETY OF GEOLOGICAL CO_2 STORAGE FROM NATURAL ANALOGUES

[CFSES] Marc A. Hesse[1], Kiran Sathaye[1], Martin Cassidy[2], Daniel Stoeckli[1], Daria Akhbari[1]
[1]Department of Geological Sciences, The University of Texas at Austin, Austin, Texas
[2]Department of Earth and Atmospheric Sciences, University of Houston, Houston, Texas

Bravo Dome is a large natural CO_2 field in northeastern New Mexico. The field contained approximately 1.3 $GtCO_2$ before production began in 1981. The field contains 99.9 % pure CO_2 with traces of methane, nitrogen and noble gasses. The reservoir is hosted in a Permian red sandstone and capped by a regional anhydride layer. The field, therefore, provides an analogue for large scale and long term CO_2 storage. We use apatite U-Th/He thermochronology to determine that filling of the reservoir ended 1.2 Million years ago. Given the lack of evidence for leakage on the surface this suggests that more than one giga-ton of CO_2 has been stored safely for more than one million years. Hydraulic isolation of the reservoir is also evidenced by the abnormally low reservoir pressures. We estimate that approximately 22% of the emplaced CO_2 has been dissolved into the reservoir brine. This provides field evidence for large-scale dissolution trapping, a process commonly invoked to suggest that storage security increases over time. The dissolution rate at Bravo Dome, however, appears much slower that might be expected from the density driven convective currents commonly observed in numerical simulations.

2:50 PM

D-V-5: INDUCED SEISMICITY DUE TO LOW PRESSURE-GRADIENT FLUID INJECTIONS: LINKING LABORATORY-SCALES WITH FIELD-SCALE OBSERVATIONS

[GSCO2] Volker Oye[1], Bettina Goertz-Allmann[1], Sergey Stanchits[2], Pierre Cerasi[3], Robert A. Bauer[4]
[1]NORSAR, Kjeller, Norway; [2]Schlumberger Research Center, Salt Lake City, UT; [3]SINTEF, Trondheim, Norway; [4] University of Illinois at Urbana-Champaign

The occurrence of induced and triggered microseismicity world-wide is of increasing concern to the general public. The underlying human causes are numerous and include hydrocarbon production and geological storage of CO_2. The concerns of induced seismicity are the potential hazards from large seismic events and the creation of fluid pathways. However, microseismicity is also a unique tool to gather information about real-time changes in the subsurface, a fact generally ignored by the public. The ability to detect, locate and characterize microseismic events provides a snapshot of the stress conditions within and around a geological reservoir. In addition, data on rapid stress changes like microseismic events can be used as input to hydro-mechanical models, often used to map fluid propagation. Our aim is to investigate how the occurrence of the microseismic events is related to the creation or re-activation of faults and fractures by stress changes imposed by pressure transients as a response to fluid injection. This will be realized by combining laboratory-scale experiments with novel numerical modelling for upscaling. Furthermore, acoustic emissions recorded in the laboratory experiments will illustrate which attribute(s) trigger microseismicity, and the results will be related to field-scale observations of microseismicity. Detailed characterization of the type of microseismicity will provide constraints on the pressure changes, extent, and stress front changes in the geologic storage formation associated with injection of CO_2. This new knowledge will assist in risk mitigation related to the triggering potential of felt earthquakes and in informing the public.

E. MATERIALS AND CHEMISTRY BY DESIGN

SESSION I: MONDAY, OCTOBER 26, 2015; 1:10 – 2:50 PM; LINCOLN 5

1:10 PM

E-I-1: MULTISCALE MODELING OF SURFACE REACTIVITY IN NANOPOROUS ALLOYS

[IMASC] Matthew Montemore[1], Branco Zugic[2], Giacomo Faclucci[3], Fairoja. C. Kabeer[4], Wei Chen[1], Cynthia. M. Friend[2], Efthimios. Kaxiras[1,5], Juergen Biener[6], Robert Madix[1], Sauro Succi[7], Alexander Tkatchenko[4]

[1] School of Engineering and Applied Sciences, Harvard University; [2] Department of Chemistry and Chemical Biology, Harvard University; [3] Department of Engineering, University of Naples, Italy; [4] Fritz-Haber Institute, Germany; [5] Department of Physics, Harvard University; [6] Lawrence Livermore National Laboratory; [7] National Research Council, Italy

The central theme of IMASC is to develop a detailed understanding of mechanisms and dynamics of catalyzed transformations, and to contribute to the design and controlled synthesis of catalytic structures, using a multiscale approach. These goals are being met by determining new paradigmatic models for controlling activity and selectivity of sustainable, complex reaction pathways for hydrogenation and oxidation reactions. The modeling effort includes microscopic and macroscopic components, which will be linked to inform the system description from both perspectives. At the microscopic level, we report on representative surface reactions in nanoporous Ag/Au and Pd/Cu alloys, and the effect of surface morphology and composition on the reaction and diffusion rates. These calculations involve density-functional-theory models of partial hydrogenation and oxidation reactions on pure, oxygen-covered and alloy surfaces. An important feature of the calculations is the inclusion of van der Walls interactions, which have a significant effect on the ordering of surface binding energies. At the macroscopic level, we model the reactive flow patterns in nanoporous structures, using the lattice Boltzmann equation approach for fluid dynamics, to capture the reactivity patterns in nanoporous ingots, in 2D and 3D geometries. We will discuss initial efforts to link the different scales and to extract information from the model studies toward the optimization of catalyst design. We also describe how the theoretical modeling follows closely experimental investigations of the nanoporous surface alloy systems, and is used to select the optimal combinations of composition and geometry of the catalytic device.

1:30 PM

E-I-2: TOWARD DESIGN OF MOLECULAR ELECTROCATALYSTS BY COMPUTATIONS

[CME] Simone Raugei[1], Ming-Hsun Ho[1], Shentan Chen[1], Neeraj Kumar[1], Michel Dupuis[1,2], R. Morris Bullock[1]

[1]*Pacific Northwest National Laboratory*; [2]*Current Address: Department of Chemical and Biological Engineering, University at Buffallo*

Electrocatalysts based on inexpensive, earth-abundant metals that rapidly and efficiently interconvert electrical energy and fuels are envisioned to play a critical role in renewable energy utilization systems. The rational design of catalysts requires a systematic approach to designing ligands with specific functionalities and precisely tailored electronic and steric properties. Efficient catalysts have flat free energy profiles that avoid high activation barriers due to low- and high-energy intermediates. Given that many reactions such as H_2 oxidation and production,

O_2 reduction, and N_2 reduction involve electrons, protons, and hydrides, we propose a framework for the systematic design of catalysts. In this framework, the relative free energy of intermediates in the catalytic cycle directly result from thermodynamic properties such as acidities, redox potentials, and hydricities. These properties are connected to each other by thermodynamic cycles, and can be estimated with quantum mechanical calculations and/or linear free energy relationships. Using examples from our work on electrocatalytic processes for H_2 oxidation and production, we will show that using *ab initio* molecular dynamics, free energy calculations and microkinetic modeling, it is possible to exhaustively characterize the complete reaction network and determine the factors controlling catalysis. We will present design principles that allow us to avoid catalytically inefficient pathways and reduce the overpotential by enforcing the requirement of a flat energy profile, which can be efficiently calculated using linear free energy relationships.

1:50 PM – Graduate Student Finalist

E-I-3: REVEALING THE SUGAR ISOMERIZATION MECHANISM ON HOMOGENEOUS SN-SILICATE CATALYSTS

[CCEI] Tyler Josephson[1], Kramer Brand[2], Jay Labinger[2], Mark Davis[2], Dion Vlachos[1], Stavros Caratzoulas[1]
[1]*University of Delaware,* [2]*California Institute of Technology*

The isomerization of glucose to fructose has recently emerged as an important route for the conversion of cellulose to intermediate platforms.[1] Sn-Beta zeolite catalyst has been active for transforming glucose into its isomer fructose, as well as its epimer mannose.[2] The active sites in these heterogeneous materials are difficult to characterize, especially under reaction conditions.[3,4] We developed a homogeneous catalyst model to isolate, characterize and test different types of active sites, and compare these to heterogeneous catalysts. These stannasilsequioxane catalysts, or Sn-Cubes, are active for glucose isomerization and epimerization, although they differ in selectivity from Sn-Beta.

In conjunction with experimental work, we performed electronic structure calculations to investigate numerous isomerization and epimerization pathways on this Sn-Cube catalyst. We modelled the full catalytic cycle, including ring-opening of glucose, hydride transfer and Bilik reactions to form fructose and mannose, and ring-closing of these products. The complete reaction network was analyzed using the energetic span model to estimate the relative rates of isomerization and epimerization. We found agreement between our predictions and kinetic measurements, as well as ^{13}C labelling experiments that distinguish among the different possible pathways for producing fructose and mannose.

The properties of these Sn-Cubes are compared to those of Sn-Beta in order to close the gap between molecular analogues of a heterogeneous catalyst and the actual material. A key feature of the active open site in Sn-Beta is the stannanol group which facilitates proton transfers in ring-opening and ring closing reactions, and a silanol group which facilitates the hydride transfer reaction steps.[2,5] These Sn-Cubes have an inert methyl group in place of a stannanol, but this does not preclude them from catalyzing this reaction. Instead, ring-opening and ring-closing are facilitated via a Sn-O-Si bridge, which accepts a proton from a glucose hydroxyl, breaks the bridge, and forms a silanol, which can participate in later reactions as the Sn-Beta open site silanol does. In addition, while the Sn-Cubes deactivate when exposed to water, the zeolite framework in Sn-Beta stabilizes the open site, preventing deactivation.

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[2] Bermejo-Deval, R.; Assary, R. S.; Nikolla, E.; Moliner, M.; Roman-Leshkov, Y.; Hwang, S.-J.; Palsdottir, a.; Silverman, D.; Lobo, R. F.; Curtiss, L. a.; Davis, M. E. *Proc. Natl. Acad. Sci.* **2012**, *109* (25), 9727–9732.

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[4] Bermejo-Deval, R.; Gounder, R.; Davis, M. E. *ACS Catal.* **2012**, *2* (12), 2705–2713.
[5] Rai, N.; Caratzoulas, S.; Vlachos, D. G. *ACS Catal.* **2013**, *3* (10), 2294–2298.

2:10 PM

E-I-4: UNDERSTANDING AND PREDICTING THE INTERFACIAL STRUCTURE AND DYNAMICS IN CAPACITIVE ENERGY SYSTEMS UTILIZING MODEL-INTEGRATED SYNTHESIS, CHARACTERIZATION AND EXPERIMENT

[FIRST] Peter T. Cummings[1], Matthew W. Thompson[1], Yu Zhang[1], Nina Balke[2], Jennifer Black[2], Paul Kent[2], Michael Naguib[2], Lukas Vlcek[2], Hsiu-Wen Wang[2], Yu Xie[2], Stuart Winikoff[3], Matthew Neurock[3], Adri Van Duin[4], Alireza Ostadhossein[4], Yoon Kichul[4], Boris Dyatkin[5], Katherine Van Aken[5], Yury Gogotsi[5], Kun Liu[6], Justin Neal[6], Cheng Zhan[6], De-en, Jiang[6], Jianzhong Wu[6], Joel Rosenthal[7], Guang Feng[8], Song Li[8]
[1]Vanderbilt University, [2]Oak Ridge National Laboratory, [3]University of Minnesota, [4]The Pennsylvania State University, [5]Drexel University, [6]University of California, Riverside, [7]University of Delaware, [8]Huazhong University of Science and Technology, China

In the FIRST Center, we have developed a paradigm for studying fluid/solid interfaces relevant to energy storage that we refer to as *model-integrated synthesis, characterization and experiment* (MISCE). Of the almost limitless number of possible electrolyte/electrode and other fluid/solid interfacial systems, the FIRST team collectively chooses systems (fluid, solid, geometry) that are amenable to computational modeling. Frequently, the geometries chosen also facilitate the applications of molecular probes, such as neutron and x-ray scattering and scanning probe microscopy. Additionally, the fluids and solids chosen may require synthesis. These highly integrated studies have led to insights into experiments as well as laying the foundation for predicting the structure and function of energy-relevant fluid-solid interfaces. In this presentation, we will describe several examples of the MISCE approach.

2:30 PM

E-I-5: MOLECULAR AND DISSOCIATIVE ADSORPTION OF WATER ON $(TiO_2)_N$ CLUSTERS

[UNCAGE-ME] Mingyang Chen[1], Tjerk P. Straatsma[1], David A. Dixon[2]
[1]National Center for Computational Sciences, Oak Ridge National Laboratory; [2]Department of Chemistry, The University of Alabama

The interactions of acid gases with metal oxides, carbon, MOFs, and ZIFs are the core research of UNCAGE-ME. These gases including water can adsorb molecularly or dissociatively. A goal of the Center is to determine which processes are dominant. Small clusters can serve as models of larger clusters as well as surface defect sites, and can be used to benchmark different computational approaches (density functional theory vs CCSD(T)). The low energy structures of the $(TiO_2)_n(H_2O)_m$ ($n \le 4$, $m \le 2n$) clusters were predicted using a new global geometry optimization approach combining molecular docking with a hybrid genetic algorithm. Water can molecularly or dissociatively adsorb to form different clusters. Dissociative adsorption is the dominant reaction for the initial H_2O additions, which eliminate the under-coordinated Ti centers. As more waters are added, dissociative adsorption becomes less exothermic leading to loss of the cluster structure and molecular adsorption becomes more energetically favored. Molecular adsorption of water occurs through Lewis acid-base Ti-O(H_2) bonds or O•••H hydrogen bonds. The Lewis acid-base binding energy at a 4-coordinate Ti center is ~ 15 kcal/mol and the hydrogen bonded interaction is ~ 7 kcal/mol, in comparison to the ~ 10 kcal/mol for the dissociative binding energy at a 4-coordinate Ti center. A number of models have been

developed to explain the reactivity. For example, intramolecular dehydration coupled with aggregation is thermodynamically allowed for hydrated $(TiO_2)_n$ clusters with all of the Ti centers 4-coordinate.

SESSION II: MONDAY, OCTOBER 26, 2015; 3:20 – 5:00 PM; LINCOLN 5

3:20 PM

E-II-1: TESTING AND APPLICATIONS OF THE SCAN METAGGA, AN ACCURATE AND EFFICIENT NONEMPIRICAL DENSITY FUNCTIONAL

[CCDM] Jianwei Sun[1], Haowei Peng[1], Richard C. Remsing[2], Akila C. Thenuwara[2], Laszlo Frazer[2], Zhaoru Sun[1], Songsong Zhou[3], Arpita Paul[4], Zenghui Yang[1], Jian Han[3], Alejandro J. Garza[5], Ioana Buda[6], Christopher A. Lane[6], Hasnain Hafiz[6], Bernardo Barbiellini-Amidei[6], Adrienn Ruzsinszky[1], Xifan Wu[1], Umesh Waghmare[4], Michael Zdilla[2], Eric Borguet[2], Gustavo E. Scuseria[5], Arun Bansil[6], David J. Srolovitz[3], Daniel R. Strongin[2], Michael L. Klein[1,2], John P. Perdew[1,2]

[1]Physics, Temple U., [2]Chemistry, Temple U., [3]MSE, U. Penn, [4]Theoretical Sciences Unit JNCASR, [5]Chemistry, Rice U., [6]Physics, Northeastern U.

The Kohn-Sham density functional theory (DFT) is a widely-used electronic structure theory in quantum chemistry and condensed matter physics. DFT is needed for electronic properties of large systems, studies of dynamical behavior, and especially for high-throughput searches of materials properties. DFT's accuracy and computational efficiency are limited by the approximation to its exchange-correlation energy. Currently, the local density approximation (LDA) and the generalized gradient approximations (GGAs) dominate applications in materials science, due partly to their reasonable accuracy but mainly to their efficiency. The recently developed nonempirical SCAN (strongly constrained and appropriately normed) meta-GGA is comparable in efficiency to LDA and GGAs, and significantly improves over LDA and the standard Perdew-Burke-Ernzerhof (PBE) GGA for geometric and energetic properties of some standard data sets that include molecules and solids. In this talk, SCAN and its applications to various systems (e.g., ice, Si, and MnO_2 of different solid phases) for different properties (e.g., geometric, energetic, dynamical, and ferroelectric) will be presented and discussed. The results are such that we expect use of this functional to have a broad impact on materials science, especially on the materials genome initiative. We will also present applications of SCAN to explain experimental data and its usage as a basis for further theoretical development.

3:40 PM

E-II-2: SEARCHING FOR NEW CORRELATED MATERIALS FOR SUPERCONDUCTIVITY

[CES] Lucas Wagner

Department of Physics, University of Illinois

While genomic approaches to materials design have made significant headway in creating solutions for application areas like batteries and transparent conducting materials, so far strongly correlated materials have not been studied much in this way. The challenges in doing this are that conventional electronic structure methods are not accurate enough and that the genome is not mapped out, particularly for unconventional superconductors. We will report on progress in constructing a system consisting of coupled high level theory that can describe correlated electrons accurately linked to experimental setups that can test the predictions with quick turnaround, with a focus on materials that may be superconducting.

4:00 PM

E-II-3: INCORPORATING METASTABILITY INTO MATERIALS BY DESIGN

[CNGMD] William Tumas[1], Gerbrand Ceder[2,8], David Ginley[1], John Perkins[1], Andriy Zakutayev[1], Stephan Lany[1], Vladan Stevanovic[1,5], Kristin Persson[2,8], Tonio Buonassisi[3], Alexie Kolpak[3], Roy Gordon[4], Daniel Nocera[4], Brian Gorman[5], Janet Tate[6], Michael Toney[7]
[1]National Renewable Energy Laboratory, [2]UC-Berkeley, [3]Massachusetts Institute of Technology, [4]Harvard University, [5]Colorado School of Mines, [6]Oregon State University, [7]SLAC National Accelerator Laboratory, [8]Lawrence Berkeley National Laboratory

Our EFRC aims to *dramatically transform the discovery of functional energy materials through multiple-property search, incorporation of metastable materials into predictive design, and the development of specific theory to guide materials synthesis*. We address four critical scientific gaps for making *Materials by Design* a robust tool to discover and synthesize novel functional materials, including non-equilibrium systems, in a predictive manner: 1) ***multiple-property design***, 2) ***accuracy and relevance***, 3) ***metastability***, and 4) ***synthesizability***. Many technologically relevant materials are kinetically stabilized and not at their true thermodynamic minimum yet exhibit improved functionality over their thermodynamically stable counterparts. To develop a fundamental understanding to incorporate non-equilibrium materials systems into materials by design, we are investigating three types of metastability: polymorphism, semiconductor alloys, and defects. Theory is used to explore polymorph space and to suggest synthesis routes that are then tightly coupled to targeted growth of specific polymorphs using homogeneous solution precipitation, electrodeposition, and vapor phase deposition processes. By coupling theory and *in-situ* characterization to probe materials growth pathways, we aim to understand and predict the thermodynamics of intermediate states (e.g., nucleation) or transient and local conditions (e.g., high chemical potentials of species established by decomposition of reactive precursors) to explain which polymorphs form under particular synthesis conditions. Work is focusing on several target systems involving Ti-O, V-O and Mn-O. Preliminary results from a broad search for new ternary pnictides with useful opto-electronic properties combining high-throughput computation with combinatorial synthesis will also be presented.

4:20 PM

E-II-4: INORGANOMETALLIC CATALYST DESIGN CENTER

[ICDC] Laura Gagliardi[1], Joseph T. Hupp[2]
[1]Dept. Chemistry, Supercomputing Institute, & Chemical Theory Center, University of Minnesota, Minneapolis; [2]Dept. Chemistry, Northwestern University

The Inorganometallic Catalyst Design Center (ICDC) computationally guides the discovery of a new class of energy-science-relevant catalytic materials and understands the underlying structure-function relationships that will lead to further catalyst discovery. Our efforts focus on reactions related to the natural gas conversion, namely selective oxidation of light alkanes to alcohols, especially methane to methanol; dehydrogenation of light alkanes to give alkene intermediates; hydrogenation of alkene intermediates and selective oligomerization reactions. We aim at developing supported single-site catalysts. Some of the supports of choice of ICDC are metal-organic frameworks (MOFs), crystalline porous materials consisting of inorganic nodes and organic linkers. We will give a presentation of the various thrusts of ICDC and the ongoing synergistic activities.

4:40 PM

E-II-5: HOW TO QUANTIFY SIMILARITY IN NANOPOROUS MATERIALS

[CGS] Yongjin Lee[1,3], Kathryn H. Bellwald[2], Berend Smit[1,3]
[1]Dept. Chemistry, University of California, Berkeley; [2]Dept. Mathematics, Ecole Polytechnique Fédérale de Lausanne; [3]Dept. Chemistry, Ecole Polytechnique Fédérale de Lausanne

In different applications of Metal Organic Frameworks (MOFs) and other nanoporous materials one would like to find the best pore structure for a given application. Given that one can synthesize millions of possible MOFs by combining different linkers and metal sites, it is important to obtain some fundamental knowledge on what constitutes the optimal pore shape for a given application. One approach to answer this question is to generate libraries of hypothetical MOFs and screen these libraries using brute force simulation techniques. An alternative approach would be that, once one has a material with a certain performance, one would like to identify all materials in these libraries that look similar as this reference material. In this presentation we focus on the question on how to quantify similarity and how one can use similarity to screen for materials with similar performance in different applications.

SESSION III: TUESDAY, OCTOBER 27, 2015; 8:30 – 10:10 AM; LINCOLN 5

8:30 AM

E-III-1: DESIGNING FUNCTIONAL TWO-DIMENSIONAL MATERIALS BY BENDING

[CCDM]] Liping Yu[1], Adrienn Ruzsinszky[1], John P. Perdew[1], Matthäus Wolak[1], Dan Trainer[1], Ian McKendry[2], Maria Iavarone[1], Michael Zdilla[2], Daniel R.Strongin[2]
[1] Physics, Temple U., [2] Chemistry, Temple U.

The two-dimensional (2D) materials show great potential for flexible electronics and energy applications. They have remarkable mechanical, electronic, and optical properties, which are often coupled to each other. Previous studies suggest that mechanical strain can be used to engineer the electronic properties (e.g., direct-indirect gap transition in MoS_2, the gigantic pseudo-magnetic field in graphene nanobubbles). In this talk, we shall present our recent study on the bending effects in the electronic structure of 2D materials from first-principles calculations and ongoing experiments. We consider graphene, phosphorene, and MoS_2, representing 2D materials of one-atomic layer, two atomic layers, and three atomic layers, respectively. Since the atoms are covalently bonded, we rely upon density functional calculations with the PBE generalized gradient approximation (GGA). Theoretically, we found that the bending can induce very non-uniform strains, resulting in extraordinary electronic properties. For example, when phosphorene is bent along the zigzag direction, in-gap states and a direct-indirect gap transition will occur and are tunable by bending. The band gap and effective masses of carriers can also vary remarkably when 2D materials are bent. In addition, an unambiguous definition of 2D material thickness will also be given based on our results. Experimentally, we will address the effect of bending on the catalytic properties of the materials. The strain in MoS_2 films grown on piezoelectric substrates will also be addressed with scanning probes and Raman spectroscopy. Our results are of fundamental and technological relevance and provide guidance for designing functional 2D materials for applications in which flexuosity is essential.

8:50 AM

E-III-2: TWO-DIMENSIONAL TRANSITION METAL DICHALCOGENIDE MATERIALS THROUGH CHEMICAL VAPOR DEPOSITION SYNTHESIS

[CE] Xiang Ji[1], Xi Ling[1], Yuxuan C. Lin[1], Lin Zhou[1], Kai Xu[1], Ahmad Zubair[1], Tomas Palacios[1], Mildred S. Dresselhaus[1,2], Jing Kong[1]

[1]*Department of Electrical Engineering and Computer Sciences, Massachusetts Institute of Technology;* [2]*Department of Physics, Massachusetts Institute of Technology*

In recent years tremendous efforts have been devoted to the research on two dimensional materials. Among them transition metal dichalcogenides (TMDs) have attracted significant attention owing to their unique structures, remarkable properties, and great potential for a wide range of applications in electronics, optoeletronics, valleytronics, catalysis, etc. The synthesis of high quality large area mono- and few-layer TMD materials is highly desirable for their applications. In this talk I will present the chemical vapour deposition (CVD) approach we have developed to synthesis these TMD materials, two examples, MoS2 and MoTe2 will be discussed. The synthesis strategy of the heterostructures of MoS2 with other 2D materials will also be presented.

9:10 AM

E-III-3: SPIN-POLARIZATION, TOPOLOGICAL, WATER-SPLITTING AND PHOTO-CATALYTIC PROPERTIES OF ULTRATHIN FILMS OF TRANSITION METAL DICHALCOGENIDES WITH OVERLAYERS AND ADSORBATES

[CCDM] Arun Bansil[1], John Perdew[2], Adrienn Ruzsinszky[2], Jianwei Sun[2], Gustavo Scuseria[3], David Srolovitz[4], Maria Iavarone[2], Xiaoxing Xi[2], Alex Gray[2], Goran Karapetrov[5], Mikko Haataja[6], Linyou Cao[7], Weitao Yang[8], Yimei Zhu[9], Eric Borguet[10]

[1]*Physics, Northeastern U.,* [2]*Physics, Temple U.,* [3]*Chemistry, Rice U.,* [4]*MSE, U. Penn,* [5]*Physics, Drexel, MAE & PRISM Princeton U.,* [6]*MSE, NC State U.,* [7] *Chemistry, Duke U.,* [8]*BNL,* [9]*Chemistry, Temple U.*

The ongoing research activities cutting across a number of groups within the CCDM [1-6], which will be discussed in this talk, concern the first-principles modeling of ultrathin films based on transition metal dichalcogenides [TMDs] with various overlayers and adsorbates. Our starting point has been to delineate the thickness dependencies of the electronic structures and spin-polarization of MX_2 films [M=Mo or W; X=S, Se and Te]. Monolayer films are found to display nearly 100% spin-polarized, spin-split states around the valence band maxima with spins aligned oppositely along the out-of-the-plane direction. In bilayer films, polarization of this spin-orbit-coupling induced band-splitting can be switched via an out-of-the-plane external electric field. In bulk MX_2 compounds, the interlayer coupling of the spin-polarized states is weak. We have also examined systematically the electronic structures and topological properties of thin films of elements of groups III-VI, including effects of strains, substrates, and passivations. Ongoing work is aimed at exploring the evolution of spin resolved states in TMD films and their transport and topological characteristics in the presence of overlayers/adsorbates of a variety of elements and alloys [1] using the new functionals being developed within the CCDM [2] for improved modeling of electronic structures. We are exploring the feasibility of experimental synthesis of selected films [3], and working to understand their electronic and morphological characteristics through modeling [4], and scanning tunneling spectroscopy/microscopy and angle-resolved photoemission measurements [3]; water-splitting [5] properties of the films and photo-catalytic properties of noble metal nano-particles placed on the films are also being considered [6].

[1-6] Collaborating groups within the CCDM.

[1] Bernardo Barbiellini[1], Robert Markiewicz[1], Ray Wang[1], Chris Lane[1], Hafiz Hasnai[1], and Baokai Wang[1], [2] Haowei Peng[2], Ana Sousa Alencar[3] and Alejandro Garza[3], [3] Dan Trainer[2], Aleksei Putilov[2] and Matt Wolak[2], [4] Shuyang Dai[5], Jian Han[5], Songsong Zhou[5], and Joel Berry[6], [5] Guoqing Li[7] and Du Zhang[8], [6] Devika Sil[10], Safiya Sylla[10], Ethan Glor[10], Kyle Gilroy[10], Zahra Fakhraai[10] and Svetlana Neretina[10].

9:30 AM

E-III-4: TWO-DIMENSIONAL CHARGE TRANSPORT IN METAL-ORGANIC FRAMEWORKS

[CE] Lei Sun[1], Dennis Sheberla[1], Melis Tekant[1], Efren Navarro-Moratalla[2], Wenbin Li[1], Cong Su[3], Zongyou Yin[3], Dong-Gwang Ha[1], Pablo Jarillo-Herrero[1], Ju Li[1], Marc Baldo[1], Mircea Dincă[1]

[1] Center for Excitonics, Massachusetts Institute of Technology; [2] Depth. Physics, Massachusetts Institute of Technology; [3] Dept. Nuclear Science and Engineering, Massachusetts Institute of Technology

Metal-organic frameworks (MOFs) are crystalline materials made from tunable organic and inorganic building blocks, which together define porous structures with very high pore volume and internal surface area. However, because of poor orbital and energetic overlap between the inorganic and organic components, these materials typically exhibit very poor electrical conductivity. Recently, we have demonstrated that MOFs with two-dimensional structures resembling that of graphite show very high electrical conductivity rivaling graphite itself. Unlike graphite and graphene, however, our bottom-up synthetic materials have intrinsic band gaps that can be tuned by varying the organic ligand and the connecting metal ions. Efforts towards understanding the fundamental transport properties of bulk and single-flake 2D MOFs will be presented, along with the potential applications for such materials.

9:50 AM

E-III-5: SPATIO-TEMPORAL IMAGING OF SPIN, VALLEY, AND THERMAL ENERGY IN TWO-DIMENSIONAL MATERIALS

[SHINES] Max Grossnickle, Fatemeh Barati, Javier Garay, Nathaniel Gabor

University of California, Riverside

Charge carriers in materials are often described as quasiparticles similar to free electrons. This description, however, fails to fully explain the physics of topological materials. For instance, valley-polarized electrons in certain two-dimensional (2D) materials such as transition metal dichalcogenides (TMDs, e.g. MoS_2, WSe_2) and heterostructures (e.g. G/h-BN, bilayer graphene) experience an effective Lorentz force even in the absence of an applied magnetic field. Our vision is to understand and utilize electron topology and its interaction with light to directly manipulate the flow of energy within this new class of materials, and begin to probe the underlying physics of a radically new class of optoelectronic devices. With the emergence of synthesis techniques for 2D materials and their heterostructures, this topological behavior can be readily accessed and exploited; yet new experimental techniques must be developed. We discuss our experiments that probe electron-hole excitations and their transmission within 2D electronic surfaces. Our newly developed microscopy – which combines low temperature transport with a 3T magnetic field and spatially resolved ultrafast photoluminescence, photocurrent, and reflectance spectroscopy - aims to directly image the in-plane flow of energy and charge current at time scales relevant to electronic transport (10^{-2} – 10^{3} ps). The impact of harnessing the valley degree of freedom for optoelectronics ("valleytronics") will be similar to the impact of utilizing the spin degree of freedom in electronics (i.e. spintronics), and the direct imaging of spin, valley, and energy propagation is the first key step toward realization of this vision.

SESSION IV: TUESDAY, OCTOBER 27, 2015; 10:40 – 12:00 PM; LINCOLN 5

10:40 AM – Postdoctoral Researcher Finalist

E-IV-1: PREDICTING AND CONTROLLING POLYMORPHISM IN TRANSITION METAL OXIDES

[CNGMD] Lauren M. Garten[1], Hong Kevin Ding[2], Laura T. Schelhas[3], Kevin Stone[3], Prashun Gorai[1], Paul Ndione[1], Kristin Persson[2], Michael F. Toney[3], Vladan Stevanović[1,4], David S. Ginley[1]
[1] National Renewable Energy Laboratory; [2] Lawrence Berkeley National Laboratory; [3] SSRL Materials Science Division, SLAC National Accelerator Laboratory; [4] Colorado School of Mines

Computational materials design is accelerating the development of technologically relevant materials but, in fact, many materials currently in applications are actually kinetically stabilized (i.e. metastable), thus motivating the CNGMD EFRC to address how metastability can be incorporated computationally. Polymorphism (i.e. different energy structures with the same composition) is a key form of metastability and we seek the ability to synthesize a specific functional polymorph from a set of structures close in energy. We report on a new predictive model describing the energy manifold of polymorphic families. This couples to a computational geometric model to identify substrates for growth of specific polymorphs and ultimately to incorporating both surface energy and kinetics.

Vanadium oxide, VO_2, was chosen as a model system for computation and experiment due to its extensive polymorphism and relevant electronic functionality. Metastable phases of VO_2 (analogous to the Brookite and Columbite polymorphs of TiO_2) are predicted to form within 15 kJ/mol of the ground state but have not been experimentally observed.[1] Epitaxial stabilization of these phases would establish how far above the convex hull substrate templating can be effective and how accessible are novel phases of a complex correlated material. A computational approach to lattice geometry was developed to target polymorphs. The selection boundary conditions limit the two-dimensional strain to less than 9% and the coincident lattice area to less than 1000 Å. TiO_2-Anatase, TiO_2-Brookite, $SrTiO_3$, and $LaAlO_3$ were identified through this modeling as candidates for the stabilization of VO_2 polymorphs. Pulsed Laser Deposition (PLD) was employed to simultaneously deposit on an array of substrates under identical processing parameters. Varying the substrate, under the same processing conditions, did indeed lead to the formation of different polymorphs. Further, TiO_2-Anatase was correctly predicated to stabilize the metastable A VO_2 phase which lies 70 meV/atom above the convex hull and TiO_2-Brookite was predicated to produce a Brookite VO_2 phase, but rather stabilized the high temperature rutile phase of VO_2. The resulting films indicate that the metal-insulator transition was successfully suppressed to below room temperature in these polymorphs. To further build upon this geometric model, the impact of the deposition kinetics on the phase formation in VO_2 was investigated. Amorphous VO_2 films were deposited under varying laser frequency during PLD. *In-situ* synchrotron x-ray diffraction during rapid thermal annealing and traditional annealing indicated variations in the final phase formation due to initial structural differences in films deposited at different frequencies, providing additional insight into the kinetic pathways for phase formation in VO_2.

[1] Mehta, P., Salvador, P. A., and Kitchin, J. R., *Identifying Potential BO2 Oxide Polymorphs for Epitaxial Growth Candidates.* ACS Applied Materials & Interfaces, 2014. **6**(5): p. 3630-3639.

11:00 AM

E-IV-2: DAMAGE PRODUCTION IN SINGLE-PHASE CONCENTRATED SOLID SOLUTION ALLOYS

[EDDE] Lumin Wang[1], Chenyang Lu[1], Yanwen Zhang[2], Roger Stoller[2], Hongbin Bei[2], William J. Weber[2,3], Mo Rigen[4], Shi Shi[4], Ian M. Robertson[4]
[1]*University of Michigan;* [2]*Oak Ridge National Laboratory;* [3]*University of Tennessee;* [4]*University of Wisconsin-Madison*

Computer simulations and modeling have determined that in single-phase concentrated solid-solution alloys, NiFe, NiCo, NiCoFeCr, the presence of the different atomic species induces site-to-site lattice distortions as well as locally disorder environments and these modify the electron, phonon and magnetic systems. These changes impact the energy dissipation processes, which in turn dictate the response to irradiation. For example, the increase in the lifetime of the thermal spike reduces defect production, defect lifetimes are reduced due to changes in thermal expansion, and the formation energy of extended defects, barriers to defect migration as well as the driving force for self-recovery are increased. Consequently, it is predicted that the defect evolution driven by energetic particle bombardment will be dependent on the alloy complexity. Experiments have been conducted to test these predictions.

The formation of extended defects, dislocation loops stacking-fault tetrahedra, voids and ion tracks under different irradiation conditions, particle type, ion mass and ion energy, irradiation temperature have been probed across length scales using multiple different experimental probes. These experiments have shown that in comparison to pure Ni, the production of damage, the depth at which it is produced, and the defect migration rate are decreased in these single-phase concentrated solid solution alloys in the following order NiCoFeCr, NiCo, NiFe and Ni. These dependencies as well as others will be illustrated through detailed analysis of the defect state generated under different irradiation conditions and explained using the insights gained from the companion simulation and modeling efforts.

11:20 AM

E-IV-3: METASTABLE HETEROSTRUCTURAL ALLOYS

[CNGMD] Janet Tate[1], Aaron Holder[2], Bethany Matthews[1], Sebastian Siol[2], John Perkins[2], Andriy Zakutayev[2], Stephan Lany[2], Laura Schelhas[3], Mike Toney[3], Roy Gordon[4], Chuanxi Yang[4], Xizhu Zhao[4], Sang Bok Kim[4], Brian Gorman[5], John Mangum[5], William Tumas[2]
[1]*Oregon State University,* [2]*National Renewable Energy Laboratory,* [3]*SLAC National Accelerator Laboratory,* [4]*Harvard University,* [5]*Colorado School of Mines*

The tailoring of materials properties by alloying is routinely utilized for materials design, i.e. to tune the properties (e.g., the band gap) as required for technological applications. Despite the great success of alloying in isostructural systems (e.g., GaAs/AlAs or Si/Ge), heterostructural alloying remains a fundamentally unexplored area. In heterostructural alloys, the crossover between different crystal structures enables the control of the atomic structure by variation of the composition. The deliberate manipulation of local atomic coordination symmetry introduces an additional materials design parameter. In this talk, we present a complementary theoretical and experimental investigation of novel semiconducting metal chalcogenide alloys with the goal to develop design principles and approaches for utilizing heterostructural alloying as a materials design strategy. We use *ab initio* methods to predict the structural and electronic properties of several novel metal chalcogenide heterostructural alloys with commensurate and incommensurate lattice symmetries and compute their corresponding equilibrium phase diagrams and materials properties. Different experimental deposition methods are employed to validate the predictions and to explore viable approaches for synthesizing metastable heterostructural alloys. Combinatorial sputtering, pulsed laser and atomic layer deposition are employed as non-equilibrium growth techniques to overcome thermodynamic solubility limits and produce metastable thin-film samples across the entire composition range. The prediction, combinatorial synthesis, and characterization of heterostructural alloys exemplify how our integrated research strategy is used to design and realize functional metastable materials. Our approach establishes a new route for the control of structure-property and composition-structure relationships by accessing non-equilibrium phase space to develop new materials with uniquely tailored properties.

11:40 AM

E-IV-4: MODELING PRIMARY DAMAGE PRODUCTION AND EVOLUTION IN CONCENTRATED NIFE

[EDDE] Laurent K Béland[1], Ke Jin[1], German Samolyuk[1], Artur Tamm[2], Yuri Osetsky[1], Hongbin Bei[1], Magdalena Caro[2], Alfredo Caro[2], Roger E. Stoller[1]

[1]Oak Ridge National Laboratory; [2]Los Alamos National Laboratory

Understanding the response of 50%-50% NiFe to ion irradiation is an important step in investigating the potential radiation resistance of multi-component solid solutions, also known as high-entropy alloys. Experimentally, alloying Ni with Fe seems to decrease the damage caused by ion irradiation to doses up to 1 displacement per atom. At higher doses, this alloying has the opposite effect.

In order to help explain and interpret the low dose data, molecular dynamics simulations of displacement cascades were performed. These simulations indicate that alloying Ni with Fe reduces primary damage production. This is explained by three factors: short range interatomic interactions are stiffer for Fe-Fe and Ni-Fe than for Ni-Ni, the decrease in lattice thermal conductivity caused by alloying, and the reduction of extended defect formation in very energetic collision cascades that involve the interaction of subcascades.

The long-time evolution of the defects created by these collision cascades was simulated using a mix of molecular dynamics and the kinetic Activation Relaxation Technique, an on-the-fly kinetic Monte Carlo algorithm. These simulations indicate that slower defect diffusion processes in the alloy leads to different damage accumulation rates in Ni and NiFe, which might explain experimental observations at high dose.

SESSION V: TUESDAY, OCTOBER 27, 2015; 1:30 – 3:10 PM; LINCOLN 5

1:30 PM

E-V-1: PROBING AND UNDERSTANDING THERMAL TRANSPORT AND ENERGY CONVERSION IN NANOSTRUCTURES

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

[1]Massachusetts Institute of Technology, [2]Boston College, [3]Oakridge National Laboratory, [4]Northwestern University, [5]University of Houston

This presentation will start with a brief introduction to the Solid-State Solar-Thermal Energy Conversion Center (S^3TEC) and key advances made in the center over the last year, followed by more in-depth discussion on phonon heat conduction localization in nanostructures. The S^3TEC Center focuses on understanding the thermal transport of electron, phonon, photon, and ions and exploiting the new understanding to advance materials and nanostructures for converting thermal energy into electricity via thermoelectric, thermogalvanic, and thermophotovoltaic effects. Significant progress has been made in the center over the past year in areas such as (1) first-principles simulation of phonon and electron transport and energy conversion properties, (2) understanding of chemical and electronic origins of low thermal conductivity of chalcogenide via simulation and neutron scattering, (3) optical characterization of phonon mean free path distribution by exploiting ballistic phonon transport, (4) electrochemical conversion of low-temperature heat into electricity, and (5) topological states of light. Following these examples, the talk will focus on engineering heat conduction via coherent phonon transport. We already demonstrated phonon transport in superlattices can maintain their phase in the past. Via placing nanoscale scattering centers in superlattices, we further demonstrate that phonon heat conduction can be localized. The experiments are supported by simulations based on the atomic Green's function. The ability to localize phonon heat conduction opens up new opportunities to engineer phonon thermal conductivity via wave effects.

1:50 PM

E-V-2: EXTREME CHEMICAL COMPLEXITY: A ROUTE TO THE CONTROL OF ENERGY DISSIPATION AND DEFECT EVOLUTION IN STRUCTURAL MATERIALS FOR INTENSE RADIATION ENVIRONMENTS

[EDDE] G. Malcolm Stocks[1], German D. Samolyuk[1], Hongbin Bei[1], Ke Jin[1], Brian C. Sales[1], Markus W. Daene[2], Suffian N. Khan[1], Sebastian Wimmer[3], Alfredo Caro[4], Artur Tamm[4], Shijun Zhao[1], Roger E. Stoller[1], Laurent K. Beland[1], Yanwen Zhang[1]

[1]Oak Ridge National Laboratoryl [2]Lawrence Livermore National Laboratory; [3]Ludwig-Maximilians-Universitaet, Germany; [4]Los Alamos National Laboratory

For more than 50 years, development of radiation tolerant structural alloys has relied on alloys containing a few principle elements and minor solute concentrations to obtain multi-phase, engineered microstructures with enhanced properties. Development of a class of single-phase concentrated solid-solution alloys (SP–CSA) provides a new paradigm by exploiting chemical complexity to affect the dissipation of incident radiation energy and the resulting production and accumulation of radiation damage. Of particular interest are the equi-atomic multi-component SP-CSA comprising subsets of the transition metal elements Cr, Mn, Fe, Co, Ni, and Pd that form on an underlying FCC lattice. These include the recently discovered high entropy alloys NiFeCoCr and NiFeCoCrMn. Reduced defect production has been observed due to increasing complexity in Ni, NiCo, NiFe and NiFeCoCr SP-CSAs. We will discuss the effects of disorder on the underlying electronic, magnetic and vibrational states, as well as electron-phonon coupling. The results of *ab initio* Korringa-Kohn-Rostoker coherent-potential-approximation calculations of the electronic structure and electron transport properties are employed. Depending on the number and specific species of alloying elements, the mean free path of electrons can be greatly reduced with a corresponding reduction in the ability of electrons to dissipate energy. To access the relative roles of the intrinsic chemical disorder, we compare the calculated residual resistivity with the experimental measurements. We also show results for the electronic thermal conductivity inferred from the Wiedermann-Franz law, and demonstrate that alloying leads to a reduction of the alloy lattice thermal conductivity compared to pure Ni.

2:10 PM

E-V-3: PHONON THERMAL TRANSPORT IN THERMOELECTRIC MATERIALS FROM FIRST PRINCIPLES

[S^{3}TEC] Olle Hellman[1], Giuseppe Romano[2], Alexie Kolpak[2], Chunhua Li[3], David Broido[3]
[1]Linköping University; Sweden, [2]Massachusetts Institute of Technology, [3]Boston College

Our collaborative research effort for the S3TEC Center has been focused on using predictive computational methods to develop fundamental understanding of phonon thermal transport in materials, and to aid in identifying new candidate materials for thermoelectric (TE) applications. We are using a first principles theoretical approach to calculate phonon thermal conductivity, k_{ph}. This approach combines an accurate determination of interatomic forces from density functional theory with a full solution of the Boltzmann transport equation for phonons. Such *ab initio* methods have demonstrated excellent agreement with measured values for a large number of materials, but to date, most calculations have examined materials with relatively simple crystal structures. Recently our group has been collaborating with other S3TEC members to study more complex crystals that are of interest for TE applications. Among these are traditional thermoelectrics such as Bi_2Te_3 and its alloys, and a promising new class of materials: layered transition metal phosphates (TMPs). S3TEC co-PI Alexie Kolpak and her group have found high electron mobility in one such TMP—$(ZrHPO_3)_2$. In collaboration with Alexie and S3TEC member, Giuseppe Romano, we are working to calculate the k_{ph} for $(ZrHPO_3)_2$. Examination of such materials requires development of advance computational techniques to capture e.g. temperature dependence of anharmonicity and phonon-phonon scattering in systems with large numbers of phonon bands. The anticipated advances will open the door for predictive computational studies of thermal transport in a host of existing complex TE materials as well as facilitating the search for new ones.

2:30 PM

E-V-4: SPECTRALLY SELECTIVE SEMICONDUCTOR ABSORBERS FOR SOLAR THERMAL ENERGY CONVERSION

[LMI] Nathan H. Thomas[1], Austin J. Minnich[1]
[1]California Institute of Technology

Spectrally selective solar absorbers are used in solar thermal energy conversion to convert the energy in sunlight to heat, which can then be used to generate electricity or to provide hot water for domestic use, among many other applications. These absorbers are designed to absorb as much energy from sunlight as possible while minimally emitting in the infrared wavelengths to reduce heat loss. Most selective surfaces cannot reach temperatures greater than 200°C under unconcentrated sunlight due to radiative losses, but achieving these temperatures without concentration is of great interest for higher energy conversion efficiency

and for providing process heat. Here, we develop a 1-D photonic structure of thin films dielectrics with an Ag back-reflector as a selective absorber for high-temperature, non-concentrated solar thermal applications. The simulated structure shows 92% absorptance at normal incidence in the visible regime up until the optical gap of amorphous silicon at 730nm and a sharp transition to an angle averaged thermal absorptance of 6% at longer wavelengths. The thin films are deposited via magnetron sputtering, and the measured room temperature absorptance spectrum of the fabricated structure at an incident angle of 25° exhibits close agreement to the theoretical prediction. The measured IR reflectance shows no appreciable change at temperatures from 50°C up to 500°C and is thermally stable after a 5 hour anneal in air at 450°C. Our approach could enable solar thermal energy conversion with high temperatures without requiring optical concentration.

2:50 PM

E-V-5: TOPOLOGICAL SPIN SEEBECK EFFECT IN TOPOLOGICAL INSULATOR/YTTRIUM IRON GARNET HETEROSTRUCTURES

[SHINES] Zilong Jiang[1], Cui-Zu Chang[2], Massoud Ramezani Masir[3], Chi Tang[1], Yadong Xu[1], Jagadeesh S. Moodera[2], Allan H. MacDonald[3], Jing Shi[1]

[1]University of California, Riverside; [2]Massachusetts Institute of Technology; [3]Department of Physics, University of Texas at Austin

Spin-momentum locking in protected surface states enables efficient electrical detection of magnon decay at a magnetic-insulator/topological-insulator heterojunction. We demonstrate this property by applying a temperature gradient across a thin film of yttrium iron garnet, an insulating ferrimagnet, and forming a heterojunction with $(Bi_xSb_{1-x})_2Te_3$, a topological insulator. The non-equilibrium magnon population which is established at the interface can decay in part by interactions of magnons with electrons near the Fermi energy of the topological insulator. When this decay channel is active, a large electromotive force emerges in the direction perpendicular to the in-plane magnetization of yttrium iron garnet. We refer to this particularly simple and direct example of an electromotive force induced by a temperature gradient in a magnetic system, as the topological spin Seebeck effect. By varying the Bi fraction x from 0 to 1 to shift the surface state Dirac point and the Fermi energy relative to the bulk topological insulator bands, $(Bi_xSb1_{-x})_2Te_3$ is tuned from an electron-doped metal, to a topological insulator, and finally to a hole-doped metal. We show experimentally that whereas neither Bi_2Te_3 (x=1) nor Sb_2Te_3 (x=0) generates a sizable spin Seebeck signal, the thermally induced electromotive force strengthens precipitously as the topological insulator approaches a bulk insulating state from either side. The enhanced, tunable spin Seebeck effect which occurs when the Fermi level lies in the bulk gap offers unique advantages over the usual spin Seebeck effect in metals for highly efficient spin-electrical conversion and therefore opens up new possibilities in spintronics.

F. CATALYSIS

SESSION I: MONDAY, OCTOBER 26, 2015; 1:10 – 2:50 PM; LINCOLN 3/4

1:10 PM

F-1-1: ELECTRON BIFURCATION IN MANAGING EFFICIENT CONVERSION OF ELECTROCHEMICAL POTENTIAL INTO CHEMICAL BONDS

[BETCy] Michael Adams[1], Diep Nguyen[1], Gerti Schut[1], Gina Lipscomb[1], John Hoben[2], Anne-Frances Miller[2], Cara Lubner[3], David Mulder[3], Michael Ratzloff[3], Katherine Chou[3], Pin-Ching Maness[3], Paul King[3], David Jennings[4], Anne K. Jones[4], Kathryn Fixen[5], Yanning Zheng[5], Carrie Harwood[5], Rhesa Ledbetter[6], Lance Seefeldt[6], Saroj Poudel[7], Monika Tokmina-Lukaszewska[7], Amaya Garcia-Costas[7], Oleg Zadornyy[7], Zachary Jay[7], Ross Carlson[7], Eric Boyd[7], Brian Bothner[7] and John Peters[7]

[1]University of Georgia, [2]University of Kentucky, [3]National Renewal Energy Laboratory, [4]Arizona State University, [5]University of Washington, [6]Utah State University, [7]Montana State University

Until recently it was thought that all cellular energy-requiring processes are coupled directly or indirectly to the hydrolysis of the high energy chemical adenosine triphosphate (ATP) to adenosine diphosphate (ADP, $\Delta G^{0\prime}$ = - 30 kJ/mol). In 2009, a new ATP- independent mechanism of energy conservation known as electron bifurcation was discovered. Electron bifurcation involves the coupling of exergonic and endergonic redox reactions resulting in the efficient use of the available free energy in the coupled reaction. Two redox steps are coupled together such that the intermediate state is exceedingly unstable, i.e. a highly reactive one-electron intermediate is generated that can drive low oxidation reduction potential reactions. For example, bifurcating hydrogenases oxidize the biological electron carrier ferredoxin (E_0' = - 0.50 V) and spontaneously reduce protons to hydrogen (E_0' = - 0.42 V). Simultaneously, the free energy that is released ($\Delta G^{0\prime}$ = - 15 kJ/mol) couples the unfavorable oxidation of a second biological electron carrier, NADH (E_0' = - 0.32 V), to proton reduction to hydrogen. Bifurcating enzymes are of key importance in managing electron flow resulting in the conservation of energy and efficient conversion of electrochemical potential to chemical bonds. However, the mechanisms of enzymatic electron bifurcation are not understood. In the BETCy EFRC, bifurcating enzymes are being investigated by biochemical, spectroscopic, kinetic and structural techniques. An understanding of electron bifurcation in nature's catalysts could have profound implications in controlling electron flow in the design and implementation of highly efficient energy conservation and energy production processes.

1:30 PM

F-I-2: SINGLE-SITE NICKEL HYDROGENATION CATALYST SUPPORTED ON A METAL-ORGANIC FRAMEWORK PRODUCED *VIA* ATOMIC LAYER DEPOSITION

[ICDC] Omar K. Farha[1,2], Zhanyong Li[1], Varinia Bernales[3], Aaron B. League[3], Neil M. Schweitzer[1], Aaron W. Peters[1], Andrew "Bean" Getsoian[4], Aleksei Vjunov[5], John Fulton[5], Ana E. Platero-Prats[6], Timothy C. Wang[1], Karena W. Chapman[6], Jeffrey T. Miller[4,7], Johannes A. Lercher[5], Christopher J. Cramer[3], Laura Gagliardi[3], Joseph T. Hupp[1]

[1]Department of Chemistry, Northwestern University; [2]Department of Chemistry, Faculty of Science, King Abdulaziz University, Saudi Arabia; [3]Department of Chemistry, Supercomputing Institute, and Chemical Theory Center, University of Minnesota, Minneapolis; [4]Chemical Science and Engineering Division, Advanced Photon Source, Argonne National Laboratory; [5]Institute for Integrated Catalysis, Pacific

Northwest National Laboratory; [6]X-ray Science Division, Advanced Photon Source, Argonne National Laboratory; [7]School of Chemical Engineering, Purdue University

Developing supported single-site catalysts is an important goal in heterogeneous catalysis, since the well-defined active sites afford opportunities for detailed mechanistic studies, thereby facilitating the design of improved catalysts. Compared to conventional catalyst supports such as zeolites and activated carbons, metal–organic frameworks (MOFs), a versatile class of crystalline porous materials consisting of inorganic nodes and organic linkers, are more readily tuned structurally by rational design to impart functionalities. In this presentation, we will describe the process of conducting atomic layer deposition (ALD) in a MOF (AIM) to install nickel ions uniformly and precisely within mesoporous NU-1000, denoting as Ni-AIM. The modified node structure in Ni-AIM is proposed, revealing the single-site nature of the nickel atoms. Of particular note, after a pretreatment with H_2 at 200 °C under flow condition, Ni-AIM exhibits remarkable ethylene hydrogenation activity, stability, and regenerability. A quantum chemical characterization of the catalyst and the catalytic process complements the experimental results. Given the large number of available ALD precursors and the generality of the AIM methodology, this contribution is a starting point for the development of a new class of single-site heterogeneous catalysts for the transformation of volatile substrates, *e.g.*, hydrocarbons derived from the exploitation of shale oil deposits. With validation of computational modeling protocols, this emerging class of materials should prove ripe for the discovery of additional new catalysts guided by theoretical predictions.

1:50 PM

F-I-3: USING SECOND-COORDINATION SPHERE STRUCUTRAL DYNAMICS TO CONTROL H_2 PRODUCTION RATES IN $[\mathrm{NI}(\mathrm{P}^{R}_{2}\mathrm{N}^{R'}_{2})_{2}]^{2+}$ CATALYSTS

[CME] Molly O’Hagan, Allan Jay P. Cardenas, Monte L. Helm, R. Morris Bullock
Pacific Northwest National Laboratory

Understanding how to precisely control substrate delivery and product removal from the active site of molecular catalysts is an important aspect of catalyst design. In the Center for Molecular Electrocatalysis, we have focused on using pendant amines in the secondary coordination sphere of nickel complexes to relay protons to and from the metal center for H_2 production and oxidation catalysis, similar to the [Fe-Fe]-hydrogenase active site. We utilize NMR spectroscopy to map and quantify the pathways of proton movement in these systems both intra- and intermolecularly. We have found that intermolecular proton transfer can represent a bottleneck in H_2 production catalysis due to protonation being kinetically preferred at nonproductive sites. Catalytic rates can be increased in these systems by disfavoring nonproductive protonation, which can be achieved by changing the reaction medium to include water. Current work has found that controlling the catalyst’s structural dynamics can also be used to disfavor protonation at nonproductive sites, and therefore, dramatically affect the catalytic rates observed facilitating rates greater than 10^6 s^{-1} in organic solvents as well as aqueous protic ionic liquids.

2:10 PM

F-I-4: DEFINING DETERMINANTS OF CATALYTIC BIAS IN ENZYME CATALYZED PROTON-COUPLED ELECTRON TRANSFER REACTIONS

[BETCy] Anne Jones[1], Garrett Williams[1], Jacob Artz[2], Saroj Poudel[2], David Mulder[3], Eric Boyd[2], Paul King[3] and John Peters[2]
[1]Arizona State University, [2]Montana State University, [3]National Renewable Energy Laboratory

Catalytic bias describes the phenomenon in which a catalyst has an inherent property of lowering the activation barrier and affecting the rate of a reaction differently in the forward and reverse reactions. We believe this to be an important property in proton-coupled electron transfer reactions and an important factor in directing efficient coupling of electrochemical potential to chemical bond formation. Hydrogenases catalyze reversible hydrogen oxidation, the simplest proton-coupled electron transfer reaction and, as such, are ideal model systems for investigations aimed at delineating the structural determinants of catalytic bias is enzyme catalyzed reactions. Our hypothesis is that catalytic biases of enzymes that catalyzes proton-coupled electron transfer reactions can be modulated by differences in the amino acid environment of the metal cluster sites, differences in the oxidation-reduction potentials, and the nature and availability of proton donor and acceptor groups at the active site. We are using a pair of hydrogenases with a high degree of primary amino acid sequence conservation that have been shown to have markedly different catalytic biases. Structural comparisons of these related hydrogenases reveal key differences in the active site and accessory cluster environments that are being probed as hypothetical determinants through a combination of biochemical, spectroscopic and electrochemical approaches.

2:30 PM

F-I-5: CENTER FOR BIO-INSPIRED ENERGY SCIENCE

[CBES] Samuel I. Stupp[1-4]
[1]Department of Chemistry, Northwestern University; [2]Department of Materials Science and Engineering, Northwestern University; [3]Department of Biomedical Engineering, Northwestern University; [4]Simpson Querrey Institute, Northwestern University

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 members have innovated in the areas of self-assembly, the interface of biology and materials science, as well as in theory and simulation of materials. CBES is scientifically organized into three main thrusts on materials with biomimetic functions, colloidal machines, and biomimetic modes of charge transport. **Thrust 1** will focus on materials with biomimetic functions related to inter-conversion between chemical and mechanical energy (as muscles do), particles inspired by biological organelles that utilize feedback mechanisms to mediate chemical reactions, and adaptive materials. **Thrust 2** investigates active matter in the form of colloidal machines, which are systems of nanometer to micrometer scale colloids that behave collectively far from equilibrium. **Thrust 3** explores artificial matter that could exhibit bio-inspired mechanisms of electron and ion transport, such as those of transmembrane ion pumps, ratchets, and photosynthetic systems.

SESSION II: MONDAY, OCTOBER 26, 2015; 3:20 – 5:00 PM; LINCOLN 3/4

3:20 PM – Postdoctoral Researcher Finalist

F-II-1: DYNAMIC EVOLUTION OF NANOPOROUS GOLD CATALYSTS DURING ACTIVATION AND SELECTIVE OXIDATION REACTIONS

[IMASC] Branko Zugic[1], Lucun Wang[1], Michelle L. Personick[1], Matthew Montemore[2], Christian Heine[3], Luan Nguyen[4], Nare Janvelyan[1], Dmitri Zakharov[5], Eric Stach[5], Miquel Salmeron[3], Monika M. Biener[6], Juergen Biener[6], Franklin (Feng) Tao[4], Efthimios Kaxiras[2], Robert J. Madix[2], Cynthia M. Friend[1, 2]

[1]Department of Chemistry and Chemical Biology, Harvard University; [2]School of Engineering and Applied Sciences, Harvard University; [3]Materials Science Division, Lawrence Berkeley National Laboratory; [4]Department of Chemical and Petroleum Engineering and Department of Chemistry, University of Kansas; [5]Center for Functional Nanomaterials, Brookhaven National Laboratory; [6]Nanoscale Synthesis and Characterization Laboratory, Lawrence Livermore National Laboratory

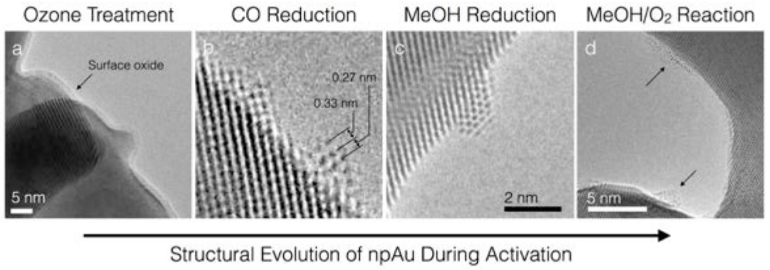


Figure 1. E-TEM study showing the structural rearrangements of the npAu surface after (a) ozone treatment (activation) (b) reduction by CO, showing removal of oxide and presence of defects (c) further reduction by MeOH, resulting in crystallization and (d) methanol oxidation reaction conditions, showing the fully evolved catalyst structure with regions of 'activity'.

Bimetallic catalysts are critical to the development of tunable material properties in order to address energy inefficiencies in catalytic processes. The dynamic nature of these materials has often been overlooked in their design. Nanoporous gold (npAu) is an unsupported metallic Au alloy with dilute Ag content. It requires activation with ozone in order to selectively catalyze the O-assisted coupling of methanol and other alcohols. We have shown that treatment of npAu by ozone at 150 °C followed by exposure to a methanol-oxygen mixture results in highly active and stable catalysts.[1] To understand the structural evolution and catalytic activity after ozone treatment, we have used a combination of reactor studies, theoretical calculations, atmospheric pressure X-ray photoelectron spectroscopy (AP-XPS), and electron microscopy (including environmental-TEM). The results show that dynamic structural changes take place at the npAu surface at different stages of the activation process as shown in Figure 1.[2] The ozone treatment causes near-complete oxidation of the npAu surface that results in amorphous layers of silver/gold oxides. This oxide layer gives rise to non-selective products (i.e. combustion). However, the 'oxidic' oxygen can be removed by CO titration, leading to metastable structures that are reactive selectively to methanol. These quasi-ordered structures appear to be responsible for the selective oxidation activity of npAu and are predicted by DFT studies. The results represent the potential of correlated *in-situ*/DFT studies and highlight their ability to improve our understanding of the dynamics of bimetallic catalysts.

[1] Personick, M. L.; Zugic, B.; Biener, M. M.; Biener, J.; Madix, R. J.; Friend, C. M. *ACS Catalysis*. July 2, 2015, pp 4237–4241.

[2] Zugic, B.; Personick, M. L.; Janvelyan, N.; Wang, L.-C.; Zakharov, D.; Stach, E. A.; Madix, R. J.; Friend, C. M. *In Preparation.*

3:40 PM

F-II-2: UNIFORM HETEROBIMETALLIC ACTIVE SITES IN METAL-ORGANIC FRAMEWORKS

[ICDC] Connie C. Lu[1], Anthony B. Thompson[1], Dale Pahls[1], Camille D. Malonzo[1], Stephen J. Tereniak[1], Timothy Wang[2], Laura Gagliardi[1], Andreas Stein[1], R. Lee Penn[1], Omar K. Farha[2], Joseph T. Hupp[2]
[1]*Department of Chemistry, Supercomputing Institute, and Chemical Theory Center, University of Minnesota;* [2]*Department of Chemistry, Northwestern University*

Nature uses heterometallic clusters of earth abundant metals to catalyze challenging chemical reactions of energy relevance. We seek to configure heterobimetallic oxide clusters with exacting control and selectivity inside metal-organic frameworks (MOFs), focusing primarily on first-row transition metals because of their availability and low cost. One outcome of this work will be a diverse library of potentially catalytic materials featuring heterobimetallic active sites. The porosity and crystallinity of MOFs are exploited to create uniform sites that are permanently isolated and accessible.

We have demonstrated the feasibility of using a heterobimetallic organometallic complex as a synthetic precursor for simultaneously installing two different metals in the MOF, NU-1000. The synthesis involves immobilizing a well-defined heterobimetallic complex in NU-1000, and subsequent calcination to remove the organic ligand and create a naked, heterobimetallic oxide cluster, which represents a potential catalytic site. The proof of concept of this approach was demonstrated for the Co-Al pairing. Both the CoAlL@NU-1000 material (where L is the organic ligand used to stabilize the bimetallic coordination complex) and its calcined analogue, $CoAlO_x$@NU-1000, have been characterized by a suite of physical methods, suggesting that a single Co-Al group is installed per Zr_6-node in the MOF.

Catalytic studies are underway to discover and understand reactivity differences between Co-O-Al, Co-O-Co, and Al-O-Al sites in NU-1000. Computational studies are ongoing to elucidate both the structure and reactivity of active sites. We are also developing more thermally robust, all inorganic supports by nanocasting $CoAlO_x$@NU-1000 with silica precursors and subsequent processing to remove the organic linkers.

4:00 PM

F-II-3: NMR STUDIES OF HETEROGENEITY, DYNAMICS, AND PHASE EQUILIBRIA IN MOFS

[CGS] Jeffrey A. Reimer[1,2], Jun Xu[1], Velencia Witherspoon[1], Eric Scott[1], Thomas Popp[2]
[1]*Department of Chemical and Biological Engineering, University of California, Berkeley;* [2]*Department of Chemistry, University of California, Berkeley*

Gas separations in metal-organic frameworks (MOFs) are well known to be sensitive to the number, type, and distribution of metal atoms linkers that comprise them. Transport of gases in these materials is partially governed by the local dynamics of adsorbates within the framework, and adsorption into MOFs is governed by the thermodynamic behavior of the adsorbate. In collaboration with our co-PIs, I will show how we have addressed these three topics using solid-state NMR spectroscopy of relaxometry. The apportionment of linkers within multivariate-MOFs has already been establish by us [2013 *Science* v341 882-885], and we are now working on discerning the apportionment of metal atoms in mixed metal MOF-74 (organic linker = 2,5-dioxido-1,4-benzenedicarboxylate). In the case of Ni/Mg MOF-74, super-transferred hyperfine coupling constants may emerge as the mechanism for ascertaining their apportionment. Variable temperature NMR studies of gas adsorbates, and methane and CO_2 in particular, reveal detailed pictures of how these molecules interact with the MOF moieties (e.g. diamine-appended Mg_2(dopbdc), dopbdc^{4-} = 4,4′-dioxidobiphenyl-3,3′-dicarboxylate). Finally, we were surprised to discover that the critical point of benzene and xylenes can be systematically adjusted when they are adsorbed within MOF-5 (organic linker = 1,4-benzenedicarboxylate). This may be very important in gas separations and/or heterogeneous catalysis.

4:20 PM

F-II-4: PROBING ACTIVE SITES ON NPAUAG ALLOY

[IMASC] Lu-Cun Wang[1], Matthew Montemore[2], Michelle L. Personick[1], Efthimios Kaxiras [2,3], Robert J. Madix[1]

[1] Department of Chemistry and Chemical Biology, Harvard University; [2] School of Engineering and Applied Sciences, Harvard University; [3] Department of Physics, Harvard University

Nanoporous Au catalysts have remarkable activity and selectivity for selective aerobic oxidation of alcohols. The activation of O_2 is key to the initiation of this reaction, as adsorbed atomic oxygen (O) is the active site for reaction. Nanoporous Au (npAg/Au) has a porous metallic structure with ligaments circa 20 nm in size containing a few percent by weight of silver. The residual Ag is thought to be critical for O_2 activation, but its role, and the nature and surface density of the sites for its dissociation remains unknown. We have examined the activation of molecular oxygen on np(Ag/)Au using transient pressure methods. For npAg/Au microspheres containing 1 at.% Ag, the saturation of adsorbed O plateaus at 4×10^{-3} monolayer at 425 K, indicating that the site density affecting O_2 dissociation comprises only 0.1% of the surface. Spillover of O onto the entire surface is not observed. O_2 dissociation at these sites exhibits an activation energy of 5.0 kcal/mol, and the area averaged dissociation probability of O_2 at 423 K is correspondingly low (1×10^{-7}). Following activation of the catalyst with ozone, methanol removes adsorbed oxygen in two stages. First, a very reactive state comprising over 95% of the adsorbed O is removed by both CO and methanol to form CO_2. The remaining adsorbed oxygen activates methanol selectively to formaldehyde and methyl formate. Analysis reveals that the activation of methanol to formaldehyde is proportional to the surface concentration of adsorbed O.

4:40 PM

F-II-5: ATOMIC LAYER DEPOSITION (ALD) IN METAL ORGANIC FRAMEWORKS (MOFS)

[ICDC] In Soo Kim[1], Joshua Borycz[2], Ana Platero-Prats[3], Samat Tussupbayev[2], Martino Rimoldi[4], Laura Fernandez[2], Wei-Guang Liu[2], Aaron League[2], Varinia Bernales[2], Zhangyong Li[4], Sol Ahn[4], Timothy C. Wang[4], Alexksei Vjunov[5], Johannes Lercher[5], Donald Truhlar[2], Omar K. Farha[4,6], Joseph T. Hupp[1,4] Laura Gagliardi[2], Karena Chapman[3], Christopher J. Cramer[2], Alex B. F. Martinson[1]

[1]Materials Science Division, Argonne National Laboratory; [2]Department of Chemistry, Supercomputing Institute, and Chemical Theory Center, University of Minnesota, Minneapolis; [3]X-ray Science Division, Argonne National Laboratory; [4]Department of Chemistry, Northwestern University; [5]Fundamental Computational Sciences, Pacific Northwest National Laboratory; [6]Department of Chemistry, Faculty of Science, King Abdulaziz University, Saudi Arabia

Uniform mesoscale structures which are amenable to full experimental structural characterization and rigorous computational modeling are ideal systems for catalytic studies. We present a post-synthetic functionalization strategy for large-pore (3 nm) metal organic frameworks (MOFs) that enables the accurate placement of new atoms on a crystallographically precise framework in high density. Combined with the diverse palette of atomic layer deposition (ALD) chemistries, ALD in MOF (AIM) allows access to a diversity of functional few-atom clusters – provided that unique chemical compatibility and gas diffusion challenges can be overcome. We computationally and experimentally investigate the reaction of model ALD precursors with a $[Zr_6(\mu_3\text{-}O)_4(\mu_3\text{-}OH)_4(OH)_4(H_2O)_4]^{8+}$ MOF node. In the best case we observe self-limiting, stoichiometric, and uniform reactions of the ALD precursors with node hydroxyls without significant loss of MOF crystallinity or pore volume.[1] The reaction mechanism and resulting metal locations are deduced using DFT and solved via synchrotron-based pair distribution function x-ray characterization, consistent with computation. The number density of the reactive handles (-OH and $-H_2O$) is further found to be adjustable via node dehydration at elevated temperature, which enables tunable metal loading. Metal atoms on the node are further found to be stable to post-processing under inert atmosphere up to hundreds of degrees, enabling structurally precise catalytic studies at relevant temperatures. The experiments are complemented by extensive modeling by density functional theory electronic structure calculations.

SESSION III: TUESDAY, OCTOBER 27, 2015; 8:30 – 10:10 AM; LINCOLN 3/4

8:30 AM

F-III-1: SELECTIVE METHANOL DEHYDROGENATION TO FORMALDEHYDE ACROSS A CONTINUUM OF STRUCTURES: FROM SINGLE CRYSTALS TO NANOPOROUS ALLOYS

[IMASC] Maria Flytzani-Stephanopoulos[1], JunJun Shan[1], Jilei Liu[1], Felicia Lucci[2], Charles Sykes[2], Jianchao Ye[3], Juergen Biener[3]

[1] Department of Chemical and Biological Engineering, Tufts University; [2] Department of Chemistry, Tufts University; [3] Lawrence Livermore National Laboratory

PtCu and NiCu alloys were prepared in this work as Cu nanoparticles with small amounts of the Pt or Ni added by galvanic replacement and other techniques. Both nonporous and nanoporous materials were prepared and tested for the oxygen-free dehydrogenation of methanol to formaldehyde and hydrogen. In the presence of water serving as dehydrogenation site and hydrogen stabilizer, both catalysts were 100% selective and an order of magnitude more active than monometallic Cu. The dehydrogenation activity is attributed to isolated Pt or Ni atoms acting as dehydrogenation sites and the weak binding of formaldehyde on the Cu surface.

8:50 AM

F-III-2: ADVANCES IN MATERIALS SYNTHESIS FOR BIOMASS CONVERSION

[CCEI] Michael Tsapatsis[1], Wei Fan[2], Dionisios G. Vlachos[3]

[1]Department of Chemical Engineering and Materials Science, University of Minnesota; [2]Chemical Engineering Department, University of Massachusetts Amherst; [3]Department of Chemical and Biomolecular Engineering, University of Delaware

The efficient conversion of biomass requires novel materials that possess porosity varying over multiple length scales, to enable fast transport and shape selectivity, and suitable active centers, to carry out selective chemical transformations. In this talk, we will present such examples of materials developed in CCEI for biomass conversion. For instance, we will discuss the first of its kind single-unit-cell Sn-MFI, with the detectable Sn uniformly distributed and exclusively located at framework sites.[1] These materials are synthesized in a direct, single-step synthesis based on repetitive branching caused by rotational intergrowths. We will demonstrate the performance of these materials for important thermocatalytic processes of cellulose to fuels and bioproducts.

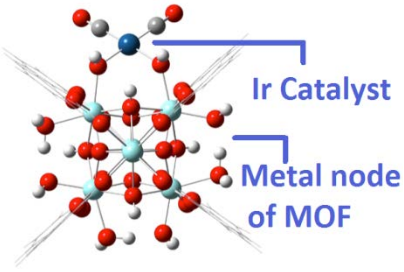
[1] L. Ren, Q. Guo, P. Kumar, M. Orazov, D. Xu, S. M. Alhassan, K. A. Mkhoyan, M. E. Davis, and M. Tsapatsis, "Self-Pillared, Single-Unit-Cell Sn-MFI Zeolite Nanosheets and Their Use for Glucose and Lactose Isomerization," *Angewandte Chemie International Edition,* **54(37)**, 10848-10851, (2015). [DOI:10.1002/anie.201505334]

9:10 AM – Postdoctoral Researcher Finalist

F-III-3: METAL-ORGANIC FRAMEWORK NODES AS NEARLY IDEAL SUPPORTS FOR MOLECULAR CATALYSTS: NU-1000- AND UIO-66-SUPPORTED IRIDIUM COMPLEXES FOR ETHYLENE HYDROGENATION AND DIMERIZATION

[ICDC] Samuel O. Odoh[1], Dong Yang[2], Timothy Wang[3], Omar K. Farha[3], Joseph T. Hupp[3], Christopher Cramer[1], Bruce C. Gates[2], Laura Gagliardi[1]

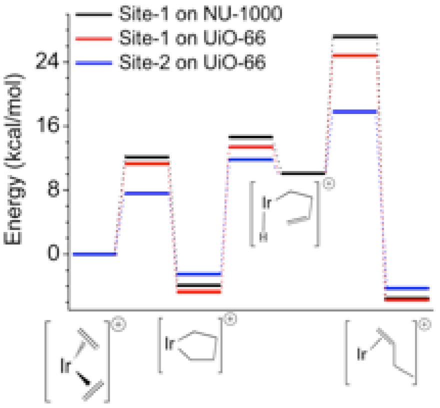
[1]*Department of Chemistry, Chemical Theory Center, and Supercomputing Institute, University of Minnesota*; [2]*Department of Chemical Engineering & Materials Science, University of California, Davis*; [3]*Departments of Chemistry and Chemical and Biological Engineering, Northwestern University*



Iridium sites at the Zr6 nodes of NU-1000.

The Inorganometallic Catalyst Design Center (ICDC) guides the discovery of supported cluster catalysts by integrating computational modeling with experiments in pristine systems that are amenable to high-throughput search and discovery methods. Metal-organic frameworks (MOF) with Zr_6 nodes, UiO-66 and NU-1000, were investigated as supports for $Ir(CO)_2$ and $Ir(C_2H_4)_2$ complexes. Quantum chemical calculations based on density functional theory (DFT) were employed to explore the local structure of the Ir-based catalysts at the MOF nodes, the number and nature of sites in each MOF. They provided results that are in good agreement with infrared and X-ray absorption fine structure spectra.

DFT calculations were also employed to investigate the mechanism for ethylene dimerization and hydrogenation at different catalytic sites. The reactivity of node-supported $Ir(CO)_2$ with C_2H_4 and the catalytic activity and selectivity of the species initially present as $Ir(C_2H_4)_2$ for ethylene hydrogenation and dimerization are affected by the node. We are currently performing DFT computations to show that the catalytic activity of Ir species deposited in the NU-1000 MOF can be improved by pre-treating this MOF with aluminum. In this case, the Lewis acidity of the aluminumlayer modifies the Ir sites, and thereby modulates the catalytic pathway of ethylene dimerization.



Calculated mechanism for ethylene dimerization at the Iridium sites deposited on MOF nodes.

Reference: Yang D., Odoh S. O., Wang, T.C., Farha O. J., Hupp J., Cramer, C. J., Gagliardi L., Gates B. C., "Metal-organic framework nodes as nearly ideal supports for molecular catalysts: NU-1000- and UiO-66-supported iridium complexes" *J. Am. Chem. Soc.* **2015**, 137, 7391.

9:30 AM – Postdoctoral Researcher Finalist

F-III-4: ACID GAS INTERACTION WITH OXIDE NANOSHAPES WITH WELL-DEFINED SURFACE FACETS

[UNCAGE-ME] Uma Tumuluri[1], Meijun Li[1], Brandon Cook[2], William Mounfield[3], Joshua D. Howe[3], Bobby Sumpter[2], Krista S. Walton[3], David S. Sholl[3], Sheng Dai[1], Zili Wu[1,2]

[1] Chemical Science Division, Oak Ridge National Laboratories; [2] Center for Nanophase Material Science, Oak Ridge National Laboratories; [3] School of Chemical & Biomolecular Engineering, Georgia Institute of Technology

Acid gases such as CO_2, SO_2, NO_x are ubiquitous in the energy applications. Nanoshaped oxides such as CeO_2, TiO_2 are widely used as adsorbents and catalysts in the energy applications. Prolonged interaction with the corrosive acid gases affects the surface and bulk properties of both metal catalysts and oxide supports. Fundamental understanding on how the acid gases interact with the catalysts and the effect of the surface structure, defects and dopants on the acid gas interaction is very important for designing more stable catalysts/adsorbents. To gain a fundamental understanding of how CeO_2 and TiO_2 are affected by the acidic CO_2/SO_2, we investigated the effect of the surface structure of CeO_2/TiO_2 on the nature and the strength of adsorbed CO_2 and adsorbed SO_x using in situ IR spectroscopic and mass spectrometric techniques. CeO_2 nanoparticles with different morphologies: rods, cubes, and octahedra and metal organic framework (MOF)-derived CeO_2 were used to represent different CeO_2 surfaces. TiO_2 nanoparticles with different morphologies: rods, disks, and octahedra and carbide-derived TiO_2 were used to represent different TiO_2 surfaces. IR spectroscopic studies indicate that SO_2 adsorbs in the form of surface and bulk sulfite/sulfates on CeO_2 and TiO_2 nanoparticles, and CO_2 adsorbs in the form of carbonates (monodentate, bidentate and bridged). The degree of the formation of adsorbed species depends on the shape of the CeO_2 and TiO_2 nanoparticles. The IR results were well substantiated by theoretical calculations of the structures and adsorption strength of the CO_2/SO_x species on intact and oxygen-vacancy involved CeO_2/ TiO_2 nanoparticles.

9:50 AM

F-III-5: INFORMING CATALYST DESIGN THROUGH FUNDAMENTAL STUDIES

[IMASC] Cynthia.M. Friend[1], Fanny Hiebel[1], Bonggeun Shong[1], Stavros Karakolas[1], Yunfei Xu[1], Matthew Montemore[2], Efthimios Kaxiras[2,3], Robert.J. Madix[1]

[1] Department of Chemistry and Chemical Biology, Harvard University; [2] School of Engineering and Applied Sciences, Harvard University; [3] Department of Physics, Harvard University

Fundamental surface science experiments in conjunction with atomistic theory are used to develop a molecular-scale mechanism for bonding and reactivity on Au(111) and (110) and on nanoporous Au (npAu), an alloy with ~3% Ag. The key for bond activation on gold is adsorption of oxygen atoms that lead to selective reaction on all surfaces investigated. Key factors that control bonding and reactivity include weak (van der Waal's) interactions between molecular species and the surface, surface reconstruction, and the relatively weak bonding of molecules to Au. The binding and reactivity of key oxygen-containing molecules, e.g. alcohols and organic acids, were studied. For example, methanol is selectively coupled to methyl formate on both Au(111) and Au(110) that are pre-covered by adsorbed O. The selectivity for methyl formate production depends on the initial coverage of oxygen. Similar reactivity is also observed for npAu both under ultrahigh vacuum conditions and in a flow reactor at atmospheric pressure. These studies establish a bridge between ultrahigh vacuum surface studies on well-defined surfaces and complex materials, e.g npAu, that function as robust working catalysts at atmospheric pressure. The work described provides a road map for relating fundamental studies to catalytic behavior that can be broadly applied.

SESSION IV: TUESDAY, OCTOBER 27, 2015; 10:40 – 12:00 PM; LINCOLN 3/4

10:40 AM

F-IV-1: DIELS-ALDER AND DEHYDRATION REACTIONS OF BIOMASS-DERIVED FURAN AND ACRYLIC ACID FOR THE SYNTHESIS OF BENZOIC ACID

[CCEI] Eyas Mahmoud[1], Jingye Yu[2], Raymond J. Gorte[2], Raul F. Lobo[1]
[1]Department of Chemical and Biomolecular Engineering, University of Delaware; [2]Department of Chemical and Biomolecular Engineering, University of Pennsylvania

Routes to benzoic acid starting from furan—obtained from hemicellulose-derived furfural—and methyl acrylate are reported. These routes involve Diels-Alder and dehydration reactions of furan and methyl acrylate (or acrylic acic) in a two-step reaction protocol that minimizes side reactions. The Diels-Alder reaction of furan and methyl acrylate (or acrylic acid) was run at 298 K and was catalyzed by Lewis acidic (Hf-, Zr- and Sn-Beta) zeolite catalysts achieving a relatively high turnover frequency (~2 h^{-1}) with no side reactions detected. The dehydration of the product oxanorbornene was performed homogeneously at low temperatures (298 to 353 K) in mixtures of methanesulfonic acid and acetic anhydride in 96% yield. This is much more favorable than the 1.7% yield of methyl benzoate obtained for the dehydration of the oxanorbornene in neat methanesulfonic acid. The effect of oxanorbornene concentration and stereochemistry were found not to decrease yield to aromatics while dehydration of the carboxylic acid form of the oxanorbornene led to a drop in selectivity to 43% at complete conversion in mixtures of methanesulfonic acid and acetic anhydride. This reaction sequence could be an important entry point for selectively directing high-yield, hemicellulose-derived furans to aromatic products used in the existing chemical process industry.

11:00 AM

F-IV-2: DELIVERING FIT-FOR-PURPOSE BIOFUELS

[C3Bio] John Degenstein[1], Priya Murria[2], Mckay Easton[1], Richard Caulkins[1], Ian Smith[1], Emre Gencer[1], Taufik Ridha[1], Hanyu Zhu[2], John Nash[2], Rakesh Agrawal[1], Fabio Ribeiro[1], W. Nicholas Delgass[1], Hilkka I. Kenttämaa[2], Maureen C. McCann[3]
[1]Department of Chemical Engineering, Purdue University, [2]Department of Chemistry, Purdue University, [3]Department of Biological Sciences, Purdue University.

Biofuels are currently blended with conventional fuels because they have different combustion characteristics and properties. To replace liquid hydrocarbon fuels such as jet fuel or gasoline with drop-in biofuels, conversion processes are required that convert intact lignocellulosic biomass to an oxygen-free, energy-dense liquid fuel, using a minimal number of steps in potentially dispatchable (mobile) reactor units. Such fuels must be fully compatible with existing and future engines such that their use is invisible to the user. C3Bio researchers have developed a process incorporating fast-hydropyrolysis followed with a catalytic hydrodeoxygenation (HDO) step and demonstrated that only these two consecutive steps are needed to obtain stable, oxygen-free C_{4+} hydrocarbon molecules in high yield; the liquid product fraction is of high energy density and shippable; the process is agnostic to the type of biomass; the ratio of aromatic to non-aromatic molecular species can be adjusted over a wide range in the bio-oil; because of high reaction rates at the temperatures used (~500°C for pyrolysis and ~300°C for catalytic HDO), the reactions can be performed in small-volume compact reactors. Integrated capabilities in mass spectrometric analyses of pyrolysis reaction products and energy systems modeling are leading to new insights for a compact and high-yielding biomass-to-liquid hydrocarbon process.

11:20 AM

F-IV-3: METAL/LEWIS BIFUNCTIONAL CATALYSTS FOR LOW TEMPERATURE UPGRADE OF BIOMASS

[CCEI] Alexander V. Mironenko[1], Matthew J. Gilkey[1], Paraskevi Panagiotopoulou[2], Glen R. Jenness[2], Bingjun Xu[1], Dionisios G. Vlachos[1]

[1]Department of Chemical and Biomolecular Engineering, University of Delaware; [2]Catalysis Center for Energy Innovation, University of Delaware

C-O bond hydrogenolysis as a means to reduce oxygen content is ubiquitous in biomass upgrade. Recently, we have developed a low-temperature, moderate-pressure, liquid-phase catalytic transfer hydrogenolysis process to convert furfural to 2-methyl furan (2-MF) with a yield of ~80%, utilizing secondary alcohols as hydrogen donors over a Ru/RuO_2 catalyst. 2-MF is a renewable platform chemical that can be used as a drop-in fuel or can be further converted to jet fuels, lubricants, and aromatics. In this talk, we unravel the mechanism and the functionalities of hydrogenolysis in metal/oxide catalysts by combining density functional theory, microkinetic modeling, and isotopic labeling experiments. We find that furfural undergoes Meerwein-Ponndorf-Verley (MPV) reduction over RuO_2 Lewis acid sites to form furfuryl alcohol (FA). In the subsequent FA hydrogenolysis to 2-MF, we elucidate the role of RuO_2 oxygen vacancies. A radical mechanism of C-O bond hydrogenolysis is exposed in agreement with deuterium distribution obtained in our H/D labeling experiments. Crystal Orbital Hamilton Population, Born-Haber, and spin density analyses identify key factors responsible for high hydrogenolysis activity over metal/metal oxide catalysts.

11:40 AM

F-IV-4: SELECTIVE CONVERSION OF LIGNIN FIRST IN TOTAL UTILIZATION OF BIOMASS TO MAKE FUELS AND CHEMICALS

[C3Bio] Trenton Parsell[1,2], Ian Klein[1,2], Hao Luo[1], John Degenstein[3], Hilkka I. Kenttämaa[1], Fabio Ribeiro[3], Rakesh Agrawal[3], Clint Chapple[4], Richard Meilan[5], Mahdi M. Abu-Omar[1,2]

[1]Department of Chemistry, Purdue University, [2]Spero Energy, Inc., [3]Department of Chemical Engineering, Purdue University, [4]Department of Biochemistry, Purdue University, [5]Department of Forestry & Natural Resources, Purdue University

Transition metal catalysts have been an integral part of the success story of the petrochemical industry in the past century. Two grand challenges for this century are renewable energy and the utilization of green resources. Approximately 1.4 billion tons of lignocellulosic biomass is an annually renewable source of energy and feedstock in the U.S. alone. The major components of biomass are cellulose, hemicellulose/xylan, and lignin - all polymeric and contain high percentage of oxygen. Current biomass utilization processes do not make use of lignin beyond its heat value. We have developed selective catalysts that convert lignin in intact wood and grass biomass species directly into two methoxyphenol chemicals, DHE (dihydroeugenol) and DMPP (2,6-dimethoxypropylphenol or propyl syringol), leaving behind polysaccharide solid residue. The lignin-derived methoxyphenols can be deoxygenated further to aromatic hydrocarbon fuels and chemicals. Furthermore, the oligosaccharide residue can be hydrolyzed and converted to fuels and chemicals precursors via simple cascade catalytic reactions. Based on these results, a synergistic biorefinery can be proposed in which both the lignin and carbohydrate fractions are utilized to make fuels and chemicals.

SESSION V: TUESDAY, OCTOBER 27, 2015; 1:30 – 3:10 PM; LINCOLN 3/4

1:30 PM

F-V-1: UNRAVELING NITROGENASE ENERGY CONVERSION AND ELECTRON TRANSFER

[BETCy] Lance Seefeldt[1], Kathryn Fixen[2], Rhesa Ledbetter[1] Yanning Zheng[2], Derek Harris[1], Sudipta Shaw[1], Zachary Jay[3], Natasha Pense[3], Ross Carlson[3], John Peters[3], Carrie Harwood[2]
[1]Utah State University, [2]University of Washington, [3]Montana State University

Nitrogenase is a remarkable catalyst comprised of a series of metal clusters embedded precisely in a protein matrix. This biological catalyst evolved to utilize cellular energy in the form of ATP to reduce the incredibly stable N_2 triple bond to NH_4. One of the goals of BETCy is to understand how nitrogenase converts cellular energy into the reductive equivalents capable of achieving this difficult chemistry. Nitrogenase is a promiscuous catalyst that has the ability to couple ATP hydrolysis to the reduction of a number of other unreactive compounds including CO and CO_2. Insights into this fundamentally important enzyme are critical in understanding how chemical reduction reactions can be performed under benign conditions. We are also working to understand how to couple the light-driven formation of ATP to nitrogenase catalyzed C-H and N-H and H-H bond formation.

1:50 PM

F-V-2: DEFECTS MATTER: CO-PRECIPITATED AND IMPREGNATED SUPPORTED WO_3/TiO_2 AND V_2O_5-WO_3/TiO_2 CATALYSTS FOR SELECTIVE REDUCTION (SCR) OF NO WITH NH_3

[UNCAGE-ME] Minghui Zhu[1], Michael E. Ford[1], Yuanyuan He[1], Uma Tumuluri[2], Zili Wu[2], Israel E. Wachs[1]
[1]Operando Molecular Spectroscopy & Catalysis Lab, Dept. Chemical & Biomolecular Engineering Lehigh University; [2]Chemical Science Division and Center for Nanophase Materials Sciences, Oak Ridge National Laboratory

The molecular structures, surface acidity and catalytic activity for NO/NH_3 SCR of WO_3/TiO_2 and V_2O_5-WO_3/TiO_2 catalysts were compared for two different synthesis methods: co-precipitation of aqueous vanadium and tungsten oxide precursors with $TiO(OH)_2$ and by incipient wetness impregnation of the aqueous precursors on a reference TiO_2 P_{25} support. *In situ* Raman and IR spectroscopy revealed that the vanadium and tungsten oxide active components were present as surface mono-oxo $O=VO_3$ and $O=WO_4$ species on the TiO_2 supports. Co-precipitation also produced new surface VO_4 and WO_4 sites anchored at defects of the TiO_2 support. IR spectroscopy showed that the most abundant active intermediates were surface $NH_4^{+}*$ and NH_3* on Brønsted and Lewis acid sites, respectively. TPSR spectroscopy demonstrated that the specific SCR kinetics was controlled by the redox surface VO_4 species and that the specific kinetics was independent of TiO_2 synthesis method or presence of surface WO_5 sites. The surface WO_5 species possessed minimal redox activity and their primary function was to increase the number of surface $NH_4^{+}*$ intermediates for the SCR reaction by the surface VO_5 species. The NO reactant was weakly adsorbed on the catalyst for its reaction with the adsorbed ammonia (Langmuir-Hinshelwood reaction mechanism). The major difference between the co-precipitated and impregnated catalysts is the presence of surface titania defects on the W- and V-containing co-precipitated catalysts that enhance the concentration of the adsorbed ammonia species and, thus, allowing for greater overall rates of N_2 formation.

2:10 PM

F-V-3: EXPLORING THE ROLE OF PENDANT AMINES IN METAL COMPLEXES FOR N_2 REDUCTION AND NH_3 OXIDATION

[CME] Michael T. Mock, Papri Bhattacharya, Demyan E. Prokopchuk, R. Morris Bullock, Eric S. Wiedner, Liezel A. Labios
Pacific Northwest National Laboratory

The reduction of dinitrogen to ammonia carried out by the Haber-Bosch process, uses N_2 and H_2 feedstocks and a heterogeneous Fe catalyst, in an energy intensive process requiring high pressures and high temperatures. In contrast, nitrogenase enzymes generate NH_3 from N_2, protons, and electrons under ambient conditions. The development of energy efficient, well-defined, molecular catalysts for N_2 reduction using protons and electrons remains a formidable challenge because of the need to generate and stabilize a large number of $M\text{-}N_xH_y$ intermediates during catalysis. We are interested in understanding the role of the pendant bases in the second coordination sphere of metal complexes to (1) facilitate intramolecular proton movement to metal-bound dinitrogen ligands and, (2) to promote N-H bond cleavage reactions in the electrochemical oxidation of ammonia. This talk will describe the development of group 6 complexes supported by phosphine ligands containing non-coordinating pendant amines (e.g., PNP, $(R_2PCH_2)_2N(R')$ and $P^R{}_2N^{R'}{}_2$, substituted 1,5-diaza-3,7-diphosphacyclooctanes) for N_2 reduction and NH_3 oxidation. In particular, the synthesis and reactivity of these complexes will be described, with an emphasis on our current understanding of how the steric and electronic properties of the pendant amine containing ligands impact the formation of protonated $M\text{-}N_xH_y$ intermediates.

2:30 PM

F-V-4: ATOMIC LATER EPITAXY OF Fe_2O_3 FOR NEW FRONTIERS IN PHOTO-ASSISTED WATER OXIDATION

[ANSER] Jonathan D. Emery[1], Christian Schlepuetz[2], Peijun Guo[3], Shannon Riha[1], R.P.H. Chang[3], Alex Martinson[1]
[1] Materials Science Division, Argonne National Laboratory; [2] X-ray Science Division, Argonne National Laboratory; [3] Department of Materials Science and Engineering, Northwestern University

There are a limited number of earth-abundant materials known to satisfy the demands required of a photoabsorber for practical photoelectrochemical (PEC) water oxidation. In an effort to expand this palate we report the growth and characterization of an uncommon bixbyite phase of iron(III) oxide ($\beta\text{-}Fe_2O_3$) epitaxially stabilized via atomic layer deposition on an conductive, transparent, and isomorphic template (Sn-doped In_2O_3). $\beta\text{-}Fe_2O_3$ is reported to possess a bandgap (E_g) as low as 1.7 eV, suggesting the possibility that it could provide superior solar absorption as compared to $\alpha\text{-}Fe_2O_3$ (E_g = 1.9-2.2 eV) and therefore be more suitable photoanode. This smaller bandgap makes $\beta\text{-}Fe_2O_3$ an outstanding candidate for use in tandem photoelectrochemical cells, for which recent modelling studies predict will optimally require a 1.7 eV bandgap top cell. Despite these promising signs, $\beta\text{-}Fe_2O_3$ had not previously been considered for PEC water splitting applications largely due to its synthetic elusivity. In addition, three distinct epitaxially-oriented $\beta\text{-}Fe_2O_3$ films were found to transform to $\alpha\text{-}Fe_2O_3$ under high temperature annealing with preservation of ordering. This allows for the first access to oriented thin film hematite for the investigation of anisotropic hole transport and crystal facet effects. Our EFRC's recent results will be discussed in the context of the current state of iron oxide photoelectrochemistry.

2:50 PM

F-V-5: MOLECULAR CATALYSTS FOR THE OXYGEN REDUCTION REACTION (ORR)

[CME] James M. Mayer[1,2], Michael L. Pegis[1,2], Bradley A. McKeown[1,2], Gannon P. Connor[1], Elizabeth A. Mader[1,2], Carlos Rodriguez[2], Derek J. Wasylenko[2], Matthew L. Rigsby[2], Neeraj Kumar[3], Simone Raugei[3], Aaron M. Appel[3], John A. S. Roberts[3,4], Eric S. Wiedner[3]

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Improved electrocatalysis of the oxygen reduction reaction (ORR), $O_2 + 4e^- + 4H^+ \rightarrow 2H_2O$, is a key challenge in energy technologies such as fuel cells. Molecular electrocatalysts are being studied to derive new understanding of the ORR, because soluble molecular species can be much more easily tailored and studied than heterogeneous analogs. Iron porphyrin ORR electrocatalysis can be fast and selective, but they operate at high overpotentials. Changing the porphyrin substituent has allowed tuning of the $Fe^{3+/2+}$ reduction potential and the introduction of proton relays in the second coordination sphere, such as 2-carboxyphenyl, 2-pyridyl, and related amide derivatives. Turnover frequencies from $3\ s^{-1}$ to $5 \times 10^6\ s^{-1}$ have been determined by electrochemical foot-of-the-wave analysis. Comparisons between different catalysts, between the same catalyst in different media, and between the same complex as a chemical and electrochemical catalyst have all been quite informative. For soluble catalysts, the rate is directly dependent on the $Fe^{3+/2+}$ reduction potential and therefore the overpotential of the reaction, even though electron transfer from the electrode is not rate determining. This analysis depends on knowledge of the thermochemical potential for the ORR in organic solvents, which we have determined for the first time. Our experimental results, together with computational studies, provide insight into the influence of proton relays on electrocatalysis.

G. SYNTHESIS OF FUNCTIONAL MATTER

SESSION II: MONDAY, OCTOBER 26, 2015; 3:20 – 5:00 PM; LINCOLN 2

3:20 PM

G-II-1: APPROACH TO THE TARGETED IDENTIFICATION AND SYNTHESIS OF TRANSITION METAL OXIDE POLYMORPHS

[CNGMD] David Ginley[1], Kristin Persson[2,8], Vladan Stevanovic[1,5], John Perkins[1], Lauren Garten[1], Paul Ndione[1], Gerbrand Ceder[2,8], Daniil Kitchaev[3], Zamyla Chan[4], Daniel Nocera[4], Roy Gordon[4], Lu Sun[4], Brian Gorman[5], John Mangum[5], Ann Deml[5], Prashun Gorai[5], Janet Tate[6], James Haggerty[6], Chiyuki Sato[6], Laura Schelhas[7], Kevin Stone[7], Johanna Nelson Weker[7], Michael Toney[7], Hong Kevin Ding[8], Wenhao Sun[8], William Tumas[1]

[1]National Renewable Energy Laboratory, [2]UC-Berkeley, [3]Massachusetts Institute of Technology, [4]Harvard University, [5]Colorado School of Mines, [6]Oregon State University, [7]SLAC National Accelerator Laboratory, [8]Lawrence Berkeley National Laboratory

CNGMD is focused on developing approaches to the identification and synthesis of functional metastable materials. Polymorphic systems present a class where the composition remains constant and the structure type and resultant electronic properties change. Considering many families with rich polymorphism, we have chosen three for our original focus: VO_2, TiO_2 and MnO_2. These systems exibit a broad pallet of structures and diverse functionality. For example TiO_2 crystallizes in Rutile, Anatase and Brookite structures; all of which occur naturally with Rutile a the key pigment in paint, Anatase a widely used opto-electronic material with a low effective mass and Brookite as a photocatalyst. Other polymorphic systems are equally rich. We will discuss our work addressing the key design questions for such polymorphic systems including: 1) how to identify the structures, properties and enthalpies/free energies for a polymorphic composition; 2) how to choose a substrate that is suitable for growth of a specific polymorph and 3) how to select an appropriate growth technique to target a specific polymorph in a set of energetically close spaced structures. Specifically we will discuss a set of new computational tools which when coupled with and informed by a set of growth techniques (PLD, hydrothermal, electrodeposition, and ALD) attempt to answer these questions. Currently, we developing a polymorph sampler, a substrate picker and we are computationally exploring which parameter spaces intersect for different growth techniques. In combination, these tools present a targeted approach for predicting synthesis of new functional polymorphs.

3:40 PM

G-II-2: SHAPE DIRECTED DYNAMICS OF ACTIVE COLLOIDS

[CBES] Syeda Sabrina[2], Alan Brooks[2], Matthew Spellings[1], Sharon C. Glotzer[1], Kyle J.M. Bishop[2]

[1]Department of Chemical Engineering, Biointerfaces Institute, and Department of Materials Science and Engineering, University of Michigan; [2]Department of Chemical Engineering, Pennsylvania State University

Active matter comprised of many self-driven units can exhibit emergent collective behaviors such as pattern formation and phase separation in both biological (e.g., mussel beds) and synthetic (e.g., colloidal swimmers) systems. We describe how the three-dimensional shape of colloidal particles can be used to program both their individual trajectories and their collective behaviors. Shape-directed particle activity can be powered by diverse energy inputs such as chemical reactions, electric fields, acoustic waves, and/or hydrodynamic shear. Through simulation and experiment, we demonstrate a wide variety of particle motions (linear, rotational, helical, etc.) as determined by the symmetry of the particle and that of the stimulus (e.g., a applied electric field). We explore the complex behaviors that arise in ensembles of rotating particles where energy input at the particle level gives rise to rotational particle motion. We show that mixtures of counter-rotating particles can organize dynamically to form larger, self-propelled excitations (vortex doublets). These results highlight opportunities for designing life-like properties in active materials subject to distributed actuation.

4:00 PM

G-II-3: AGGREGATION AND SOLUBILITY OF CLUSTERS OF ACTINIDES IN WATER

[MSA] Peter C. Burns[1], Travis Olds[1], Sarah Hickam[1], Haylie Lobeck[1], Christine Wallace[1], Tianbo Liu[2], Yunyi Gao[2], Jennifer A. Soltis[3], R. Lee Penn[3], Laura Gagliardi[3], Varinia Bernales[3], Rene Johnson[4], William H. Casey[4]

[1]Dept. Civil and Environmental Engineering and Earth Sciences, University of Notre Dame; [2]Dept. Polymer Science, The University of Akron; [3]Dept. Chemistry, University of Minnesota; [4]Dept. Earth and Planetary Sciences, Dept. Chemistry, University of California, Davis

An extensive family of nanoscale uranyl peroxide cage clusters is providing novel insights into actinide cluster behavior in aqueous solution. Subsequent to self-assembly in solution, these cage clusters persist through intense gamma irradiation or thermal treatment, and remain present in solution for several months under ambient conditions. Upon dissolution of crystals containing cage clusters, some of their counter ions are released and their effective charges are concentration dependent. Aging or addition of salt triggers cation-mediated aggregation into stable hollow spherical macro-ion assemblies called blackberries with sizes and morphologies that are cation and cluster dependent, as demonstrated by cryogenic transmission electron microscopy and light scattering. Where uranium is contained within cage clusters, total uranium concentrations in aqueous solution under alkaline conditions can exceed 300,000 ppm. The total concentration of clusters that can be achieved in aqueous solution is strongly dependent on the choice of counter ion, as crystallization is also a counter-ion mediated process for these anionic clusters. Conditions conducive to cluster formation tend to cause scavenging of simple uranyl species from solution for incorporation into cages, thereby accelerating the dissolution of various uranium-bearing solids in water.

4:20 PM

G-II-4: DISPERSION AND HIGH-RESOLUTION TRANSITION ELECTRON MICROSCOPY OF CARBON NANOTHREADS

[EFree] Stephen Juhl[1], Xiang Li[2], Nasim Alem[1], John V. Badding[2]

[1]Department of Materials Science and Engineering, Pennsylvania State University; [2]Department of Chemistry, Pennsylvania State University

Low-dimensional carbon nanomaterials such as fullerenes, nanotubes, graphene and diamondoids have extraordinary physical and chemical properties. Compression-induced polymerization of aromatic molecules could provide a viable synthetic route to ordered carbon nanomaterials, but despite almost a century of study this approach has produced only amorphous products. We recently reported recovery to ambient pressure of macroscopic quantities of a crystalline one-dimensional sp^3 carbon nanomaterial formed by high-pressure solid-state reaction of benzene. Preliminary characterization revealed close-packed bundles of subnanometer-diameter sp^3-bonded carbon threads capped with hydrogen, crystalline in two dimensions and short-range ordered in the third. Further investigation of this new 1-D carbon material has been conducted through a battery of techniques, including high-resolution transmission electron microscopy. These experiments have confirmed the preliminary characterization results and further revealed the structure of the carbon nanothreads. Determining the structure and reaction mechanism behind carbon nanothreads may help to develop a new class of ordered sp^3 nanomaterials synthesized by kinetic control of high-pressure solid-state reactions.

4:40 PM – Graduate Student Finalist

G-II-5: Structural Evolution of Uranyl Peroxide Nano-Cage Fullerene: U60, at Elevated Pressures

[MSA] Katlyn M. Turner[1], Yu Lin[1], Fuxiang Zhang[2], Brendan T. McGrail[3], Wendy Mao[1], Peter C. Burns[3], Rodney C. Ewing[1]

[1] Dept. Geological Sciences, Stanford University; [2] Dept. of Earth & Environmental Sciences, University of Michigan; [3] Dept. Civil & Environmental Engineering & Earth Sciences, University of Notre Dame

U60 is a uranyl peroxide nano-cage that adopts a highly symmetric fullerene topology. The topological isomer of U60 is the same as C60 buckminsterfullerene. Several studies on the aqueous-phase of U60 clusters, $[UO_2(O_2)(OH)]_{60}^{60-}$, have shown the persistence and stability of the compound in complex solutions[1] and over lengthy time scales. U60 (Fm-3) crystallizes at ambient conditions with approximate formula: $Li_{68}K_{12}(OH)_{20}[UO_2(O_2)(OH)]_{60}(H_2O)_{310}$. In this investigation, we have used the diamond anvil cell (DAC) to examine U60 *in situ* in order to understand the stability of this cluster at high pressures. We used a symmetric DAC with 300 µm culet diamonds and two different pressure-transmitting media: a 4:1 mixture of methanol + ethanol and silicone oil. By using a combination of *in situ* Raman spectroscopy and synchrotron powder x-ray diffraction (XRD), and electrospray ionization mass spectroscopy (ESI-MS) *ex situ*, we have determined the pressure-induced evolution of the U60 cluster. Crystalline U60 undergoes an irreversible phase transition to a tetragonal structure at 4.1-4.4 GPa, and irreversibly amorphizes between 11-14 GPa. This amorphous phase likely consists of clusters of U60. Above pressures of ~15 GPa, the U60 nano-cage is irreversibly destroyed—ESI-MS shows that this phase consists of several species that likely have between 10-20 uranium atoms. The Raman spectroscopy of crystalline U60 shows two dominant modes[2]: a symmetric stretch of the uranyl U-O triple bond at ~810 cm^{-1}, and a symmetric stretch of the $U\text{-}O_2\text{-}U$ peroxide bond at ~820-850 cm^{-1}. As pressure is increased, these two modes shift to increasing wavenumbers, and eventually overlap at ~4 GPa. At ~15 GPa, the intensity of these modes decreases below detection. These vibrational results complement the synchrotron XRD measurements. U60 degrades quickly in methanol and ethanol mixtures, as evidenced by broad, diffuse diffraction patterns even at low pressures, however, in silicone oil, crystalline U60 remains intact for several hours. In both studies, a phase transition was observed at 4 GPa. In methanol and ethanol, U60 amorphizes between 10-13 GPa, but in silicone oil, the amorphization pressure is slightly higher: 13-14 GPa. In both studies, the phase transition and amorphization were irreversible. These experiments reveal several novel behaviors: U60 undergoes irreversible phase transitions, the tetragonal phase of U60 is exclusively a high-pressure phase, and the amorphization of the U60 compound occurs before the collapse of the U60 cluster topology. Notably, this is different from the behavior of solvated C60 with increasing pressure, which maintains a hexagonal structure at high pressure (up to 30 GPa), while the clusters become disordered[3]. These results suggest that uranyl nano-cage clusters may be very persistent once formed, regardless of the state of the cluster—crystalline, amorphous, or even in solution.

[1] Flynn, Shannon L., *et al*. "Experimental measurements of U60 nanocluster stability in aqueous solution." *Geochim. et Cosmo. Acta.* **156** (2015): 94-105.

[2] McGrail, Brendan T., *et al*. "Raman Spectroscopic and ESI-MS Characterization of Uranyl Peroxide Cage Clusters." *Inorg. Chem.* **53**.3 (2014): 1562-1569.
[3] Wang, Lin, *et al*. "Long-range ordered carbon clusters: a crystalline material with amorphous building blocks." *Science* **337**.6096 (2012): 825-828.

SESSION V: TUESDAY, OCTOBER 27, 2015; 1:30 – 3:10 PM; LINCOLN 2

1:30 PM – Postdoctoral Researcher Finalist

G-V-1: ULTRAFAST SYNTHESIS METAL-ORGANIC FRAMEWORKS CRITICAL FOR ENERGY-EFFICIENT CO_2 CAPTURE

[CGS] L. Maserati[1], S. M. Meckler[1,2] , C. Li[1,3], J. R. Long[2,4] and B. A. Helms[1]
[1]The Molecular Foundry, Lawrence Berkeley National Laboratory; [2]Department of Chemistry, University of California, Berkeley; [3]Department of Chemical Engineering, University of California, Berkeley; [4]Materials Sciences Division, Lawrence Berkeley National Laboratory

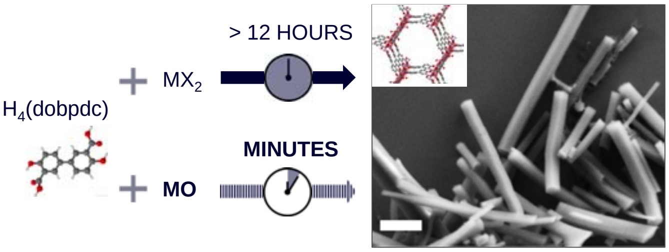


Fig. 3 M_2(dobpdc) synthesis concept and realization.

Metal-organic frameworks (MOFs) are microporous crystalline solids constructed from metal ions or clusters, which are covalently linked by organic ligands[1]. The tunability of their composition, architecture and properties has revolutionized the way we approach carbon capture and storage at CO_2-emitting power plants[2,3]. M_2(dobpdc) MOFs—and in particular their diamine-modified derivatives—have shown exceptional promise for energy-efficient CO_2 capture[4]. However, today's multi-hour synthetic procedures prevent their expedient and scalable production, which limits our ability to validate these materials in pilot-scale prototypes.

To address this challenge, we developed an exceptionally rapid synthesis of high quality M_2(dobpdc) where (dobpdc = 4,4′-dioxido-3,3′-biphenyldicarboxylate) that co-opts conventional divalent metal salts in favor of divalent metal oxides: MO = MgO, MnO, CoO, NiO, or ZnO. Our (pseudo)halide-free route avoids the generation of acidic by-products otherwise inherent to conventional M_2(dobpdc) syntheses[5]; as a result, the reaction time needed decreases significantly — in some cases, by several orders of magnitude (Fig. 1). We show that M_2(dobpdc) formation proceeds via a dissolution-precipitation mechanism. Through our analysis of MO precursor morphology, surface area, and composition-dependent etch rate, we determined that MO dissolution is rate-limiting. Notably, then, scaling the dimensions of the MO precursor to nanoscopic dimensions allows these MOFs to be prepared in high quality in mere minutes without residual MO. As a penultimate demonstration, we synthesized Zn_2(dobpdc) MOFs from 7 nm ligand-stripped[6] ZnO colloidal nanocrystals (NCs) in less than 1 minute. Our discovery highlights the role for basic science to guide methods of production of critical materials for energy-efficient CO_2 capture.

[1] Rowsell, J. L. C. & Yaghi, O. M. Metal–organic frameworks: a new class of porous materials. *Met.-Org. Open Framew.* **73,** 3–14 (2004).
[2] Boot-Handford, M. E. *et al.* Carbon capture and storage update. *Energy Environ. Sci.* **7,** 130–189 (2014).

[3] Sumida, K. *et al.* Carbon Dioxide Capture in Metal–Organic Frameworks. *Chem. Rev.* **112,** 724–781 (2012).
[4] McDonald, T. M. *et al.* Cooperative insertion of CO2 in diamine-appended metal-organic frameworks. *Nature* **519,** 303–8 (2015).
[5] Chalati, T., Horcajada, P., Gref, R., Couvreur, P. & Serre, C. Optimisation of the synthesis of MOF nanoparticles made of flexible porous iron fumarate MIL-88A. *J Mater Chem* **21,** 2220–2227 (2011).
[6] Doris, S. E. *et al.* Mechanistic Insight into the Formation of Cationic Naked Nanocrystals Generated under Equilibrium Control. *J. Am. Chem. Soc.* **136,** 15702–15710 (2014).

1:50 PM

G-V-2: PRINTING FUNCTIONAL MATERIALS

[LMI] Jennifer A. Lewis[1], Mark Scott[1], Nanjia Zhou[1], Alex Valentine[1]
[1]*Harvard University*

The ability to pattern functional materials in planar and three-dimensional forms is of critical importance for several emerging applications, including photovoltaics, solid-state lighting, flexible electronics, and sensors. We have developed a multimaterial 3D printing platform that enables the rapid design and fabrication of devices in arbitrary shapes without the need for expensive tooling, dies, or lithographic masks. In this talk, I will describe several viscoelastic ink designs based on conductive, resistive, elastomeric, and reactive epoxy materials that can be patterned at the mesoscale. In addition, I will discuss new microfluidic printheads that are capable of active mixing and switching between multiple inks "on-the-fly" during printing to enable rapid fabrication of designer materials architectures. Finally, I will introduce a new laser-assisted 3D printing approach for producing freely supported, 3D metal structures.

2:10 PM

G-V-3: ADVANCES IN 2-DIMENSIONAL POROUS LAYERS FOR GAS SEPARATION MEMBRANES

[CGS] Feng Xue[1], Meera Shete[1], Hao Li[2], Hong-Cai Zhou[2], Michael Tsapatsis[1]
[1]*Department of Chemical Engineering and Materials Science, University of Minnesota;* [2]*Department of Chemistry, Texas A&M University*

Crystalline molecular sieve nanosheets with nm-thickness are 2-dimensional materials that hold promise for enabling large scale, low cost fabrication of high-flux, high-selectivity gas, vapor and liquid separation membranes [1-6]. A focus of CGS is to explore the potential of such membranes for energy efficient separations. Fabrication of thin film membranes consisting of 2D molecular sieves relies on: (i) the synthesis of high aspect ratio nanosheets with well-defined pore sizes; (ii) the development of deposition techniques by which these nanosheets can be transferred on porous supports to form compact films and (iii) defect-healing methods to create functional membranes. In this talk, we will present examples of synthesis and structural characterization of 2D porous metal-organic-frameworks (2D-MOF) and 2D microporous silicates (2D-zeolites) and we will assess their potential in novel thin film permselective membrane fabrication.

[1] Varoon *et al.* Dispersible Exfoliated Zeolite Nanosheets and Their Application as a Selective Membrane. Science **334**, 72-75 (2011)
[2] Zhang *et al.* Direct Synthesis of Self-Pillared Zeolite Nanosheets by Repetitive Branching. Science **336**, 1684-1687 (2012)
[3] Tsapatsis M. 2-Dimensional Zeolites. AIChE Journal **60**, 2374-2381 (2014)

[4] Rodenas *et al.*, Metal-organic Framework Nanosheets in Polymer Composite Materials for Gas Separation. Nature Materials, **14**, 48-55 (2015)
[5] Peng *et al.*, Metal-organic framework nanosheets as building blocks for molecular sieving membranes. Science **346**, 1356-1359 (2014)

2:30 PM

G-V-4: SYNTHESIS OF PERIODIC MESOPOROUS SILICA WITH CRYSTALLINE PORE WALLS

[EFree] Manik Mandal[1], Yiqun Liu[1], Vincenzo Stagno[2], Cong Liu[1], Yingwei Fei[3], Kai Landskron[1]
[1] Department of Chemistry, Lehigh University; [2] Ehime University, Japan; [3] Geophysical Laboratory, Carnegie Institution of Washington

The motivation for the synthesis of periodic mesoporous silica materials (with pore sizes from 2 to 50 nm) 20 years ago was to replace the microporous zeolites (which have pore sizes of < 2 nm) in petroleum cracking applications, because the larger pore size of mesoporous materials allows for faster transport of larger molecules. However, these mesoporous materials could not replace zeolite materials because they showed lower hydrothermal stability and lower catalytic activity. This reduced performance has been attributed to the amorphous nature of the mesoporous materials' channel walls. Here, we have developed a synthetic route to mesoporous aluminosilica with crystalline pore walls via "nanocasting at high pressure" at 2 GPa and a temperature of 650 ^{o}C. This method requires the use of a mesostructure as the so called "hard template". The synthesized mesoporous aluminosilica materials are steam stable and are resistant to shrinkage under harsh conditions of hydrothermal treatment at 800 ^{o}C. In addition, we are growing mesoporous quartz single crystal under hydrothermal conditions with porous carbon as the hard template.

2:50 PM

G-V-5: DESIGNING PHOTOCATHODE MATERIALS FOR DYE-SENSITIZED PHOTOELECTROSYNTHESIS CELLS

[UNC] Cory J. Flynn[1], Candy C. Mercado[2], Shannon M. McCullough[1], Lesheng Li[1], Byron H. Farnum[1], Leila Alibabaei[1], Robert Dillon[1], EunBi Oh[1], [1]Gerald J. Meyer, John M. Papanikolas[1], Thomas J. Meyer[1], Arthur J. Nozik[2,3], Yosuke Kanai[1], James F. Cahoon[1]
[1]Department of Chemistry, University of North Carolina at Chapel Hill; [2]Renewable and Sustainable Energy Institute, and Department of Chemistry and Biochemistry, University of Colorado; [3]National Renewable Energy Laboratory

Dye-sensitized photoelectrosynthesis cells (DSPECs) generate solar fuels using the energy from sunlight to drive catalytic synthetic transformations. The DSPEC concept pursued at the UNC Center for Solar Fuels uses molecules to absorb light and perform redox catalysis, and the molecules are attached to two types of mesoporous semiconductors. At the photoanode, an n-type metal oxide, such as TiO_2, is used to transport electrons from the molecular chromophore-catalysts that perform water oxidation. At the photocathode, a p-type metal oxide is used to transport holes from the molecular chromophores and catalysts that perform CO_2 reduction. Although photoanode systems have exhibited good efficiency, most photocathode materials examined to-date exhibit relatively poor characteristics. Here, we address this problem through the rational design of p-type metal oxide composition and morphology. For the widely-used photocathode NiO, we demonstrate a method termed targeted atomic deposition (TAD) for site-selective passivation of the defect sites on the material's surface. As shown by a comparison of experiments and first-principles calculations, the TAD process passivates oxygen dangling bonds adjacent to metal vacancies, leading to a dramatic change in the color of the material and a

three-fold improvement in devices. In addition, we develop a new photocathode material, the spinel $ZnCo_2O_4$. Prepared as both a thin film and mesoporous structure using mechanochemical synthesis methods, the material exhibits performance comparable to NiO in initial tests, suggesting excellent promise for further development. Continued rational design of photocathode materials should lead to mesoporous structures that can be used in high-performance DSPEC devices.

H. BIOSCIENCE

SESSION II: MONDAY, OCTOBER 26, 2015; 3:20 – 5:00 PM; LINCOLN 6

3:20 PM

H-II-1: PRIMARY CELL WALL STRUCTURE IN PLANTS: NEW CONCEPTS, SOME REMAINING ENIGMAS

[CLSF] Daniel J. Cosgrove[1], Tian Zhang[1], Yunzhen Zheng[1], Yong Bum Park[1], Charles T.Anderson[1], Linghao Zhong[2], Shi-Chun Huang[3], Janna Maranas[3], Tuo Wang[4], Mei Hong[4]

[1]Department of Biology, Pennsylvania State University; [2]Department of Chemical Engineering, Pennsylvania State University, [3]Department of Chemistry, Pennsylvania State University at Mont Also, [4]Department of Chemistry, Massachusetts Institute of Technology

Much of the carbon and energy captured in photosynthesis is locked away in cell walls (CW), a large-scale material with biofuel potential. Plant cells construct a primary CW from cellulose microfibrils, xyloglucan and pectins, followed by a secondary CW within the confines of the primary CW. Extensibility of the primary CW limits plant growth and the potential for secondary CW deposition. Until recently primary CWs were believed to be constructed of a scaffold of well-separated cellulose microfibrils, coated and tethered by xyloglucans and embedded in a gel-like pectin matrix. Based on new results we come to different conclusions about how CWs are constructed and how wall extensibility arises. Results with enzymes and biomechanics indicate that most of the xyloglucan is not load bearing and that extensibility is controlled at the meso-scale at limited junctions where microfibrils are tightly connected. Molecular dynamics simulations indicate that such junctions contribute substantially to CW strength. Studies of hydrated CWs by multi-modal atomic force microscopy show a poly-lamellate construction; microfibrils within each lamella are bundled in short domains and oriented in a similar direction, differing between lamellae. Genetic lesions in xyloglucan synthesis change microfibril order. Solid-state NMR shows that much of the cellulose surface is in contact not with xyloglucan but with pectins, some of which have rigid domains with ^{13}C T1 relaxation times similar to that of cellulose. SANS experiments complement these results, which all together point to new principles of CW organization, and raise new questions of how CWs are assembled.

3:40 PM

H-II-2: STRUCTURE AND SYNTHESIS OF CELLULOSE

[C3Bio] Phillip Rushton[1], Anna Olek[1], Catherine Rayon[1], Tânia Shiga[1], Priya Murria[2], John Degenstein[3], Bryan Penning[4], Haibing Yang[5], Hui Wei[6], Lee Makowski[7], John Badger[8], Cynthia Stauffacher[3], Bryon Donohoe[6], Michael Crowley[6], Hilkka I. Kenttämaa[2], Rakesh Agrawal[3], Mel Tucker[6], Wendy Peer[5], Angus Murphy[5], Maureen McCann[3], Nicholas Carpita[1]

[1]Department of Botany & Plant Pathology, Purdue University, [2]Department of Chemistry, Purdue University, [3]Department of Chemical Engineering, Purdue University, [4]Department of Biological Sciences, Purdue University,[5]Department of Horticulture & Landscape Architecture, Purdue University, [6]Biosciences Center, National Renewable Energy Laboratory, [7]Department of Bioengineering and Department of Chemistry and Chemical Biology, Northeastern University, [8]DeltaG Technologies

Newly discovered technologies to deconstruct lignin from intact cell walls have refocused our efforts to understand and reduce the nature of biomass recalcitrance. We are establishing the structure of cellulose synthase complexes, and how the crystalline microfibrils they synthesize might be modified, to improve cellulose deconstruction during catalytic conversion processes. Small-angle x-ray scattering and molecular docking experiments provided a solution structure of

a rice cellulose synthase catalytic domain (CatD). The catalytic core fits into the central portion of a two-domain structure; a smaller domain functions in dimerization of two CatDs, forming the fundamental scaffolding unit in construction of the complex. The Plant-Conserved Region is a non-canonical coiled-coil with a large connecting loop containing a trio of aromatic residues that are predicted to face the catalytic core distal to the dimerization domain. The size and structure of the microfibril synthesized is controversial. We have modified a TEMPO-catalyzed oxidation method followed by sodium borodeuteride reduction to identify disordered amorphous chains, ordered crystalline surface chains, and anhydrous crystalline core chains. Microfibril bundling in the secondary wall results in significantly higher crystalline, anhydrous core domains. We are surveying diverse populations of maize and genetic variants of poplar to determine if bundling is a genetically tractable trait. Iron pretreatments of biomass, or genetic variants in which iron catalysts have been targeted biologically to the cell wall, defibrillate cell wall architecture and improve recovery of glucose from cellulose. Tomographic images combined with computational modeling of these materials give new targets for catalytic deconstruction of microfibrils.

4:00 PM – Postdoctoral Researcher Finalist

H-II-3: STRUCTURAL STUDIES OF PLANT CELLULOSE SYNTHASE SUPPORT 18 SYNTHASES IN THE CELLULOSE SYNTHESIS COMPLEX

[CLSF] Venu Gopal Vandavasi[1], B. Tracy Nixon[2], Daniel K. Putnam[3], Katayoun Mansouri[4], Jung-Goo Lee[4], Abhishek Singh[4], Juan Du[2], Eric M. Roberts[5], Alison W. Roberts[6], Erin Slabaugh[4], Jonathan K. Davis[4], Qiu Zhang[1], Loukas Petridis[1], William T. Heller[1], Udaya Kalluri[1], Leighton Coates[1], Paul Langan[1], Jeremy C. Smith[1], Jens Meiler[3], Yaroslava G. Yingling[4], Candace H. Haigler[4] Hugh O'Neill[1,7]
[1]Oak Ridge National Laboratory; [2]Pennsylvania State University; [3]Vanderbilt University; [4]North Carolina State University; [5]Rhode Island College; [6]University of Rhode Island; [7]University of Tennessee

Cellulose is the most important structural component of plant cell walls and constitutes the Earth's largest store of biorenewable material for liquid biofuel production for the transportation sector of the economy, yet the mechanism of its synthesis by plants is poorly understood. The plant cellulose synthesis complex (CSC), also called a 'rosette' because of its hexameric appearance in electron microscope images, is a large multi-subunit transmembrane protein complex responsible for synthesis of cellulose chains and their assembly into microfibrils. The number of cellulose synthase (CESA) proteins in the CSC and the number of cellulose chains in a microfibril have been debated for years. This work reports analysis of CSCs obtained using refined methods in freeze facture transmission microscopy (FF-TEM) and structural studies of a recombinant cytosolic domain of plant CESA in solution. Together, these studies provide new insights into the structure and oligomeric state of CESAs and the probable number of cellulose chains in the microfibril. Class averaging of the FF-TEM images of individual lobes in the CSC combined with computational modeling of the transmembrane helical (TMH) region of CESA revealed each lobe of the CSC likely contains three CESAs. Analysis of the individual lobes in the FF-TEM images indicates that the lobe-lobe interactions are relatively weak suggesting the forces that hold the CSC together must be due to protein-protein interactions in the cytosolic portion of CESA and/or glucan chain interactions near the plasma membrane surface. Small-angle neutron and X-ray scattering were used to study the solution structure of the cytosolic domain of Arabidopsis CESA1 (CESAcatD). *Ab initio* models for CESAcatD derived from the SANS and SAXS data provide the first experimental evidence to support the self-assembly of CESAcatD monomers into stable homotrimer complexes. By combining small-angle scattering data with computational approaches, possible configurations for the arrangement of CESAcatD monomers in the homotrimer were obtained. Several candidate trimers were identified with monomers oriented such that that newly synthesized cellulose chains project towards the cell membrane. In these models, the class specific region is found at the periphery of the complex and the

plant-conserved region forms the base of the trimer. Comparison of the FF-TEM images with the sizes of a TMH trimer and a CESACatD trimer provides compelling evidence that each lobe of a CSC contains three CESAs. The combined data from the two studies refutes the long-standing model of 36 CESAs within the rosette CSC and strongly supports the 'hexamer of trimers' model for rosette CSC that synthesizes an 18-chain cellulose microfibril as the fundamental product of cellulose synthesis in plants.

4:20 PM

H-II-4: ALTERED LIGNIN BIOSYNTHESIS TAILORS PLANT CELL WALL ARCHITECTURE FOR EFFICIENT CATALYTIC CONVERSIONS TO FUELS AND CHEMICALS

[C3Bio] Bryon Donohoe[1], Peter Ciesielski[1], Hideyo Inouye[2], Yan Zhang[2], Ian Klien[3], Barron Hewetson[4], Ximing Zhang[4], Nicholas Anderson[5], Nicholas Bonawitz[5], Jeong Im Kim[5], Lee Makowski[2], Mahdi Abu-Omar[3], Nathan Mosier[4], Rick Meilan[6], Clint Chapple[5]

[1]Biosciences Center, National Renewable Energy Laboratory, [2]Department of Bioengineering and Department of Chemistry and Chemical Biology, Northeastern University, [3]Department of Chemistry, Purdue University, [4] Department of Agricultural & Biological Engineering, Purdue University, [5]Department of Biochemistry , Purdue University, [6]Department of Forestry & Natural Resources, Purdue University.

Efficient production of fuels and products from lignocellulosic biomass will benefit from learning to control the chemical and physical complexity of plant cell walls. Modifying lignin composition and structure is one key strategy to control cell wall architecture. Using multi-scale, multi-mode microscopy and quantitative image analysis, we have shown how catalytic conversion treatments alter the meso and nanostructure of wild-type and genetically modified cell walls. We investigated several genetic variants of *Arabidopsis*: the wild type, which makes a lignin polymer of guaiacyl (G) and syringyl (S) monomeric units, the *fah1* mutant, which makes lignin from almost exclusively G subunits, and a ferulate 5-hydroxylase (F5H) over-expressing line (C4H:F5H) that makes lignin predominantly from S subunits. In addition, these lines have been combined with disruption of the genes encoding two cinnamyl alcohol dehydrogenases (CADs), resulting in the atypical incorporation of hydroxycinnamaldehydes into lignin. These Arabidopsis samples, and similar lines in *Populus*, were exposed to catalytic treatments designed for lignin, xylan, or cellulose depolymerization. Increased cell-cell dislocation, cell wall surface roughness, delamination, nanofibrillation, and cellulose microfibril spacing revealed by direct observation confirms the mesoscale changes in cell wall architecture that underlie the superior performance of some catalytic treatments used in combination with modified cell walls. In addition, we have explored how changes in 3D nanoporosity impact catalyst access to cell wall biopolymers and have used microscopic analysis as a foundation for building improved models of biomass particles.

4:40 PM

H-II-5: MECHANISM OF CELLULOSE SYNTHESIS AND MEMBRANE TRANSLOCATION

[CLSF] Joshua T. McNamara[1]*, Jacob L.W. Morgan[1]*, Michael Fischer[2], Jamie Rich[2], Hong-Ming Chen[2], Stephen G. Withers[2], Jochen Zimmer[1]

*[1] Center for Membrane Biology, Molecular Physiology and Biological Physics, University of Virginia School of Medicine; [2]Department of Chemistry, University of British Columbia; *These authors contributed equally to this work.*

Cellulose is an extracellular polysaccharide that is primarily produced by vascular plants but also by some algae, bacteria and even tunicates. It is a linear glucose polymer that is synthesized and

secreted by cellulose synthase. While bacterial cellulose is an important component of many biofilms, cellulose found in primary and secondary plant cell walls is bundled into cable-like structures, which form the primary load bearing structure of the cell wall.

Cellulose biosynthesis most likely occurs by an evolutionarily conserved mechanism. Resting and activated structures of the bacterial BcsA-B cellulose synthase complex at intermediate states during cellulose synthesis and translocation provided unique insights into how the enzyme couples the elongation of the nascent polysaccharide chain with its translocation across the membrane.

We used *in crystallo* enzymology with the bacterial BcsA-B complex to obtain structural snapshots of a complete cellulose biosynthesis cycle. Substrate and product-bound states of BcsA reveal the basis for substrate recognition and demonstrate the stepwise elongation of cellulose. Our structural and functional analyses reveal that BcsA translocates cellulose into its transmembrane channel via a ratcheting mechanism involving a “finger helix” that contacts the polymer's terminal glucose. Together with a conserved gating loop, the finger helix moves ‘up’ and ‘down’ in response to substrate binding and polymer elongation, respectively, thereby pushing the elongated polymer into the transmembrane channel.

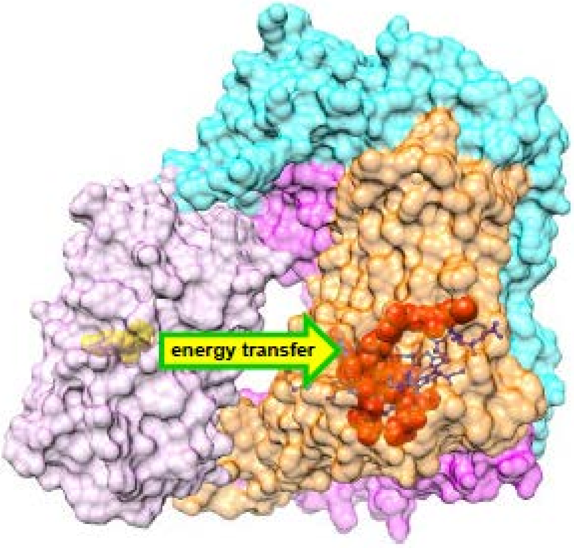
Session III: Tuesday, October 27, 2015; 8:30 – 10:10 AM; Lincoln 6

8:30 AM – Graduate Student Finalist

H-III-1: Expanding the Range of Light Absorbers for Bacterial Photosynthesis: YFP-Enhanced Charge Separation at the Rhodobacter Sphaeroides Reaction Centre

[PARC] Kaitlyn M. Faries[1], Katie J. Grayson[2], Pu Qian[2], Preston Dilbeck[1], Elizabeth Martin[2], Jonathan M. Yuen[1], Dariusz M. Niedzwiedzki[3], Dewey Holten[1], Christine Kirmaier[1] and C. Neil Hunter[2]

[1]Dept. Chemistry, Washington University, St. Louis; *[2]Dept. Molecular Biology and Biotechnology, University of Sheffield, UK*; *[3]Photosynthetic Antenna Research Center, Washington University, St. Louis*



Idealized schematic model of the Rb. sphaeroides *RC with polypeptide subunits H (cyan), M (magenta) and L (cyan) and pigments (orange/purple) plus attached YFP with protein (light pink) and integral pigment (yellow).*

Native light-harvesting systems of photosynthetic organisms are very efficient at light collection and transfer of energy to a reaction centre (RC) for conversion to chemical energy via charge separation across a membrane. However, that efficiency is often limited to certain color ranges of solar light because of gaps in the visible and near-infrared spectrum where the antenna pigments do not absorb. Although incorporation of synthetic chromophores to complement the absorption spectrum of native light-harvesting proteins in biohybrid architectures is promising, the approach is challenging and generally involves pigment integration post purification of proteins from the organism and *in vitro* assembly. However, fluorescent proteins such as green fluorescence protein (GFP) and derivatives offer the advantage of *in vivo* incorporation and production. In this study, we incorporated a yellow fluorescent protein (YFP) derivative (sYFP2) gene at the C-terminus of the gene for the H-polypeptide subunit of the RC in the purple photosynthetic bacterium *Rhodobacter sphaeroides*. The engineered organism grows photosynthetically. The strong YFP emission has excellent spectral overlap with the visible-region (Q_X) absorption bands of the RC, allowing for energy transfer from YFP to RC via a long-range dipole-dipole trough- space (Förster) mechanism. We used a number of complementary static and ultrafast time-resolved absorption and fluorescence techniques to quantify the yield of energy transfer from YFP to the RC, which was found to $\Phi_{EET} = 0.4 \pm 0.1$. Using Förster theory, including the YFP emission and RC absorption spectral overlap, a Förster radius R_0 (distance at which $\Phi_{EET} = 0.5$) of 55 Å was obtained for the YFP/RC energy donor/acceptor pair. The values $\Phi_{EET} = 0.4$ and $R_0 = 55$ Å give an estimated distance between the YFP and RC pigments of R = 60 Å. This work demonstrates the viability of incorporating fluorescent proteins into the genome of photosynthetic systems to complement production of their existing suite of light-harvesting proteins and chromophores, thereby conferring new capabilities on the native organisms.

8:50 AM

H-III-2: FLAVINS ARE SINGLE-MOLECULE SWITCHES THAT COUPLE ELECTRON TRANSFER, PROTON TRANSFER, CONFORMATIONAL GATING AND ENERGY REALLOCATION IN SUPPORT OF VERSATILE HIGH-EFFICIENCY ENERGY TRANSDUCTION

[BETCy] Anne-Frances Miller[1], John Hoben[1], Deissel Duan[1], Cara Lubner[2], Michael Ratzloff[2], Paul King[3], David Jennings[3], Anne K. Jones[3], Gerti Schut[4], Michael Adams[4], Saroj Poudel[5], Amaya Garcia-Costas[5], Eric Boyd[5], John Peters[5]

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

Flavins are heterocyclic molecules used as active site cofactors by diverse enzymes, wherein they carry out redox reactions coupling electron transfer to proton transfers, conformational gating, reconciliation of spins and even absorption of light. Whilst most organic redox reactions involve pairs of electrons, flavins can also do one-electron chemistry. This special ability explains why they are found at crucial junctures of biological energy transduction, enabling energy associated with 1-e^- processes to be fed into 2-e^- reactions that generate chemical bonds. Flavins are also proposed to be the points of electron transfer bifurcation in the newly-identified bifurcating enzymes under study by the BETCy EFRC because flavins can concentrate the total energy of a pair of electrons on one of the electrons, with exergonic transfer of the other 'paying' for the energizing of the first. This can be understood in terms of the stability of the semi-reduced ('semiquinone') state of the flavin, which is exquisitely tunable via interactions with the protein. Bifurcating enzymes must also gate electron transfer such that only one of the two electrons can take the exergonic route; flavoenzymes provide precedent for this too. Moreover flavin electronics and interactions can be studied via diverse spectroscopic and time-resolved methods. Thus flavin systems studied by BETCy afford unique opportunities to understand the fundamental determinants of electron transfer bifurcation and pave the way to tuning the properties of flavins to 'upgrade' the energy of half the electrons they deliver, enabling demanding chemical reactions.

9:10 AM

H-III-3: NEUTRON SCATTERING STUDIES OF PHOTOSYNTHETIC ANTENNA SYSTEMS

[PARC] Volker S. Urban[1], Laura-Roxana Stingaciu[1], Michelle Liberton[2], Hugh O'Neill[1], Michael Ohl[1], Himadri B. Pakrasi[2], Jerilyn A. Timlin[3], Peter G. Adams[4], Aaron M. Collins[4], Tuba Sahin[5], Vijaya Subramanian[6], Pothiappan Vairaprakash[5], Yongming Tian[4,7], Deborah G. Evans[6], Andrew P. Shreve[6], Gabriel A. Montaño[4]

[1] Biology and Soft Matter Division, Oak Ridge National Laboratory; [2] Department of Biology, Washington University, St. Louis; [3] Department of Bioenergy and Defense Technologies, Sandia National Laboratories, Albuquerque; [4] Center for Integrated Nanotechnologies, Los Alamos National Laboratories; [5] Department of Chemistry, North Carolina State University; [6] Center for Biomedical Engineering, University of New Mexico; [7] Department of Chemistry, New Mexico Institute of Mining and Technology

The efficiency with which photosynthetic organisms capture sunlight and convert it to chemical energy depends on sophisticated hierarchical structures with optimized organization from the atomic to the cellular length scale. Moreover, these biological structures exhibit many degrees of dynamic response to changes in environmental factors. Understanding the complexity of this wide space of structure, dynamics and function requires the collaborative use of many different experimental, computational and theoretical tools. Notably, neutron scattering and diffraction are well placed in this context to provide critical insights, because they allow localization of

specific hydrogen atoms and hydrogen bonding networks, and provide possibilities for distinguishing components with nano-scale to meso-scale structure based on hydrogen content and contrast variation through deuterium exchange and labeling. In addition, low-energy neutrons that are available at cold neutron sources of the Department of Energy's neutron user facilities provide well matched length-scale and energy-resolution of the neutron probe in a single experiment. This combination of neutron capabilities has been widely utilized in several collaborative efforts within the framework of the Photosynthetic Antenna Research Center (PARC), including work on natural antennas as well as bio-inspired synthetic systems. Most recently, we have used the Neutron Spin-Echo technique (NSE) to observe motions of photosynthetic membranes inside live cyanobacteria. The degree of mobility that is exhibited by these cell-internal membranes depends on light intensity and appears to correlate with photosynthetic activity.

9:30 AM

H-III-4: DESIGNING SELF-REGULATING MICROCAPSULES THAT HARNESS CHEMICAL ENERGY TO UNDERGO BIMIMETIC COLLECTIVE MOTION

[CBES] Henry Shum[1], Victor V. Yashin[1], Anna C. Balazs[1]
[1]*Department of Chemical & Petroleum Engineering, University of Pittsburgh*

One of the intriguing challenges in designing active matter is devising systems that not only self-organize, but also exhibit self-regulation. Inspired by biological regulatory networks, we design a collection of self-organizing, self-regulating microcapsules that move in response to self-generated chemical signals. Three microcapsules act as localized sources of distinct chemicals that diffuse through surrounding fluid. Production rates are modulated by the "repressilator" regulatory network motif: each chemical species represses the production of the next in a cycle. Depending on the maximum production rates and capsule separation distances, we show that immobile capsules either exhibit steady or oscillatory chemical production. We then consider movement of the microcapsules over the substrate, induced by gradients in surface energy due to adsorbed chemicals. We numerically simulate this advection-diffusion-reaction system with solid-fluid interactions by combining lattice Boltzmann, immersed boundary and finite difference methods, and thereby, construct systems where the three capsules spontaneously assemble to form a close-packed triad. Chemical oscillations are shown to be critical to this assembly. By adjusting parameters, the triad can either remain stationary or translate as a cohesive group. Stationary triads can also be made to "turn off", producing chemicals at minimal rates after assembly. With large numbers of these self-regulating microcapsules, we find that the system produces spiral chemical waves, which induce the collective motion of these assemblies. Notably, this mode of self-organization closely mimics the behavior of slime molds. These findings provide design rules for creating synthetic material systems that encompass biomimetic feedback loops, which enable dynamic collective behavior.

9:50 AM

H-III-5: PHYCOBILISOME DEGRADATION IN A FAST GROWING CYANOBACTERIUM

[PARC] Aparna Nagarajan[1], Michelle Liberton[1], Jon M. Jacobs[2], Richard D. Smith[2], David W. Koppenaal[3], Himadri B. Pakrasi[1]

[1]Department of Biology, Washington University, St. Louis; [2]Biological Sciences Division, Pacific Northwest National Laboratory; [3]Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory

Phycobilisomes (PBSs) are natural light-harvesting antenna in cyanobacteria, with pigmented phycobiliproteins and linker proteins that assemble to form massive complexes. PBSs account for 50% of the total soluble protein and possess tremendous plasticity that allows cyanobacteria to adjust to changes in environmental factors such as nutrient deprivation (1). The phenomenon of PBS degradation was observed over two decades ago, in which cyanobacteria undergo bleaching during nutrient deprivation. Previous studies on PBS degradation have been in model organisms where this process occurs over a period of 48 hours.

In *Synechoccous elongatus* UTEX 2973, a recently identified fast growing cyanobacterium (2), the process of PBS degradation is very rapid. We have observed that 80% of PBSs per cell are degraded in 6 hours and continuous translation of protein factors is essential for PBS degradation. A modulation of photosystems as an immediate consequence of nitrogen depletion was also observed. We have collected various time points during PBS degradation and re-synthesis process to understand the physiological changes during this time period. Additionally, we have used a quantitative Liquid Chromatography – tandem Mass Spectrometry (LC-MS/MS) top down global proteomics approach to gain insights on whole protein modifications and truncations, primarily those associated with PBSs. The outcome of this study will aid in improving the current understanding of the mechanism of this extensive and tightly controlled degradation process.

(1) Grossman, AR. et al. (1993) *Microbiol. Rev*. 57, 725-749
(2) Yu, J. et al., *Sci. Rep*. 2015 Jan 30; 5:8132. doi: 10.1038/srep08132

I. SEPARATIONS

SESSION III: TUESDAY, OCTOBER 27, 2015; 8:30 – 10:10 AM; LINCOLN 2

8:30 AM

I-III-1: CLUSTER-BASED URANIUM SEPARATION USING GREEN CHEMISTRY PRINCIPLES

[MSA] Harrison A. Neal[1], Jennifer E.S. Szymanowski[2], Jeremy B. Fein[2], May Nyman[1]
[1] Department of Chemistry, Oregon State University; [2] Department of Civil and Environmental Engineering and Earth Sciences, University of Notre Dame

For nuclear energy to become broadly accepted, concerns of safety and the environment must be addressed. Fuel recycling, important for separating uranium from isotope decay products, includes dissolution of fuel pellets in acid, extraction into an organic phase (kerosene) as monomeric uranium complexes, and back-extraction with acid. Enhanced purification and decreased hazardous chemical wastes are goals for improving these processes. Here we describe an alternative uranium extraction chemistry that 1) utilizes ammonium hydroxide-peroxide for fuel dissolution and carbonate for back-extraction, and 2) extracts uranium into kerosene as polyoxometalate capsules with surfactant counterions. The use of less toxic chemicals and improved atom economy of extractant molecules arising from the polynuclear form of uranium demonstrate *green chemistry* principles. The uranium capsules behave differently in kerosene than in water, including low mobility of chemical species residing inside the capsules, and evolution into larger capsules. The distinct uranium capsule behavior in organic solvent yields new fundamental and applied chemistries.

8:50 AM

I-III-2: CARBON DIOXIDE CAPTURE IN DIAMINE-APPENDED METAL-ORGANIC FRAMEWORKS

[CGS] Thomas M. McDonald[1], Jarad A. Mason[1], Rachel L. Segalman[1], Xueqian Kong[2], Walter Drisdell[4], Eric D. Bloch[1], David Gygi[1], Samuel Odoh[6], Bess Vlaisavljevich[2], Allison L. Dzubak[6], Kyuho Lee[4,5], Nora Planas[6], Tod Pascal[5], Liwen F. Wan[5], David Prendergast[5], Jeffrey B. Neaton[3-5], Laura Gagliardi[6], Berend Smit[1,2,4], Jeffrey B. Kortright[4,5], Jeffrey A. Reimer[2,4], Jeffrey R. Long[1,2,4]
[1]Department of Chemistry, University of California, Berkeley; [2]Department of Chemical and Biological Engineering, University of California, Berkeley; [3]Department of Physics, University of California, Berkeley; [4]Materials Sciences Division, Lawrence Berkeley National Laboratory; [5]The Molecular Foundry, Lawrence Berkeley National Laboratory; [6]Department of Chemistry, Chemical Theory Center and Supercomputing Institute, University of Minnesota

Owing to their high surface areas, tunable pore dimensions, and adjustable surface functionality, metal-organic frameworks (MOFs) can offer advantages for a variety of gas storage and gas separation applications. In an effort to help curb greenhouse gas emissions from power plants, we are developing new MOFs for potential use as solid adsorbents in post- and pre-combustion CO_2 capture, and for the separation of O_2 from air, as required for oxy-fuel combustion. In particular, MOFs with diamine-functionalized surfaces are demonstrated to provide high selectivities and capacities for the adsorption of CO_2 over N_2 under dry flue gas conditions. Thermogravimetric cycling and multicomponent adsorption measurements further show compounds of this type remain highly effective in the presence of water, while calorimetry data reveal a low regeneration energy compared to aqueous amine solutions. Most significantly, as revealed by *in situ* nuclear magnetic resonance, infrared, and x-ray absorption spectroscopy experiments, powder x-ray diffraction crystal structure determinations, and computational simulations, the unusual stepped CO_2 adsorption isotherms exhibited by these materials are shown to arise from a unique cooperative insertion mechanism to form one-dimensional chains of metal-bound ammonium carbamates. A detailed understanding of this mechanism now enables us to design new materials for the low-energy separation of CO_2 from a wide variety of key gas mixtures, including flue gases, air, biogas, and natural gas deposits.

9:10 AM

I-III-3: IN SITU IR SPECTROSCOPIC INVESTIGATION OF ACID GAS ADSORPTION ON MOF-DERIVED CERIA AND TITANIA

[UNCAGE-ME] William P. Mounfield, III[1], Uma Tumuluri[2], Yang Jiao[1], Zili Wu[2], Krista S. Walton[1]
[1]School of Chemical & Biomolecular Engineering, Georgia Institute of Technology; [2]Chemical Science Division and Center for Nanophase Materials Sciences, Oak Ridge National Laboratory

In order to further the development of sorbent and catalytic materials for industrial applications, laboratory experiments must be conducted to probe material stability in the often harsh environments encountered in these potential applications. Metal-organic frameworks (MOFs) and metal oxides often display promising performance in ideal, one or two component systems; however, industrial adsorption and catalysis applications are almost always in the presence of acid gases that degrade the adsorbent or the catalyst. Therefore, it is necessary to understand the interaction of acid gases with MOFs and metal oxides to drive future material design. Calcination of MOFs was used to prepare porous oxides that retain the overall morphology of the parent MOF, allowing comparison of the MOF, MOF-derived oxide, and bulk oxide synthesized through traditional methods in an investigation of both the effect of morphology and the metal coordination environment on acid gas stability. A cerium-based MOF with open-metal sites, CeBTC, was chosen for creation of a MOF-derived CeO_2, and the Ti-based MIL-125 was chosen to compare to CeBTC and similarly as a parent for a derived TiO_2 for comparison with bulk TiO_2. It was shown that surface and bulk species observed during SO_2 and CO_2 adsorption with in situ IR spectroscopy on the derived oxides differed from traditional oxides due to an increased number of defects and retained porosity from the MOF parent material. SEM images taken before and after IR experiments revealed a degradation of all materials giving visual insight into the mechanism of degradation after acid gas exposure.

9:30 AM

I-III-4: UNDERSTANDING UNIQUE DIFFUSION BEHAVIOR IN HIERARCHICAL ZEOLITES

[CCEI] Peng Bai[1], Emmanuel Haldoupis[2], Paul J. Dauenhauer[1], Michael Tsapatsis[1], J. Ilja Siepmann[1,2]
[1]Department of Chemical Engineering and Materials Science, University of Minnesota; [2]Department of Chemistry and Chemical Theory Center, University of Minnesota

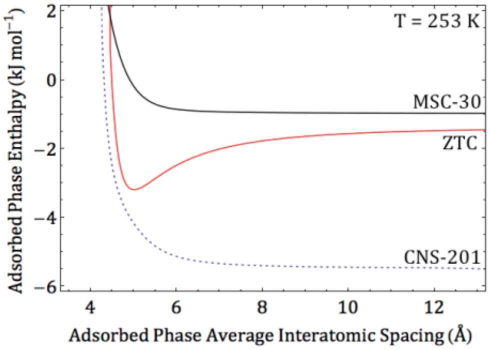
Hierarchical zeolites are materials that contain both micro (<2 nm) and meso (2—50 nm) porosity and are proposed as potential solutions to alleviate transport limitations of conventional microporous zeolites. The introduction of mesopores adds considerable complexity to the adsorption and transport behavior exhibited by these hierarchical materials. Adsorption measurements and Monte Carlo simulations demonstrate a crossover phenomenon where the sorbate loading in the conventional zeolite exceeds that in the hierarchical zeolite at low pressure, but the ordering is reversed at high pressure. Similarly, experimental measurements and molecular dynamics simulations point to unexpected transport behavior. In this talk, we present a molecular simulation study on the diffusion of linear and branched alkanes in MFI-type zeolites. Diffusion coefficients are computed at multiple temperatures from 363 – 543 K and as a function of loading. The comparison between the diffusional behaviors in conventional and hierarchical materials reveals surprising features in the latter systems, and we offer explanations in terms of free energy profiles in the two types of materials.

9:50 AM – Graduate Student Finalist

I-III-5: Anomalous Surface Thermodynamics of Gas Adsorption on Zeolite-Templated Carbon

[EFree] Maxwell Murialdo, Nicholas P. Stadie, Channing C. Ahn, Brent Fultz
California Institute of Technology

In this talk I will discuss a newly discovered effect in the field of gas adsorption and its impact on three energy-relevant gases: methane, ethane and krypton. While krypton separation (from xenon) is of critical importance to establishing "closed" nuclear fuel cycles, methane and ethane are the main components in natural gas. For natural gas-fueled cars, the ability to store the necessary quantities of natural gas in inexpensive and moderately sized onboard tanks remains a significant challenge. By filling the onboard tanks with specially designed physisorptive materials, the onboard storage capacity can be significantly improved. In particular we have synthesized a zeolite-templated carbon that is one of the best carbonaceous adsorbents for methane storage to date, yielding roughly a 50% improvement over compression alone at room temperature and 90 bars pressure.



While the adsorbed phase enthalpies on conventional carbons (MSC-30 and CNS-201) decrease monotonically with interatomic spacing, on zeolite-templated carbon it resembles a 12-6 Lennard-Jones potential, showcasing the enhanced adsorbate-adsorbate interactions.

Unlike conventional adsorbate-adsorbent systems which have isosteric enthalpies of adsorption that decrease with surface loading, our zeolite-templated carbon has isosteric enthalpies for methane, ethane and krypton adsorption that increase with surface loading [1-3]. The uniquely ordered nanostructure of our zeolite-templated carbon [4] promotes lateral interactions between the adsorbate molecules leading to this anomalous effect. By using a controlled adsorbent nanostructure to thus tune the adsorption thermodynamics, gas storage and separation properties may be favorably modified. Furthermore, to gain a better understanding of this phenomenon, we have developed more robust fitting techniques, and have used statistical mechanical estimates to corroborate our findings and develop a cooperative interaction model of the effect. These techniques are also applicable to the analysis of other adsorbents and may prove useful for understanding adsorption properties on other carbons that have been synthesized at high pressures by EFree collaborators in the Lehigh group.

[1] M. Murialdo, N.P. Stadie, C.C. Ahn, and B. Fultz, "Anomalous Thermodynamics of Krypton Adsorption on Zeolite-Templated Carbon," *Langmuir*, **31**, 7991 (2015).
[2] M. Murialdo, N.P. Stadie, C.C. Ahn, and B. Fultz, "Observation and Investigation of Increasing Isosteric Heat of Adsorption of Ethane on Zeolite-Templated Carbon," *J. Phys. Chem. C*, **119**, 994 (2015).
[3] N.P. Stadie, M. Murialdo, C.C. Ahn, and B. Fultz, "Anomalous Isosteric Enthalpy of Adsorption of Methane on Zeolite-Templated Carbon," *J. Am. Chem. Soc.* **135**, 990 (2013).
[4] N.P. Stadie, B. Fultz, C.C. Ahn, and M. Murialdo, "Nanostructured Carbon Materials for Adsorption of Methane and Other Gases," **U.S. Patent 9,067,848.** Jun. 30, 2015.

J. MESOSCALE SCIENCE

SESSION IV: TUESDAY, OCTOBER 27, 2015; 10:40 – 12:00 PM; THURGOOD MARSHALL E/N

10:40 AM

J-IV-1: INFLUENCE OF CHEMICAL DISORDER ON ENERGY DISSIPATION AND DEFECT EVOLUTION IN ADVANCED ALLOYS - PROGRESS TOWARD STRUCTURAL MATERIALS BY DESIGN

[EDDE] Yanwen Zhang[1], G. Malcolm Stocks[1], Ke Jin[1], Chenyang Lu[2], Hongbin Bei[1], Brian C. Sales[1], Lumin Wang[2], Laurent K. Beland[1], Roger E. Stoller[1], German D. Samolyuk[1], Magdalena Caro[3], Alfredo Caro[3], William J. Weber[1,4]

[1]Oak Ridge National Laboratory; [2]University of Michigan; [3]Los Alamos National Laboratory; [4]University of Tennessee

Alloy development is arguably one of the oldest sciences, dating back at least 3,000 years. Most efforts have been focused on alloys with one principal element and minor alloying elements. In sharp contrast to traditional alloys, recent advances of single-phase concentrated solid solution alloys (SP–CSAs) have opened up new frontiers in materials research. In these alloys, a random arrangement of multiple elemental species on a lattice (fcc or bcc) results in unique site-to-site lattice distortions and local disordered chemical environments.

We show that chemical disorder and compositional complexity in SP–CSAs have an enormous impact on defect dynamics through substantial modification of energy dissipation pathways. Based on a closely integrated computational and experimental study using a novel set of Ni-based SP-CSAs, we have explicitly demonstrated that increasing chemical disorder can lead to a substantial reduction in the electron mean free path and electrical and thermal conductivity. These reductions have a significant impact on energy dissipation and consequentially on defect evolution during ion irradiation. Considerable enhancement in radiation resistance with increasing chemical complexity is observed under ion irradiation. The insights into defect dynamics at the level of atoms and electrons provide an innovative path forward towards solving a long-standing challenge in structural materials. Understanding how material properties can be tailored by alloy complexity and their influence on defect dynamics may pave the way for new design principles of radiation–tolerant structural alloys for advanced energy systems, as well as for new defect engineering paradigms benefiting broader science and technology.

11:00 PM

J-IV-2: LEVERAGING EMPIRICAL AND COMPUTATIONALLY MODELED STRUCTURES TO EXPLORE PLANT CELLULOSE SYNTHASE PROTEIN FUNCTION

[CLSF] Candace H. Haigler[1], Erin Slabaugh[1], Arielle Chaves[2], Jonathan K. Davis[1], Jung-Goo Lee[3], Tess Scavuzzo-Duggan[2], Abhishek Singh[3], Carmen Wilson[1], Liza Wilson[4], Charles T. Anderson[4], Daniel J. Cosgrove[4], Alison W. Roberts[2], Yaroslava G. Yingling[3]

[1]Department of Crop Science and Department of Plant and Microbial Biology, North Carolina State University; [2]Department of Biological Sciences, University of Rhode Island; [3]Department of Materials Science and Engineering, North Carolina State University; [4]Department of Biology, The Pennsylvania State University

We will describe an integrated multi-disciplinary research program to test structure-function relationships in plant cellulose synthase (CESA) and the cellulose synthesis complex (CSC), taking advantage of new structural information about bacterial and plant cellulose synthases. Despite the predicted similarity of cellulose polymerization in bacterial BcsA and plant CESA, other aspects of plant CESAs are different and must be empirically tested to determine their mechanistic impacts on the synthesis of renewable cellulose-rich biomaterials. Computational modeling was used to generate hypotheses about CESA structure-function relationships, which were then tested through genetic complementation assays in two phylogenetically distant CESAs of *Arabidopsis thaliana* and *Physcomitrella patens*. The mesoscale properties of cellulose in genetically altered Arabidopsis lines were assessed by use of high-resolution microscopic methods. This strategy was implemented to: (a) test the role of a plant-specific region of CESA; and (b) assess the function of a region containing a broadly conserved FxVTxK motif that has a different predicted topology in CESA as compared to bacterial BcsA. The relatively high throughput testing strategy helped to clarify strong structure/function relationships in diverse CESAs. The experiments also revealed differences in: (a) the effects of analogous structural changes in diverse CESA isoforms; (b) the impacts of altering the function of one CESA versus the entire CSC; and (c) the degree of tolerance for changing the cellulose network in the context of particular developmental events. Finally, progress in generating a refined and complete model of a plant CESA will be described.

11:20 PM

J-IV-3: ADVANCED CHARACTERIZATION TECHNIQUES FOR ACTINIDE MATERIALS

[MSA] Maik Lang[1], Raul I. Palomares[1], Jacob Shamblin[1], Cameron L. Tracy[2], Rodney C. Ewing[2]
[1] *Department of Nuclear Engineering, University of Tennessee*
[2] *Department of Geological Sciences, Stanford University*

Actinide materials are subjected to extreme environments during nuclear reactor operation (intense irradiation, high temperature, and production of fission products and transuranic elements). We are currently utilizing pulsed neutrons at the Spallation Neutron Source and synchrotron X-rays at the Advanced Photon Source to investigate structural and chemical modifications induced by these conditions in a wide variety of nuclear materials. The unique combination of anion-sensitive neutron and cation-sensitive X-ray techniques yields information on the defect behavior over a range of length scales. While diffraction experiments probe the average sample structure, total scattering experiments with pair distribution function (PDF) analysis provide information on the local atomic arrangements. Neutron PDFs on lanthanide-doped UO_2 samples were used to study the effects of chemical composition on local defect structure, including changes in site occupation, coordination number, bond-distance, and bond-angle. The structural and chemical effects of high-energy heavy ion irradiation on actinide and analogue materials were analyzed using X-ray diffraction (XRD) and X-ray absorption masses and energies indicated coupling of structural damage to electronic excitation-induced cation valence changes. Heatable diamond anvil cells combined with synchrotron radiation were used to characterize the annealing of radiation damage in samples at temperature of up to 850 °C. X-ray diffraction analysis shows defect recovery in both oxides following a different trend as a function of increasing temperature with a one- and two-stage behavior for ThO_2 and CeO_2, respectively.

11:40 PM

J-IV-4: PROBING THE ARCHITECTURE OF PLANT CELL WALL IN BETWEEN THE NANOSCOPIC AND MACROSCOPIC LENGTH SCALES WITH SUM-FREQUENCY-GENERATION (SFG) VIBRATION SPECTROSCOPY

[CLSF] Christopher M. Lee[1], Kabindra Kafle[1], Shixin Huang[1], Charles T. Anderson[2], Ying Gu[3], James D. Kubicki[4], Seong H. Kim[1]

[1]Department of Chemical Engineering and Materials Research Institute, [2]Biology, [3]Biochemistry and Molecular Biology, [4]Geological Sciences, Pennsylvania State University

Plant cell walls are the most abundant biomass feedstock available for production of renewable fuels but are recalcitrant to biochemical treatment processes. This is due to the crystalline nature of cellulose and the three-dimensional arrangements with the matrix polymers hemicellulose or lignin. This level of organization takes place between the nanometer and micron length scales or “mesoscale”. The mesoscale organization of crystalline cellulose varies depending on developmental stages, cell types and species. Therefore understanding the hierarchical organization of cellulose will advance our understanding of plant cell growth and to develop methods for plant-based fuels. We use sum-frequency-generation (SFG) vibration spectroscopy which probes crystalline cellulose in intact cell walls and provides the structural information of cellulose microfibrils at the mesoscale. In this talk, we show the remarkable differences in cellulose crystal structure within intact A. thaliana primary cell walls (seedlings) and secondary cell walls (stems). In addition we investigate how cellulose organization is affected by interactions with matrix polymers and the process of microfibril formation by studying the A. thaliana mutants with deficiencies in hemicellulose production and the cellulose synthesis machinery. These structural differences would not be detected if the cellulose is first isolated from the cell walls using purification processes, which has been the main approach for structural analysis of cellulose in biomass. Therefore, SFG will provide an unprecedented opportunity to study the intact mesoscale organization of crystalline cellulose in biomass, which can be utilized as a renewable resource to meet the increase in demands for transportation fuels.

EFRC OVERVIEW POSTERS: OCTOBER 26-27, 2015

The EFRC Overview Posters will be displayed during the entire meeting. The EFRC may choose to have a presenter at the poster at one or both poster sessions, but it is not required.

P-O-1: PHOTOSYNTHETIC ANTENNA RESEARCH CENTER (PARC)
Robert Blankenship, ***Washington University in St. Louis***

P-O-2: CENTER FOR LIGNOCELLULOSE STRUCTURE AND FORMATION (CLSF)
Daniel Cosgrove, ***Pennsylvania State University***

P-O-3: CENTER FOR DIRECT CATALYTIC CONVERSION OF BIOMASS TO BIOFUELS (C3BIO)
Maureen McCann, ***Purdue University***

P-O-4: CENTER FOR BIOLOGICAL ELECTRON TRANSFER AND CATALYSIS (BETCY)
John Peters, ***Montana State University***

P-O-5: CATALYSIS CENTER FOR ENERGY INNOVATION (CCEI)
Dionisios Vlachos, ***University of Delaware***

P-O-6: MATERIALS SCIENCE OF ACTINIDES (MSA)
Peter Burns, ***University of Notre Dame***

P-O-7: ENERGY FRONTIER RESEARCH IN EXTREME ENVIRONMENTS (EFREE)
Russell Hemley, ***Carnegie Institution of Washington***

P-O-8: ENERGY DISSIPATION TO DEFECT EVOLUTION (EDDE)
Yanwen Zhang, ***Oak Ridge National Laboratory***

P-O-9: CENTER FOR NANOSCALE CONTROLS ON GEOLOGIC CO_2 (NCGC)
Donald DePaolo, ***Lawrence Berkeley National Laboratory***

P-O-10: CENTER FOR GEOLOGIC STORAGE OF CO_2 ($GSCO_2$)
Scott M. Frailey, ***University of Illinois at Urbana-Champaign***

P-O-11: CENTER FOR FRONTIERS OF SUBSURFACE ENERGY SECURITY (CFSES)
Larry Lake, ***University of Texas at Austin***

P-O-12: CENTER FOR GAS SEPARATIONS RELEVANT TO CLEAN ENERGY TECHNOLOGIES (CGS)
Jeffrey Long, ***University of California, Berkeley***

P-O-13: CENTER FOR UNDERSTANDING AND CONTROL OF ACID GAS-INDUCED EVOLUTION OF MATERIALS FOR ENERGY (UNCAGE-ME)
Krista Walton, ***Georgia Institute of Technology***

P-O-14: CENTER FOR EMERGENT SUPERCONDUCTIVITY (CES)
Peter Johnson, ***Brookhaven National Laboratory***

P-O-15: SPINS AND HEAT IN NANOSCALE ELECTRONIC SYSTEMS (SHINES)
Jing Shi, ***University of California, Riverside***

P-O-16: CENTER FOR BIO-INSPIRED ENERGY SCIENCE (CBES)
Samuel Stupp, ***Northwestern University***

P-O-17: INTEGRATED MESOSCALE ARCHITECTURES FOR SUSTAINABLE CATALYSIS (IMASC)
Cynthia Friend, ***Harvard University***

P-O-18: INORGANOMETALLIC CATALYST DESIGN CENTER (ICDC)
Laura Gagliardi, ***University of Minnesota***

P-O-19: CENTER FOR THE COMPUTATIONAL DESIGN OF FUNCTIONAL LAYERED MATERIALS (CCDM)
John Perdew, ***Temple University***

P-O-20: CENTER FOR ELECTROCHEMICAL ENERGY SCIENCE (CEES)
Paul Fenter, ***Argonne National Laboratory***

P-O-21: NANOSTRUCTURES FOR ELECTRICAL ENERGY STORAGE (NEES)
Gary Rubloff, ***University of Maryland***

P-O-22: CENTER FOR MESOSCALE TRANSPORT PROPERTIES (M2M)
Esther Takeuchi, ***Stony Brook University***

P-O-23: FLUID INTERFACE REACTIONS, STRUCTURES AND TRANSPORT CENTER (FIRST)
David Wesolowski, ***Oak Ridge National Laboratory***

P-O-24: NORTHEAST CENTER FOR CHEMICAL ENERGY STORAGE (NECCES)
M. Stanley Whittingham, ***Binghamton University***

P-O-25: CENTER FOR EXCITONICS (CE)
Marc Baldo, ***Massachusetts Institute of Technology***

P-O-26: CENTER FOR MOLECULAR ELECTROCATALYSIS (CME)
R. Morris Bullock, ***Pacific Northwest National Laboratory***

P-O-27: SOLID-STATE SOLAR-THERMAL ENERGY CONVERSION CENTER (S^3TEC)
Gang Chen, ***Massachusetts Institute of Technology***

P-O-28: CENTER FOR ADVANCED SOLAR PHOTOPHYSICS (CASP)
Victor Klimov, ***Los Alamos National Laboratory***

P-O-29: CENTER FOR SOLAR FUELS (UNC)
Thomas Meyer, ***University of North Carolina***

P-O-30: LIGHT-MATERIAL INTERACTIONS IN ENERGY CONVERSION (LMI)
Ralph Nuzzo, ***California Institute of Technology***

P-O-31: CENTER FOR NEXT GENERATION OF MATERIALS BY DESIGN: INCORPORATING METASTABILITY (CNGMD)
William Tumas, ***National Renewable Energy Laboratory***

P-O-32: ARGONNE-NORTHWESTERN SOLAR ENERGY RESEARCH CENTER (ANSER)
Michael Wasielewski, ***Northwestern University***

POETRY OF SCIENCE POSTERS: OCTOBER 26-27, 2015

The Poetry of Science Entries will be displayed during the entire meeting. The location of specific entries will be announced (labels on the poster boards) after the plenary session on Monday, October 26. The posters should be put up between the end of the plenary session and the start of Poster Session I on October 26. The entries are listed first by the juried winners and then by the remaining entries in alphabetical order by title.

FIRST PLACE

Afterlife of a Photon
EFRC: Center for Lignocellulose Structure and Formation (CLSF)
Contributors: Jochen Zimmer, Sarah Kiemle, Daniel Cosgrove

SECOND PLACE

As Above, So Below
EFRC: Center for Frontiers of Subsurface Energy Security (CFSES)
Contributors:
Poet: Jeffrey Clement Olson, UT Austin, Student
Artist: Victoria Osborne, UT Austin
Graph / data-rich element: Kim Gilbert, UT Austin, Student
Data-rich image description: Hilary Olson, UT Austin

THIRD PLACE

Ode to the Chlorosome
EFRC: Center for Excitonics (CE)
Contributors: Stéphanie Valleau

At Dawn I Rise
EFRC: Light-Material Interactions in Energy Conversion (LMI)
Contributors: Jennifer A. Dionne, Diane M. Wu

A Crystallographer's Peek
EFRC: Center for Gas Separations Relevant to Clean Energy Technologies (CGS)
Contributors: Ying-Pin Chen

Footprints on Copper
EFRC: Integrated Mesoscale Architectures for Sustainable Catalysis (IMASC)
Contributors: Nare Janvelyan

The Free Charge of AN-SER
EFRC: Argonne-Northwestern Solar Energy Research Center (ANSER)
Contributors: Nicholas Jackson, Eric Manley

Go with the Flow
EFRC: Center for Biological Electron Transfer and Catalysis (BETCy)
Contributors: Jamie Cornish, Montana State University; Amaya Garcia Costas, Montana State University; John Hoben, University of Kentucky; Rhesa Ledbetter, Utah State University; Suzi Taylor, Montana State University

In Full Color
EFRC: Solid-State Solar-Thermal Energy Conversion Center (S3TEC)
Contributors: Emma Anquillare (Poem Text)

Journey to Biomass
EFRC: Center for Direct Catalytic Conversion of Biomass to Biofuels (C3Bio)
Contributors: Nitya Kalyani Josyula

Metastability for Awesome Utility
EFRC: Center for Next Generation of Materials by Design: Incorporating Metastability (CNGMD)
Contributors: Don Gwinner, NREL; Al Hicks, NREL; Zamlya Chan, Harvard University; John Perkins, NREL

The Modern Man Runs on Lithium Ion
EFRC: Center for Electrochemical Energy Science (CEES)
Contributors: Bruno Giuliano Nicolau, University of Illinois, Urbana-Champaign; Kimberly Lundberg, University of Illinois, Urbana-Champaign; Fernando Castro, Northwestern University

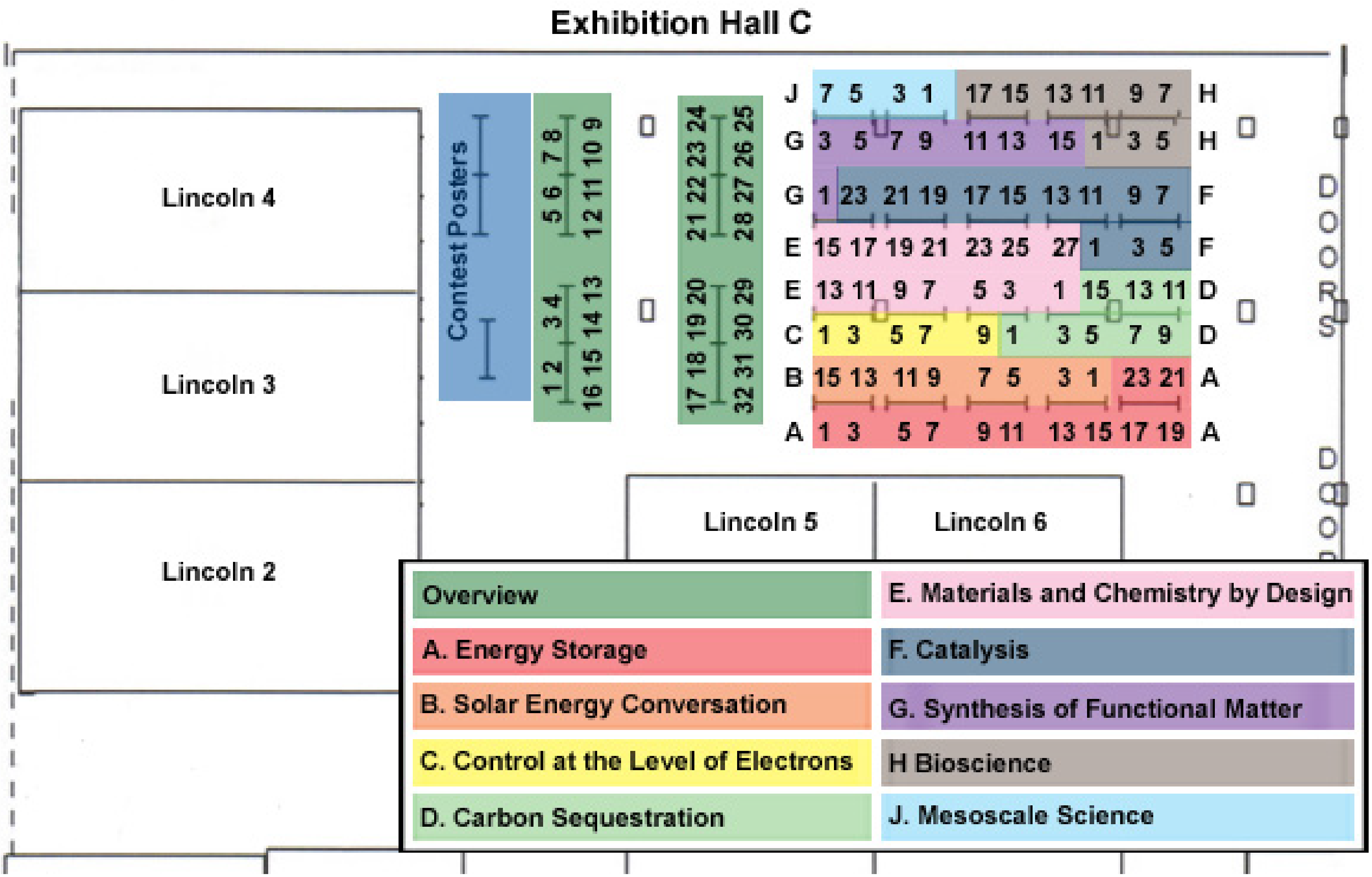
Quantum Dots for Solar Windows
EFRC: Center for Advanced Solar Photophysics (CASP)
Contributors: Ashley R. Marshall, Andrew F. Fidler

Solar Harvest
EFRC: Center for Solar Fuels (UNC)
Contributors: Christopher J. Dares, Gerald J. Meyer

Taming Vortices: Pathways to improved Superconductivity
EFRC: Center for Emergent Superconductivity (CES)
Contributors:
Image: Alexei Koshelev *et al.*, ANL
Poem: Superconducting Sleuths by Melinda Rak, UIUC
Poem: Running the East Coast in Summer by Jon Rameau, BNL

Three Ways of Looking at a Battery
EFRC: Nanostructures for Electrical Energy Storage (NEES)
Contributors: Elizabeth Lathrop, Martha J. Heil, Ernie Cleveland, Pradeep R. Rajasekaran

POSTER SESSION I: MONDAY, OCTOBER 26, 2015; 5:00 – 6:30 PM



POSTER SESSION I: MONDAY, OCTOBER 26, 2015; 5:00 – 6:30 PM, *EXHIBITION HALL C, ODD NUMBERED POSTERS*

A. ENERGY STORAGE

P-A-1: ENERGY CONVERSION IN POLYELECTROLYTE HYDROGELS

[CBES] Aykut Erbas[3], Monica Olvera de la Cruz[1-4]

[1]Department of Chemistry, Northwestern University; [2]Department of Materials Science and Engineering, Northwestern University; [3]Department of Physics and Astronomy, Northwestern University; [4]Department of Chemical and Biological Engineering, Northwestern University

P-A-3: THEORETICAL INVESTIGATION OF MANGANESE DISSOLUTION AT $LiMn_2O_4$ CATHODE INTERFACE

[CEES] Kah Chun Lau[1], Hakim Iddir[1], Chris Knight[2], Handan Yildirim[3], Robert Warburton[3], Jeff Greeley[3], Larry A Curtiss[1]

[1]Materials Science Division, Argonne National Laboratory ; [2]Argonne Leadership Computing Facility, Argonne National Laboratory; [3]School of Chemical Engineering, Purdue University

P-A-5: MULTISCALE ELECTROCHEMICAL REDUCTION FROM A SINGLE PARTICLE TO THE SYSTEMS LEVEL

[m2M] David C. Bock[1], Kevin C. Kirshenbaum[1], Zhong Zhong[1], Amy C. Marschilok[2], Kenneth J. Takeuchi[2], Esther S. Takeuchi[1,2]

[1]Brookhaven National Laboratory; [2]Stony Brook University

P-A-7: TRANSPORT IN ELECTRODES ACROSS MULTIPLE LENGTH SCALES

[NECCES] Min-Ju Choe[1], Hui-Chia Yu[1], Katsuyo Thornton[1], Nathalie Pereira[2], Glenn G. Amatucci[2], Ruhul Amin[3], Ping-Chun Tsai[3], Bohua Wen[3] , Yet-Ming Chiang[3].

[1] University of Michigan; [2] Rutgers University; [3] Massachusetts Institute of Technology

P-A-9: IN-SITU ELECTRICAL CONDUCTIVITY OF Li_xMnO_2 NANOWIRES AS A FUNCTION OF "X" AND SIZE IN ENERGY STORAGE DEVICE

[NEES] Mya Le[1], Yu Liu[2], Hui Wang[2,3], Rajen K. Dutta[2], Wenbo Yan[1], Jonathan Larson[4], Janice Reutt-Robey[4], John C. Hemminger[1], Ruqian Q. Wu[2], Reginald M. Penner[1,5]

[1] Department of Chemistry, University of California, Irvine; [2] Department of Physics and Astronomy, University of California, Irvine; [3] Department of Physics, Fudan University, China; [4] Department of Chemistry and Biochemistry, University of Maryland; [5] Department of Chemical Engineering and Materials Science, University of California, Irvine

P-A-11: ATOMIC-LAYER MODIFICATION OF ELECTRIFIED INTERFACES FOR SAFE AND RELIABLE LITHIUM-ION BATTERIES

[CEES] Xiangbo (Henry) Meng[1], Jeffrey W. Elam[1], Massimiliano Delferro[2], Madelyn Stalzer[2], Tobin J. Marks[2], Robert Warburton[3], Jeffrey P. Greeley[3], Jun Lu[4], Khalil Amine[4]

[1]Energy Systems Division, Argonne National Laboratory; [2]Department of Chemistry, Northwestern University; [3]School of Chemical Engineering, Purdue University ; [4]Chemical Sciences and Engineering Division, Argonne National Laboratory

P-A-13: *OPERANDO* NANOSCALE IMAGING OF INTERFACIAL REACTIONS USING ELECTROCHEMICAL TRANSMISSION ELECTRON MICROSCOPY AND DOUBLE LAYER FORMATION USING NEUTRON REFLECTOMETRY

[FIRST] Robert L. Sacci[1], Jennifer M. Black[1], Yu Zhang[2], Matthew Thompson[2], Pengfei Zhang[1], Mathieu Doucet[1], James F. Browning[1], Sheng Dai[1], Peter T. Cummings[2], Nina Balke[1], Gernot Rother[1], Raymond R. Unocic[1], Nancy J. Dudney[1]
[1]*Oak Ridge National Laboratory,* [2]*Vanderbilt University*

P-A-15: REALIZATION OF STABLE CATHODE-ELECTROLYTE INTERFACES IN DMSO BASED LI-AIR BATTERIES: EXPERIMENTAL AND THEORETICAL PERSPECTIVES

[NEES] Malachi Noked[1], Marshall A. Schroeder[1], Nitin Kumar[2], Alexander J. Pearse[1], Vladimir P. Oleshko[1,3], John Cumings[1], Kevin Leung[2], Sang Bok Lee[1], Gary W. Rubloff [1]
[1] *University of Maryland;* [2] *Sandia National Laboratories, Albuquerque;* [3] *Materials Science and Engineering Division, Material Measurement Laboratory, NIST*

P-A-17: ONE DIMENSIONAL MANGANESE OXIDES AS CATHODE MATERIALS IN LI-ION BATTERIES: THE ROLES OF MORPHOLOGY, PHYSICOCHEMICAL AND REDOX PROPERTIES ON ELECTROCHEMICAL PERFORMANCE

[m2M] Altug S. Poyraz[1], David Bock[1], Jianping Huang[2], Lijun Wu[1], Yimei Zhu[1], Amy C. Marschilok[2], Kenneth J. Takeuchi[2], Esther S. Takeuchi[1,2]
[1]*Brookhaven National Laboratory;* [2]*Stony Brook University*

P-A-19: UNRAVELING THE LITHIUM-ION SOLID ELECTROLYTE INTERPHASE THROUGH OPTICAL SPECTROSCOPY AND MASS SPECTROMETRY

[CEES] Bruno G. Nicolau[1], Yao-Min Liu[1], Kimberly Lundberg[1], Jen Esbenshade[1], Elizabeth Jones[1], Ralph Nuzzo[1], Nancy Sottos[1], Andrew Gewirth[1]
[1]*University of Illinois, Urbana-Champaign*

P-A-21: HOW ε-VOPO$_4$ WORKS AS TWO-ELECTRON CATHODE FOR LI-ION BATTERIES

[NECCES] Natasha A. Chernova[1],Youngmin Chung[1], Fredrick Omenya[1], Nicholas Quackenbush[1], Louis Piper[1], M. Stanley Whittingham[1], Yuh-Chieh Lin[2], Shyue Ping Ong[2], Kamila M. Wiaderek[3], Karena Chapman,[3] Bohua Wen[1,4]
[1] *Binghamton University;* [2] *University of California, San Diego;* [3] *Argonne National Laboratory;*
[4] *Massachusetts Institute of Technology*

P-A-23: ENGINEERING OF CNT/SULFUR COMPOSITES FOR LITHIUM-SULFUR BATTERIES

[NEES] Jeremy Ticey[1], Vladimir P. Oleshko[1, 2], Yujie Zhu[2], Chunsheng Wang[3], John Cumings[1]
[1] *Department of Materials Science and Engineering, University of Maryland;* [2] *Materials Science and Engineering Division, Material Measurement Laboratory, NIST;* [3] *Chemical and Biomolecular Engineering, University of Maryland*

B. SOLAR ENERGY CONVERSION

P-B-1: A PHOTOELECTROCHEMICAL CELL CONTAINING ALD-STABILIZED PERYLENE DYES AND AN IRIDIUM WATER OXIDATION CATALYST FOR LIGHT DRIVEN WATER OXIDATION

[ANSER] Kelly L. Materna[1], Rebecca Lindquist[2], Julianne Thomsen[1], William Hoffeditz[2], Benjamin Rudshteyn[1], Bradley Brennan[1], Aaron Bloomfield[1], Morgan H. Kane[1], Michael R. Wasielewski[2], Joseph T. Hupp[2], Victor S. Batista[1], Robert H. Crabtree[1], Gary W. Brudvig[1]

[1] Department of Chemistry, Yale University; [2] Department of Chemistry, Northwestern University

P-B-3: PHOTO-INDUCED CARRIER DYNAMICS IN QUANTUM DOT FILMS AND DEVICES MEASURED BY TRANSIENT PHOTOCURRENT AND PHOTOLUMINESCENCE EXPERIMENTS

[CASP] Andrew F. Fidler[1], Justin C. Johnson[2], Ashley R. Marshall[2], Jianbo Gao[1], Arthur J. Nozik[2], Matt Law[3], Matthew C. Beard[2], Victor I. Klimov[1]

[1] Chemistry Division, Los Alamos National Laboratory; [2] National Renewable Energy Laboratory;
[3] Depts. Chemistry and Chemical Engineering and Materials Science, University of California, Irvine

P-B-5: SYNTHESIS AND CHARACTERIZATION OF METASTABLE EXOTIC FORMS OF SILICON

[EFree] Lakshmi Krishna[1], Carolyn A. Koh[2], Reuben T. Collins[1], P. Craig Taylor[1]

[1] Department of Physics, Colorado School of Mines
[2] Department of Chemical and Biomedical Engineering, Colorado School of Mines

P-B-7: ELECTRON TRANSFER DYNAMICS AT DYE-SENSITIZED SnO_2/TiO_2 CORE/SHELL PHOTOANODES

[UNC] Robin R. Knauf[1], Melissa K. Gish[1], Berç Kalanyan[2], Alexander M. Lapides[1], Gregory N. Parsons[2], Thomas J. Meyer[1], John M. Papanikolas[1], Jillian L. Dempsey[1]

[1]Department of Chemistry, University of North Carolina at Chapel Hill
[2]Department of Chemical & Biomolecular Engineering, North Carolina State University

P-B-9: THREE- AND TWO-DIMENSIONAL HALIDE PEROVSKITE SOLAR CELLS

[ANSER] Duyen H. Cao[1], Constantinos C. Stoumpos[1], Feng Hao[1], Joseph T. Hupp[1], Mercouri G. Kanatzidis[1]

[1] Department of Chemistry, Northwestern University

P-B-11: TRIPLET EXCITON TRANSFER FROM TETRACENE TO SILICON

[CE] Daniel N. Congreve[1], Tony Wu[1], Markus Einzinger[1], Neil Patel[1], Nicholas J. Thompson[1], Michel Jurgen[1], Lionel C. Kimerling[1], Marc A. Baldo[1]

[1] *Center for Excitonics, Massachusetts Institute of Technology*

P-B-13: QUANTUM DOT LUMINESCENT CONCENTRATORS FOR 3RD GENERATION PHOTOVOLTAICS

[LMI] Noah D. Bronstein[1], Yuan Yao[2], Lu Xu[2], Erin O'Brien[1], Alexander S. Powers[1], Vivian E. Ferry[3], A. Paul Alivisatos[1,4], Ralph G. Nuzzo[2]

[1]University of California, Berkeley, [2]University of Illinois at Urbana–Champaign, [3]University of Minnesota, [4]Lawrence Berkeley National Laboratory

P-B-15: SYNTHETIC STRATEGIES OF MOLECULAR CHROMOPHORE-CATALYST ASSEMBLIES FOR LIGHT-ASSISTED WATER OXIDATION CATALYSIS

[UNC] Alexander M. Lapides, Benjamin D. Sherman, Christopher J. Dares, Melissa K. Gish, Kyung-Ryang Wee, Matthew V. Sheridan, Kasey R. Skinner, M. Kyle Brennaman, Joseph L. Templeton, Thomas J. Meyer
Department of Chemistry, University of North Carolina at Chapel Hill

C. CONTROL AT THE LEVEL OF ELECTRONS

P-C-1: SUPERCONDUCTING CRITICAL-CURRENT-BY-DESIGN

[CES] Maxime Leroux[1] and Karen Kihlstrom[1,2], Ivan A. Sadovskyy[1], Ying Jia[1], Jihwan Kwon[3], Hefei Hu[3], Lei Fang[1], Shaofei Zhu[4], Ulrich Welp[1], Jian-Min Zuo[3], Venkat Selvamanickam[5], George W. Crabtree[1,2], Alexei E. Koshelev[1], Andreas Glatz[1,6], Wai-Kwong Kwok[1]
[1]Materials Science Division, Argonne National Laboratory; [2]Dept. Physics, University of Illinois at Chicago

P-C-3: MAGNON-MEDIATED ELECTRIC CURRENT DRAG EFFECT IN NORMAL METAL/MAGNETIC INSULATOR/NORMAL METAL SANDWICH STRUCTURES

[SHINES] Junxue Li[1], Y.D. Xu[1], M. Aldosary[1], G. Yin[1], Y. Balars[1], S.S. Su[1], C. Tang[1], Z.S. Lin[1], R. Lake[1], S.F. Zhang[2], J. Shi[1]
[1]University of California, Riverside; [2]University of Arizona

P-C-5: ENERGY DISSIPATION AND DEFECT EVOLUTION IN ADVANCED ALLOYS

[EDDE] Hongbin Bei[1], G. Malcolm Stocks[1], Roger E. Stoller[1], German D. Samolyuk[1], Lumin Wang[2], Ian M. Robertson[3], William J. Weber[1,4], Magdalena Caro[5], Alfredo Caro[5], Alfredo Correa[6], Yanwen Zhang[1]
[1]Oak Ridge National Laboratory; [2]University of Michigan; [3]University of Wisconsin- Madison;
[4]University of Tennessee; [5]Los Alamos National Laboratory; [6]Lawrence Livermore National Laboratory

P-C-7: SPIN-ORBIT MANIPULATION OF MAGNETIZATION

[SHINES] P. Upadhyaya[1], Guoqiang Yu[1], Y. Fan[1], W. Jiang[1], Y. Liu[1], I. Barsukov[2], P.K. Amiri[1], Y. Tserkovnyak[1], I. Krivorotov[2], A.H. MacDonald[3], K.L. Wang[1]
[1]University of California, Los Angles; [2]University of California, Irvine; [3]University of Texas at Austin

P-C-9: HEAT-FLUX CONTROL AND SOLID-STATE COOLING BY REGULATING CHEMICAL POTENTIAL OF PHOTONS IN NEAR-FIELD ELECTROMAGNETIC HEAT TRANSFER

[LMI] Kaifeng Chen[1], Parthiban Santhanam[1], Sunil Sandhu[1], Linxiao Zhu[1], Shanhui Fan[1]
[1]Stanford University

D. CARBON SEQUESTRATION

P-D-1: FRACTURE PROPAGATION AND ITS IMPACT ON SEAL CAPACITY IN A NATURAL CO_2 SYSTEM

[CFSES] Hongkyu Yoon[1], Jon Major[2,3], Sanghyun Lee[4], Peter Eichhubl[3], Mary Wheeler[4], Thomas Dewers[5], Jacqueline Reber[6], Nick Hayman[6]
[1]Geoscience Research and Applications, Sandia National Laboratories; [2]Dept. Geological Sciences, The University of Texas at Austin; [3]Bureau of Economic Geology, The University of Texas at Austin; [4]The Institute for Computational Engineering and Sciences, The University of Texas at Austin; [5]Geomechanics Department, Sandia National Laboratories; [6]Institute for Geophysics, The University of Texas at Austin

P-D-3: PROBING THE MECHANISM OF CO_2 CAPTURE IN METAL-ORGANIC FRAMEWORKS USING X-RAY SPECTROSCOPY AND DFT CALCULATIONS

[CGS] Walter S. Drisdell[1], Roberta Poloni[2], Thomas M. McDonald[3], Tod A. Pascal[4], Liwen F. Wan[4], C. Das Pemmaraju[4], Bess Vlaisavljevich[5], Samuel O. Odoh[6], Jeffrey B. Neaton[4], Jeffrey R. Long[1,3], David Prendergast[4], Jeffrey B. Kortright[1]
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P-D-5: LEVEL-SET METHOD FOR IMMISCIBLE TWO-PHASE FLOW WITH DYNAMIC CONTACT ANGLE

[NCGC] Moataz Abu AlSaud[1], Cyprien Soulaine[1], Amir Riaz[1], Hamdi Tchelepi[1]
[1]*Stanford University*

P-D-7: DEVELOPING A PREDICTIVE METHOD FO LOCAL CAPILLARY TRAPPING CAPACITY ESTIMATION OF CO_2 USING INVASION PERCOLATION SIMULATIONS IN REALISTIC 3-D NUMERICAL LITHOFACIES MODEL

[CFSES] *Luca Trevisan[1], Prasanna Krishnamurthy[2], Tip Meckel[1]*
[1]Gulf Coast Carbon Center, Bureau of Economic Geology, The University of Texas at Austin
[2]Center for Petroleum and Geosystems Engineering, The University of Texas at Austin

P-D-9: DISCOVERY OF A NEW GEOLOGICAL FORMATION AND ITS IMPLICATIONS FOR MICROSEISMICITY PREDICTION IN CO_2 STORAGE PROJECTS

[GSCO2] Charles C. Monson[1,2], Jared T. Freiburg[1,3], Robert Ritzi[4], Volker Oye[5]
[1]Illinois State Geological Survey, Prairie Research Institute; [2]Department of Geoscience, University of Illinois at Urbana-Champaign; [3]Institut für Geographie und Geologie, Ernst-Moritz-Arndt Universität Greifswald, Germany; [4]Department of Earth and Environmental Sciences, Wright State University
[5]NORSAR, Kjeller, Norway

P-D-11: ANALYSIS AND MODELING OF PORE-SCALE STRUCTURES AND ASSOCIATED FLUID BEHAVIOR

[NCGC] David Cole[1], Alexander Swift[1], Bohyun Hwang[1], Salim Ok[1], Lawrence Anovitz[2], Julia Sheets[1]
[1]*Ohio State University;* [2]*Oak Ridge National Laboratory*

P-D-13: DETERMINATION OF CO_2-BRINE RELATIVE PERMEABILITY WITH AN INTEGRATED STEADY-STATE AND UNSTEADY-STATE METHOD

[CFSES] Xiongyu Chen, Amir Kianinejad, David DiCarlo
Center for Petroleum and Geosystems Engineering, The University of Texas at Austin

P-D-15: FLOW INTERACTIONS BETWEEN LIQUID CO_2 AND WATER IN HOMOGENEOUS AND HETEROGENEOUS MICROMODELS AT RESERVOIR CONDITIONS

[GSCO2] Yaofa Li[1], Farzan Kazemifar[1,2], Gianluca. Blois[1,2], Kenneth T. Christensen[1,2]
[1]University of Notre Dame
[2]International Institute for Carbon-Neutral Energy Research (I^2CNER), Kyushu University, Japan

E. MATERIALS AND CHEMISTRY BY DESIGN

P-E-1: SCAN+RVV10: A PROMISING DENSITY FUNCTIONAL FOR LAYERED MATERIALS

[CCDM] Haowei Peng[1], Zenghui Yang[1], Jianwei Sun[1], John P. Perdew[1]
[1] Physics, Temple U.

P-E-3: TOOLS ACCELERATING MATERIALS BY DESIGN

[CNGMD] Michael Toney[5], Stephan Lany[1], Aaron Holder[1], Andriy Zakutayev[1], Lauren Garten[1], David Ginley[1], John Perkins[1], Andre Bikowski[1], Vladan Stevanovic[1,4], Kristin Persson[2,6], Gerbrand Ceder[2,6], Alexie Kolpak[3], Spencer Wyant[3], Brian Kolb[3], Brian Gorman[4], Prashun Gorai[4], Ann Deml[4], Laura Schelhas[5], Kevin Stone[5], Johanna Nelson Weker[5], Wenhao Sun[6], Hong Kevin Ding[6], Patrick Huck[6], William Tumas[1]
[1]National Renewable Energy Laboratory, [2]UC-Berkeley, [3]Massachusetts Institute of Technology,
[4]Harvard University, [4]Colorado School of Mines, [5]SLAC National Accelerator Laboratory,
[6]Lawrence Berkeley National Laboratory

P-E-5: EFFECTS OF COMPOSITIONAL COMPLEXITY ON THE ION IRRADIATION RESPONSE IN NI-BASED, FACE-CENTER-CUBIC, EQUIATOMIC ALLOYS

[EDDE] Ke Jin[1], Hongbin Bei[1], Brian C. Sales[1], G. Malcolm Stocks[1], Chenyang Lu[2], Lumin Wang[2], William J. Weber[2,3], Yanwen Zhang[1]
[1]Oak Ridge National Laboratory; [2]University of Michigan; [3]University of Tennessee

P-E-7: TRIVALENT METAL LOADING VIA ATOMIC LAYER DEPOSITION

[ICDC] Joshua Borycz[2], In Soo Kim[1], Ana Platero-Prats[3], Samat Tussupbayev[2], Timothy C. Wang[4], Omar K. Farha[4,5], Joseph T. Hupp[1,4], Laura Gagliardi[2], Karena Chapman[3], Christopher J. Cramer[2], Alex B. F. Martinson[1]
[1]Materials Science Division, Argonne National Laboratory; [2]Dept. Chemistry, Supercomputing Institute, and Chemical Theory Center, University of Minnesota; [3]X-ray Science Division, Argonne National Laboratory; [4]Dept. Chemistry, Northwestern University; [5]Dept. Chemistry, Faculty of Science, King Abdulaziz University, Saudi Arabia

P-E-9: NANOSCALE CONTROL OF ACTINIDE MATERIAL DISSOLUTION

[MSA] Haylie L. Lobeck[1], Kathryn M. Peruski[1], Sarah Hickam[1], Mateusz Dembowski[1], Enrica Balboni[1], Varinia Bernales[2], Laura Gagliardi[2], Jennifer E.S. Szymanowski[1], Peter C. Burns[1]
[1] Department of Civil and Environmental Engineering and Earth Sciences, University of Notre Dame
[2] Department of Chemistry, Minnesota Supercomputing Institute, University of Minnesota

P-E-11: PHONON SCATTERING MECHANISMS IN THERMOELECTRICS

[S^3TEC] Olivier Delaire[1], Jie Ma[1], Chen Li[1], J. Hong[1], David Singh[1], Andrew May[1], Brian Sales[1], Sangyeop Lee[2], Zhiting Tian[2], Keivan Esfarjani[3], Christopher Carlton[2], Yang Shao-Horn[2], Gang Chen[2]
[1] Oak Ridge National Laboratory, [2] Massachusetts Institute of Technology, [3] Rutgers University

P-E-13: STRUCTURE-PROPERTY RELATIONSHIP OF MATERIALS PREDICTED BY THE COMB3 POTENTIAL

[UNCAGE-ME] Difan Zhang[1], Tao Liang[1], Kamal Choudhary[1], Michael R. Dutzer[2], Susan B. Sinnott[1]
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[2]*School of Chemical & Biomolecular Engineering, Georgia Institute of Technology*

P-E-15: ENHANCING THE HIGH FIELD PERFORMANCE OF CUPRATE AND IRON BASED SUPERCONDUCTORS

[CES] Ulrich Welp[1], Karen Kihlstrom[1,2], Jihwan Kwon[3], Hefei Hu[3], Lei Fang[1], Shaofei Zhu[4], Jian-Min Zuo[3], Venkat Selvamanickam[5], Alexei E. Koshelev[1], Qiang Li[7], Martin Rupich[8] and Wai-Kwong Kwok[1]
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P-E-17: FROM BENZENE TO NANOTHREADS: INTERMEDIATE POLYMERS, TOPOLOGICAL PATHWAYS AND REACTION MECHANISMS

[EFree] Bo Chen, Roald Hoffmann
Department of Chemistry and Chemical Biology, Cornell University

P-E-19: URANYL CAGE CLUSTERS: A COMPUTATIONAL STUDY OF THEIR SELF ASSEMBLY AND THEIR PROPERTIES

[MSA] Varinia Bernales[1], Surya P. Tiwari[2], David Semrouni[1], Ken Newcomb[2], Peter Winegar[1], Edward Maginn[2], Laura Gagliardi[1]
[1] *Department of Chemistry, Supercomputing Institute, and Chemical Theory Center, University of Minnesota;* [2] *Department of Chemical and Biomolecular Engineering, University of Notre Dame*

P-E-21: DIRECT OBSERVATION OF IRRADIATION RESPONSE IN NI AND NI-BASED CONCENTRATED SOLID-SOLUTION ALLOYS

[EDDE] Chenyang Lu[1], Ke Jin[2], Laurent K. Beland[2], Feifei Zhang[1], Taini Yang[1], Yanwen Zhang[2], Hongbin Bei[2], Roger E. Stoller[2], Lumin Wang[1]
[1]*University of Michigan;* [2]*Oak Ridge National Laboratory*

P-E-23: MAGNETIC RESONANCE CHARACTERIZATION OF ADSORBATE INTERACTIONS IN METAL ORGANIC FRAMEWORKS SYSTEMS

[CGS] Velencia J. Witherspoon[1], Lucy M. Yu[1], Yusu Chen[1], Jeffrey A. Reimer[1,2,3]
[1]*Department of Chemical and Biomolecular Engineering, University of California, Berkeley;* [2]*Department of Chemistry, University of California, Berkeley*
[3]*Environmental Energy Technologies Division, Lawrence Berkeley National Laboratory*

P-E-25: THE EFFECT OF SO_2 EXPOSURE ON THE EXTERNAL SURFACES OF ZIF-8

[UNCAGE-ME] Simon H. Pang[1], Christopher W. Jones[1], Ryan P. Lively[1]
[1]*School of Chemical & Biomolecular Engineering, Georgia Institute of Technology*

P-E-27: DESIGN AND DISCOVERY OF NOVEL SEMICONDUCTING NITRIDES

[CNGMD] Bernado Orvananos[1], Gebrand Ceder[2,5], Aaron Holder[3], Stephan Lany[3], Andre Bikowski[3], Andriy Zakutayev[3], Vladan Stevanovic[3,4], Brian Gorman[4], John Mangum[4], Wenhao Sun[5], William Tumas[3]
[1]*Massachusetts Institute of Technology,* [2]*UC-Berkeley,* [3]*National Renewable Energy Laboratory,* [4]*Colorado School of Mines,* [5]*Lawrence Berkeley National Laboratory*

F. CATALYSIS

P-F-1: STRUCTURAL CHARACTERIZATION OF HOMOGENEOUS AND AMORPHOUS METAL OXIDE THIN-FILM WATER OXIDATION CATALYSTS USING IN-SITU X-RAY TECHNIQUES

[ANSER] David M. Tiede[1], Gihan Kwon[1], Jier Huang[1], Jiyun Hong[2], Ke Yang[3], Adam Matula[3], Lin X. Chen[2], Robert H. Crabtree[3], Victor S. Batista[3], Gary W. Brudvig[3], Alex B. F. Martinson[4]
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P-F-3: GREENING PAINTS, PLASTICS, AND FIBERS: RENEWABLE PHTHALIC ANHYDRIDE FROM BIOMASS-DERIVED SUGARS

[CCEI] Eyas Mahmoud[1], Donald A. Watson[2], Raul F. Lobo[1]
[1]Department of Chemical and Biomolecular Engineering, University of Delaware
[2]Department of Chemistry and Biochemistry, University of Delaware

P-F-5: HIGH-POTENTIAL ELECTROCATALYTIC O_2 REDUCTION WITH NITROXYL/NO_x MEDIATORS: IMPLICATIONS FOR FUEL CELLS AND AEROBIC OXIDATION CATALYSTS

[CME] James B. Gerken, Shannon S. Stahl
University of Wisconsin-Madison

P-F-7: ACTIVATION OF O_2 AND CH_3OH ON NANOPOROUS (AG)AU CATALYSTS: A TAP REACTOR STUDY

[IMASC] Lu-Cun Wang[1], Branko Zugic[1], Michelle L. Personick[1], Nare Janvelyan[1], Cynthia M. Friend[1], Robert J. Madix[1]
[1] Department of Chemistry and Chemical Biology, Harvard University

P-F-9: EXPLORING THE MECHANISMS OF FAST PYROLYSIS REACTIONS OF LIGNIN AND HEMICELLULOSE VIA HIGH RESOLUTION TANDEM MASS SPECTROMETRY EXPERIMENTS AND QUANTUM CHEMICAL CALCULATIONS ON MODEL COMPOUNDS

[C3Bio] Priya Murria[1] , John C. Degenstein[2] , McKay Easton[2], Matthew R. Hurt[1], Huaming Sheng[1], Jinshan Gao[1], Hanyu Zhu[1] , John J. Nash[1], Rakesh Agrawal[2] , W. Nicholas Delgass[2], Fabio H. Ribeiro[2], Hilkka I. Kenttämaa[1]
[1]Department of Chemistry, [2]Department of Chemical Engineering, Purdue University

P-F-11: ON THE INTERACTION AND REACTIVITY OF FURFURAL ON THE IR(111) SURFACE

[CCEI] Glen R. Jenness[1], Ke Xiong[3], Geun Ho Gu[2], Jingguang Chen[3], Dionisios G. Vlachos[2]
[1]Catalysis Center for Energy Innovation, University of Delaware
[2]Department of Chemical and Biomolecular Engineering, University of Delaware
[3]Department of Chemical Engineering, Columbia University

P-F-13: SYNTHESIS OF MESOPOROUS DILUTE ALLOY CATALYSTS

[IMASC] Jianchao Ye[1], Tobias Michael Egle[1], Junjun Shan[2], Hang Li[2], Nare Janvelyan[3], Maria Flytzani-Stephanopoulos[2], Cynthia M. Friend[3], Monika Biener[1], Juergen Biener[1]
[1] Lawrence Livermore National Laboratory; [2] Department of Chemistry, Tufts University
[3] Department of Chemistry and Chemical Biology, Harvard University

P-F-15: UNCOVERING DESIGN PRINCIPLES OF LAYERED MATERIALS THROUGH MULTISCALE MODELING

[CCDM] Richard C. Remsing[1,2], Jianwei Sun[3], Joel Berry[4], Ian G. McKendry[2], Haowei Peng[3], David Srolovitz[5], Mikko Haataja[4], John P. Perdew[2,3], Daniel R. Strongin[2], Michael J. Zdilla[2], Michael L. Klein[1,2,3]
[1]Institute for Computational Molecular Science, Temple U., [2]Chemistry, Temple U., [3]Physics, Temple U., [4]MSE & PRISM, Princeton U., [5]MSE &, U. Penn.

P-F-17: DIELS-ALDER CYCLOADDITION OF DIMETHYLFURAN AND ETHYLENE FOR RENEWABLE PET PLASTICS

[CCEI] Kristeen E. Joseph, Katherine P. Vinter, Paul J. Dauenhauer
Department of Chemical Engineering and Materials Science, University of Minnesota

P-F-19: CALCULATION OF ELECTROCHEMICAL SOLVENT REORGANIZATION ENERGIES FOR MOLECULAR CATALYSTS AT ELECTRODE-SOLVENT INTERFACES

[CME] Soumya Ghosh, Alexander V. Soudackov, Sharon Hammes-Schiffer
University of Illinois at Urbana-Champaign

P-F-21: FIRST PRINCIPLES SIMULATIONS OF FUNCTIONALIZED FLUID-SOLID INTERFACES TOWARD SELECTIVE TRANSPORT AND DESIGN OF ELECTROCATALYTIC SYSTEMS

[FIRST] Matthew Neurock[1,2], Stuart Winikoff[1], John Dimeglio[3], Joel Rosenthal[3], Danny Lutterman[4], David Mullins[4], Steve Overbury[4], Gilbert Brown[4], Zhiyong Zhang[4], Kichul Yoon[5], Adri van Duin[5], Franz Geiger[6], Jennifer Achtyl[6], Raymond Unocic[7], Lijun Xu[2], Yu Cai[2], Muralikrishna Raju[5], Weiwei Zhang[7], Robert Sacci[7], Ivan Vlassiouk[4], Pasquale Fulvio[4], Panchapakesan Ganesh[7], David Wesolowski[4], Sheng Dai[4]
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P-F-23: BRIDGING THE PRESSURE GAP IN HETEROGENEOUS CATALYSIS-SURFACE SENSITIVE X-RAY ABSORPTION SPECTROSCOPY UNDER REALISTIC CATALYTIC CONDITIONS

[IMASC] Christian Heine[1], Branko Zugic[2], Luan Nguyen[3], Franklin Feng[3], Cynthia M. Friend[2], Miquel Salmeron[1]
[1] Lawrence Berkeley National Laboratory; [2] Dept. Chemistry & Chemical Biology, Harvard University; [3] Dept. Chemical & Petroleum Engineering, Dept. Chemistry, University of Kansas

G. SYNTHESIS OF FUNCTIONAL MATTER

P-G-1: GAS-PHASE SYNTHESIS AND PHOTOPHYSICAL PROPERTIES OF GROUP-IV NANOCRYSTALS FOR SOLAR ENERGY CAPTURE APPLICATIONS

[CASP] Katharine Hunter[1], Samantha Ehrenberg[1], Nikolay Makarov[2], Istvan Robel[2], Márton Vörös[3], Giulia Galli[3], Victor Klimov[2], Uwe Kortshagen[1]
[1] Department of Mechanical Engineering, University of Minnesota; [2] Chemistry Division, Los Alamos National Laboratory; [3] Institute for Molecular Engineering, University of Chicago

P-G-3: NEAR INFRARED 2-DIMENSIONAL LIGHT EMISSION DIODE AND PHOTODETECTOR MADE BY $\mathrm{MoTe_2}$ BILAYER P-N JUNCTION

[CE] Ya-Qing Bie[1], Gabriele Grosso[1], Yuan Cao[1], Hugh Churchill[1], Lin Zhou[1], Jing Kong[1], Dirk Englund[1], Pablo Jarillo-Herrero[1]
[1] *Center for Excitonics, Massachusetts Institute of Technology*

P-G-5: STRUCTURE TRANSITIONS OF THE $\mathrm{Zr_6(O)_8}$ CLUSTERS IN NU-1000 AND RELATED MOFS

[ICDC] Ana E. Platero-Prats[1], Leighanne C. Gallington[1], Andreas Mavrantonakis[2], Yangyang Liu[3], Joseph T. Hupp[3], Omar K. Farha[3,4], Christopher J. Cramer[2], Karena W. Chapman[1]
[1]*X-ray Science Division, Argonne National Laboratory;* [2]*Department of Chemistry, Chemical Theory Center, & Supercomputing Institute, University of Minnesota;* [3]*Department of Chemistry, Northwestern University;* [4]*Department of Chemistry, Faculty of Science, King Abdulaziz University, Saudi Arabia*

P-G-7: ULTRAFAST SYNTHESIS OF METAL-ORGANIC FRAMEWORKS CRITICAL FOR ENERGY-EFFICIENT $\mathrm{CO_2}$ CAPTURE

[CGS] Lorenzo Maserati[1], Stephen M. Meckler[1,2], Changyi Li[1,3], Brett A. Helms[1]
[1]*The Molecular Foundry, Lawrence Berkeley National Laboratory ;* [2]*Dept. Chemistry, University of California, Berkeley;* [3]*Dept. Chemical and Biomolecular Engineering, University of California, Berkeley*

P-G-9: THERMOELECTRIC PERFORMANCE OF BULK IV-VI CHALCOGENIDES (PbSe, $\mathrm{PbTe_{1-\mathit{x}}Se_{\mathit{x}}}$, SnSe)

[$\mathrm{S^3}$TEC] Eyob K. Chere[1], Qian Zhang[1], Kenneth McEnaney[2], Hee Seok Kim[1], Feng Cao[1], Jingying Sun[1], Shuo Chen[1], Yizhou Ni[1], Keshab Dahal[1], Weishu Liu[1], Mengliang Yao[3], Cyril Opeil[3], Ching-Wu Chu[1], Gang Chen[2], Zhifeng Ren[1]
[1]*Department of Physics and TcSUH, University of Houston;* [2]*Department of Mechanical Engineering, Massachusetts Institute of Technology;* [3]*Department of Physics, Boston College*

P-G-11: IMPROVING SUPERCONDUCTORS AND TESTING FOR TOPOLOGICAL PROPERTIES

[CES] Ruidan Zhong[1], J. A. Schneeloch[1], C. Zhang[1], X.Y. Shi[1], G. Du[2], H.H. Wen[2], Q. Li[1], J. M. Tranquada[1], G.D. Gu[1]
[1]*Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory*
[2]*National Laboratory of Solid State Microstructures and Department of Physics, Nanjing University*

P-G-13: SHAPE CONTROL AND COMPARTMENTALIZATION IN ACTIVE COLLOIDAL CELLS

[CBES] Matthew Spellings[1], Michael Engel[1], Daphne Klotsa[1,4], Syeda Sabrina[2], Aaron M. Drews[2,3], Nguyen H. P. Nguyen[5], Kyle J. M. Bishop[2], Sharon C. Glotzer[1]
[1]*Department of Chemical Engineering, Biointerfaces Institute, and Department of Materials Science and Engineering, University of Michigan;* [2]*Department of Chemical Engineering, Pennsylvania State University;* [3]*Department of NanoEngineering, University of California, San Diego;* [4]*Department of Chemistry, University of Cambridge;* [5]*Department of Mechanical Engineering, University of Michigan*

P-G-15: ULTRAFAST PUMP-PROBE STUDIES OF PHONON MEAN FREE PATH, PHONON COHERENCE, AND PHONON LOCALIZATION

[S^3TEC] Lingping Zeng[1], Maria N. Luckyanova[1], Kimberlee C. Collins[1], Yongjie Hu[1], John Cuffe[1,4], Alexei A. Maznev[2], Jeffrey K. Eliason[2], Jeremy A. Johnson[2], Felix Hofmann[2], Austin A. Minnich[1], Keivan Esfarjani[1], Jivtesh Garg[1], Jonathan Mendoza[1], Vazrik Chiloyan[1], Samuel Huberman[1], Adam Jandl[3], Mayank T. Bulsara[3], Roger Jia[3], Andrey A. Shchepetov[5], Mika Prunnila[5], Jouni Ahopelto[5], Clivia M. Sotomayor Torres[4], Eugene A. Fitzgerald[3], Keith A. Nelson[2], Gang Chen[1]

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H. BIOSCIENCE

P-H-1: LIGHT DRIVEN NITROGENASE CATALYZED C-H BOND FORMATION

[BETCy] Rhesa Ledbetter[1], Kathryn Fixen[2], Yanning Zheng[2], Derek Harris[1], Sudipta Shaw[1], Zach Jay[3], Ross Carlson[3], Lance Seefeldt[1], Carrie Harwood[2]

[1]Utah State University, [2]University of Washington, [3]Montana State University

P-H-3: ENGINEERING OF ARABIDOPSIS THALIANA THAT DEPOSIT ALDEHYDE-DERIVED LIGNIN

[C3Bio] Fabiola Muro-Villanueva[1], Nickolas A. Anderson[1,2], Yuki Tobimatsu[3,4,5], Peter N. Ciesielski[6], John Ralph[3,4,7], Bryon S. Donohoe[6], Clint Chapple[1]

[1]Department of Biochemistry, Purdue University, [2]Heartland Plant Innovations, [3]Department of Biochemistry, University of Wisconsin-Madison, [4]DOE Great Lakes Bioenergy Research Center, and Wisconsin Energy Institute, University of Wisconsin-Madison, [5]Research Institute for Sustainable Humanosphere, Kyoto University, [6]Biosciences Center, National Renewable Energy Laboratory, [7]Department of Biological Systems Engineering, University of Wisconsin-Madison.

P-H-5: STRUCTURE, DYNAMICS AND LOOSENING OF PLANT PRIMARY CELL WALL FROM SOLID-STATE NMR

[CLSF] Tuo Wang[1], Paul White[1], Yong Bum Park[2], Yuning Chen[2], Daniel Cosgrove[2], Mei Hong[1]

[1]Department of Chemistry, Massachusetts Institute of Technology, [2]Department of Biology, Pennsylvania State University

P-H-7: EXCITON DYNAMICS IN LH2 COMPLEXES OF PURPLE BACTERIA PROBED BY SINGLET-SINGLET ANNIHILATION

[PARC] Andrew Proppe, Evgeny E. Ostroumov, Gregory D. Scholes

Frick Chemistry Laboratory, Princeton University

P-H-9: INSIGHTS INTO THE DETERMINANTS OF CATALYTIC BIAS USING PROTEIN FILM ELECTROCHEMISTRY

[BETCy] Garrett Williams[1], Jacob Artz[2], David Mulder[3], Paul King[3], John Peters[2], Anne Jones[1]

[1]Arizona State University, [2]Montana State University, [3]National Renewable Energy Laboratory

P-H-11: STUDIES ON THE INITIATION AND MECHANICAL EFFECTS OF LIGNIFICATION

[CLSF] Sarah N. Kiemle[1], Jyotsna L. Pandey[2], Ivo Doudevski[1], Yimin Zhu[3], Charles T. Anderson[1], Daniel J. Cosgrove[1]

[1]Dept. Biology, Pennsylvania State University; [2]Agricultural & Biological Engineering, Pennsylvania State University; [3]Mathematics & Natural Sciences, Pennsylvania State University at Altoona

P-H-13: POST-TRANSLATIONAL MODIFICATION AS A MECHANISM TO MODULATE ELECTRON TRANSFER CATALYSIS TO CONTROL ELECTRON FLOW TO CHEMICAL BOND FORMATION

[BETCy] Monika Tokmina-Lukaszewska[1], Gerti Schut[2], Oleg Zadornyy[1], Eric Boyd[1], Michael Adams[2], Brian Bothner[1]
[1]*Montana State University,* [2]*University of Georgia*

P-H-15: UNDERSTANDING THE PLANT CELL WALL: MODELING CELLULOSE MICROFIBRILS

[C3Bio] Peter Ciesielski, Lintao Bu, Bryon Donohoe, Michael E. Himmel, Michael F. Crowley
Biosciences Center, National Renewable Energy Laboratory

P-H-17: PARC'S MODEL OUTREACH PROGRAM INTERESTS AND INFORMS

[PARC] Rachel M. Ruggirello
Washington University in St. Louis

J. MESOSCALE SCIENCE

P-J-1: CHARGE TRANSPORT IN SURFACE-ENGINEERED COLLOIDAL QUANTUM DOT SOLIDS AND DEVICES

[CASP] Daniel Straus[1], Jason Tolentino[2], Ashley R. Marshall[3], Ryan W. Crisp[3], Gregory Pach[3], Justin C. Johnson[3], Andrew Shabaev[4], Samuel Keene[2], Alexander Efros[4,5], Uwe Kortshagen[6], Matthew C. Beard[3], Joseph M. Luther[3], Matt Law[2], Cherie Kagan[1,7]
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P-J-3: POLYMER-DNA CONSTRUCTS FOR BIO-INSPIRED MUSCLE-LIKE MATERIALS

[CBES] Hiroaki Sai[1], David A. Walker[2-4], Ronit Freeman[1], Chad A. Mirkin[2-4], Samuel I. Stupp[1,3-7]
[1]*Simpson Querrey Institute, Northwestern University;* [2]*International Institute for Nanotechnology, Northwestern University;* [3]*Dept. Chemistry, Northwestern University;* [4]*Dept. Materials Science and Engineering, Northwestern University;* [5]*Dept. Biomedical Engineering, Northwestern University* [6]*Dept. Chemical Engineering, Northwestern University;* [7]*Dept. Medicine, Feinberg School of Medicine, Northwestern University*

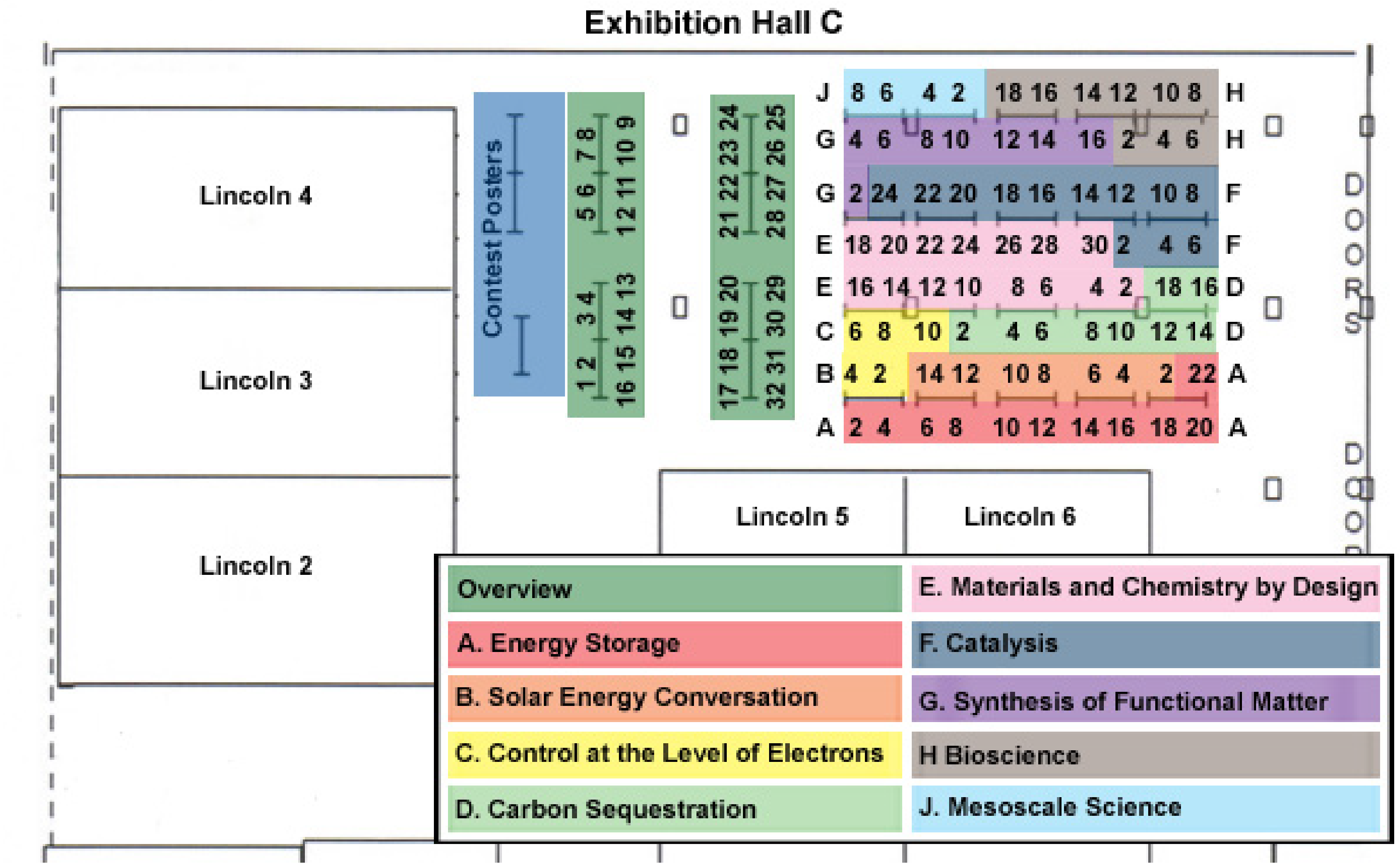
P-J-5: SIMULATING EXCITONIC SYSTEMS OF TENS OF THOUSANDS OF MOLECULES: NATURAL SYSTEMS AND NEW TECHNOLOGIES

Nicolas Sawaya[1], Joonsuk Suh[1], Takatoshi Fujita[1], Semion Saikin[1], Etienne Boulais[2], Remi Veneziano[2], Mark Bathe[2,3], Alan Aspuru-Guzik[1]
[1] *Center for Excitonics, Harvard University;* [2] *Department of Biological Engineering, MIT;* [3] *Center for Excitonics, MIT*

P-J-7: LIGHT DIRECTED SYNTHESIS OF NANO-PATTERNED SEMICONDUCTOR FILMS

[LMI] Azhar I. Carim[1], Nicolas A. Batara[1], Anjali Prekumar[1], Harry A. Atwater[1], Nathan S. Lewis[1]
[1]*California Institute of Technology*

POSTER SESSION II: TUESDAY, OCTOBER 27, 2015; 3:10 – 5:00 PM



POSTER SESSION II: TUESDAY, OCTOBER 27, 2015; 3:10 – 5:00 PM, *EXHIBITION HALL C, EVEN NUMBERED POSTERS*

A. ENERGY STORAGE

P-A-2: STATIC AND DYNAMIC ELECTRON MICROSCOPY OF ELECTRODE MATERIALS IN LI-BASED SYSTEMS
[CEES] Fernando C. Castro[1], Qianqian Li[2], Jinsong Wu[1,2], Vinayak P. Dravid[1,2]
[1]Department of Materials Science and Engineering, Northwestern University
[2]NUANCE Center, Northwestern University

P-A-4: POLARON MOBILITY AND DISORDERING OF THE NA SUBLATTICE IN NA_xFEPO_4
[EFree] Sally J. Tracy, Brent T. Fultz
Department of Applied Physics and Materials Science, California Institute of Technology

P-A-6: ROLE OF THE TUNNEL CATION IN THE ELECTROCHEMISTRY OF ONE DIMENSIONAL MANGANESE OXIDES
[m2M] Alexander B. Brady[1], Jessica L. Durham[1], Jianping Huang[1], Lijun Wu[2], Feng Xu, Yimei Zhu[2], Eric Dooryhee[2], Amy C. Marschilok[1], Esther S. Takeuchi[1,2], Kenneth J. Takeuchi [1]
[1]Stony Brook University; [2]Brookhaven National Laboratory

P-A-8: SURFACE AND SUBSURFACE TRANSFORMATIONS OF LAYERED INTERCALATION ELECTRODE MATERIALS; DESIGN RULES AND TRANSPORT IMPLICATIONS
[NECCES] Glenn G. Amatucci[1], Nicholas Faenza[1], Nathalie Pereira[1], Frederic Cosandey[1], Pinaki Mukherjee[1], Louis Piper[2], Shawn Sallis[2], Gerbrand Ceder[3], Aziz Abdellahi[3], Hena Das[3], Shin Young Kang[3]
[1] Rutgers University; [2] Binghamton University; [3] Massachusetts Institute of Technology

P-A-10: NEW LITHIUM AND MANGANESE (III, IV) ALD PRECURSORS FOR $LIMN_2O_4$ GROWTH
[CEES] Madelyn M. Stalzer[1], Massimiliano Delferro[1], Tobin J. Marks[1]
[1]Department of Chemistry, Northwestern University

P-A-12: MULTISCALE MICROSCOPY, SPECTROSCOPY AND CONTINUUM MODELING OF ELECTROACTIVE SPINEL ELECTRODES
[m2M] Christopher C. Pelliccione[1], Kevin W. Knehr[2], David C. Bock[1], Christina A. Cama[3], Kevin C. Kirshenbaum[1], Zhou Lin[3], Nicholas W. Brady[2], Christianna N. Lininger[2], Jiajun Wang[1], Wei Zhang[1], Feng Wang[1], Jun Wang[1], Alan C. West[2], Amy C. Marschilok[3], Kenneth J. Takeuchi[3], Esther S. Takeuchi[1,3]
[1]Brookhaven National Laboratory; [2]Columbia University; [3]Stony Brook University

P-A-14: LI-BASED ATOMIC LAYER DEPOSITION SOLID ELECTROLYTES FOR BEYOND-LI-ION BATTERIES
[NEES] Alexander C. Kozen[1], Alexander J. Pearse[1], Marshall A. Schroeder[1], Chanyuan Liu[1], Oliver Zhao[1], Malachi Noked[1], Chuan-Fu Lin[1], A. Alec Talin[2], Sang Bok Lee[1], Gary W. Rubloff[1,3]
[1] Department of Materials Science and Engineering, University of Maryland; [2] Sandia National Laboratories, Livermore; [3] Institute for Systems Research, University of Maryland

P-A-16: Portfolio of X-Ray Imaging Tools for Studies of Battery Materials: Development and Scientific Insight

[NECCES] Young-Sang Yu[1, 2], Andrej Singer[3], Brian May[1], Sunny Hy[3], Andrew Ulvestad[3], Fiona Strobridge[4], Clare P. Grey[4], Nathalie Pereira[5], Glenn G. Amatucci[5], Oleg Shpyrko[3], Danna Qian[3], Y. Shirley Meng[3], Jordi Cabana[1]

[1] University of Illinois at Chicago; [2] Advanced Light Source, Lawrence Berkeley National Laboratory; [3] University of California, San Diego; [4] University of Cambridge; [5] Rutgers University

P-A-18: Multi-electron Transfer Reaction and Ionic Transport in Spinel-type electrodes

[m2M] Wei Zhang[1], David C. Bock[1], Christopher Pelliccione[1], Yan Li[1], Lijun Wu[1], Yimei Zhu[1], Kenneth J. Takeuchi[2], Amy. C. Marschilok[2], Esther S. Takeuchi[1,2], Feng Wang[1]

[1]Brookhaven National Laboratory; [2]Stony Brook University

P-A-20: Relationship between Nanoporous Carbon Electrode Materials and Capacitive Energy Storage

[FIRST] Katherine L. Van Aken[1], Jennifer M. Black[2], Yu Zhang[3], Justin Neal[4], Jianzhong Wu[4], Peter T. Cummings[3], Nina Balke[2], Yury Gogotsi[1]

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

P-A-22: Investigating the Structural Dynamics during Electrochemical Cycling of Layered Metal Oxides through Operando X-ray and Neutron Measurements

[NECCES] Kamila M. Wiaderek[1], LuXi Lu[1], Hao Liu[1], Peter Chupas[1], Karena Chapman[1], Haodong Liu[2], Sunny Hy[2], Shirley Meng[2], Natalya Chernova[3], M Stanley Whittingham[3]

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

B. Solar Energy Conversion

P-B-2: Assembling Charge Transport Networks in Disordered Environments: New Metrics for Organic Photovoltaics

[ANSER] Nicholas Jackson[1], Kevin Kohlstedt[1], Thomas Fauvell[1], Pat Hartnett[1], Tianyue Zheng[1], Luping Yu[2], George Schatz[1], Lin Chen[1], Tobin Marks[1], Mark Ratner[1]

[1] Department of Chemistry, Northwestern University; [2] Department of Chemistry, University of Chicago

P-B-4: Light-driven Ca^{2+} ion pump: How does it work?

[CBES] Cheng-Tsung Eric Lai[1], Yu Zhang[1], George C. Schatz.[1,2], Igal Szleifer[3]

[1]Department of Chemistry, Northwestern University; [2]Department of Chemical and Biological Engineering, Northwestern University; [3]Department of Biomedical Engineering, Northwestern University

P-B-6: Biohybrid Molecular Architectures for Panchromatic Solar Light-Harvesting

[PARC] Yunlong Zhang[1], Rui Liu[1], Jianbing Jiang[1], Jonathan S. Lindsey[1], David F. Bocian[2], Dewey Holten[3], Paul A. Loach[4]

[1]Dept. Chemistry, North Carolina State University; [2]Dept. Chemistry, University of California, Riverside; [3]Dept. Chemistry, Washington University, St Louis; [4]Dept Molecular Biosciences, Northwestern University

P-B-8: PHOTOINDUCED DYNAMICS IN MOLECULAR ASSEMBLIES FOR SOLAR ENERGY CONVERSION

[UNC] Zachary A. Morseth[1], Gyu Leem[2], Toan V. Pho[3], Matthew V. Sheridan[1], Junlin Jiang[2], Hayden T. Black[3], Thomas J. Meyer[1], John R. Reynolds[3], Kirk S. Schanze[2], John M. Papanikolas[1]
[1]Department of Chemistry, University of North Carolina at Chapel Hill; [2]Department of Chemistry, Center for Macromolecular Science and Engineering, University of Florida; [3]School of Chemistry and Biochemistry, School of Materials Science and Engineering, Center for Organic Photonics and Electronics, Georgia Institute of Technology

P-B-10: APPLICATION OF PEROVSKITE BASED DESIGN RULES FOR NEW PV ABSORBERS

[CNGMD] Riley Brandt[1], Vladan Stevanović[2,3], Robert Hoye[1], Rachel Kurchin[1], John Perkins[3], David Ginley[3], Tonio Buonassisi[1], William Tumas[3]
[1]Massachusetts Institute of Technology, [2]Colorado School of Mines, [3]National Renewable Energy Laboratory

P-B-12: OPTICAL MATERIALS AND MODULE ARCHITECTURES FOR ULTRAHIGH-EFFICIENCY PHOTOVOLTAICS

[LMI] Kyu-Tae Lee[1], Yuan Yao[1], Junwen He[1], Lu Xu[1], Mikayla Anderson[1], Xing Sheng[1], Noah Bronstein[2], A. Paul Alivisatos[2], Ralph G. Nuzzo[1], John A. Rogers[1]
[1]University of Illinois at Urbana-Champaign, [2]Lawrence Berkeley National Laboratory

P-B-14: EVOLUTIONS AND NEW DIRECTIONS IN WIDE-BANDGAP PHOTOCATHODES FOR EFFICIENT TANDEM-DSPECS

[UNC] Cory J. Flynn[1], Shannon M. McCullough[1], Candy C. Mercado[2], Lesheng Li[1], Byron H. Farnum[1], Taylor H. Moot[1], Yejee Han[1], Carrie L. Donley[3], Gerald J. Meyer[1], Jillian L. Dempsey[1], Thomas J. Meyer[1], Arthur J. Nozik[2,4], James F. Cahoon[1]
[1]Department of Chemistry, University of North Carolina at Chapel Hill, Chapel Hill; [2]Renewable and Sustainable Energy Institute, and Department of Chemistry and Biochemistry, University of Colorado; [3]Chapel Hill Analytical and Nanofabrication Laboratory (CHANL), Department of Applied Physical; Sciences, University of North Carolina at Chapel Hill; [4]National Renewable Energy Laboratory

C. CONTROL AT THE LEVEL OF ELECTRONS

P-C-2: PHOTO-SPIN-VOLTAIC EFFECT

[SHINES] David Ellsworth[1], Lei Lu[1], Jin Lan[2,3], Houchen Chang[1], Peng Li[1], Zhe Wang[3], Jun Hu[2], Bryan Johnson[1], Yuqi Bian[1], Jiang Xiao[3], Ruqian Wu[2.3], Mingzhong Wu[1]
[1]Colorado State University; [2]University of California, Irvine; [3]Fudan University

P-C-4: UNIFIED DESCRIPTION OF ELECTRON-ION ENERGY DISSIPATION IN METALS

[EDDE] Alfredo Correa[1], Magdalena Caro[2], Artur Tamm[2], German D. Samolyuk[3], G. Malcolm Stocks[3], Alfredo Caro[2]
[1]Lawrence Livermore National Laboratory; [2]Los Alamos National Laboratory; [3]Oak Ridge National Laboratory

P-C-6: SPIN WAVE TRANSPORT STUDY BY MICROWAVE ANTENNA ON YIG

[SHINES] David Gutierrez, Howard Chiang, Mojtaba Ranjbar, Alexander Khitun
University of California, Riverside

P-C-8: NOVEL TRANSPORT IN HYDROGEN-RICH MATERIALS: EXPERIMENTS

[EFree] Maddury Somayazulu, Russell J. Hemley
Geophysical Laboratory, Carnegie Institution of Washington

P-C-10: MAGNONS AND PHONONS OPTICALLY DRIVEN OUT OF LOCAL EQUILIBRIUM IN A MAGNETIC INSULATOR

[SHINES] Kyongmo An, Kevin S. Olsson, Xi Chen, Nikita Klimovich, Sean Sullivan, Annie Weathers, Luke G. Marshall, Xin Ma, Jianshi Zhou, Li Shi, Xiaoqin Li
University of Texas at Austin

D. CARBON SEQUESTRATION

P-D-2: CHARACTERIZING 3-D FLOW VELOCITY IN EVOLVING PORE NETWORKS DRIVEN BY $CaCO_3$ PRECIPITATION AND DISSOLUTION

[CFSES] Kirsten N. Chojnicki[1], Hongkyu Yoon[1], Mario J. Martinez[2]
[1]*Geoscience Research and Applications, Sandia National Laboratories;* [2]*Engineering Sciences Center, Sandia National Laboratories*

P-D-4: THE IMPACT OF MICRO-STRUCTURE AND INTER-GRANULAR SPACING ON CO_2 TRAPPING. THE MT. SIMON AS A CASE STUDY

[GSCO2] John Tudek[1], Dustin Crandall[1], Dustin McIntyre[1], Angela Goodman[1]
[1]*National Energy Technology Laboratory*

P-D-6: RESIDUAL CO_2 TRAPPING AT SHORT TIMES AND LONG-TERM STABILITY

[NCGC] Charlotte Garing[1], Jacques de Chalendar[1], Sally M. Benson[1]
[1]*Stanford University*

P-D-8: THE WETTABILITY OF SHALE BY CO_2 AND ITS IMPACT ON GEOLOGIC CO_2 SEQUESTRATION

[CFSES] Eric Guiltinan[1], Bayani Cardenas[1], Nicolas Espinoza[2], Kirsten Chojnicki[3], Mario Martinez[4], Thomas Dewers[5], Hongkyu Yoon[3]
[1]*Department of Geological Sciences, The University of Texas at Austin;* [2]*Center for Petroleum and Geosystems Engineering, The University of Texas at Austin;* [3]*Geoscience Research and Applications, Sandia National Laboratories, Albuquerque;* [4]*Engineering Sciences Center, Sandia National Laboratories, Albuquerque;* [5]*Geomechanics Department, Sandia National Laboratories, Albuquerque*

P-D-10: CHALLENGING TRADITIONAL GEOCELLULAR MODELING METHODOLOGIES TO REPRESENT THE MULTISCALED AND HIERARCHICAL SEDIMENTARY ARCHITECTURE IN CO_2 RESERVOIRS CREATED BY FLUVIAL DEPOSITION

[GSCO2] James Damico[1], Robert Ritzi[2]
[1]*Illinois State Geological Survey, Prairie Research Institute;* [2]*Department of Earth and Environmental Sciences, Wright State University*

P-D-12: CAPILLARY AND WETTABILITY CONTROLS ON CO_2–BRINE DISTRIBUTIONS IN GEOLOGIC CARBON SEQUESTRATION

[NCGC] Timothy J. Kneafsey[1]; Shibo Wang[1], Tetsu K. Tokunaga[1;] Jiamin Wan[1], Yongman Kim[1]; Jonathan Ajo-Franklin[1]; Marco Voltlini[1]; Chun Chang[1], David Trebotich[1]
[1]*Lawrence Berkeley National Laboratory*

P-D-14: IMPACT OF NONWETTING PHASE HYSTERESIS IN RELATIVE PERMEABILITY AND CAPILLARY PRESSURE ON THE DISTRIBUTION OF CO_2

[GSCO2] Christopher Patterson[1], Naum Gershenzon[2], Robert W. Ritzi[2], and Peter Berger[1]
[1]Illinois State Geological Survey; [2]Department of Earth and Environmental Sciences, Wright State University

P-D-16: MOLECULAR ENGINEERING OF SITE-SPECIFIC CO_2 ADSORPTION

[CGS] Zachary Perry[1], Lanfang Zou[1], Hao Li[1], Shuai Yuan[1], Hong-Cai Zhou[1,2]
[1]Department of Chemistry, Texas A&M University
[2]Department of Materials Science and Engineering, Texas A&M University

P-D-18: MODIFICATION OF FRACTURE APERTURES BY REACTIVE MULTIPHASE FLOW

[NCGC] Zhenyu Xu[1], Julie Sheets[2], Timothy J. Kneafsey[3], David R. Cole[2], Laura J. Pyrak-Nolte[1]
[1]Purdue University; [2]Ohio State University; [3]Lawrence Berkeley National Laboratory

E. MATERIALS AND CHEMISTRY BY DESIGN

P-E-2: FABRICATION AND SCANNING PROBE CHARACTERIZATION OF MoS_2 THIN FILMS

[CCDM] Matthäus Wolak[1], Dan Trainer[1], Aleksei Putilov[1], Cinzia Di Giorgio[1], G. Plummer[2], Marian Precner[2], Laszlo Frazer[3], R. Chandrasena[1], F. Kronast[4], Alex X. Gray[1], Eric Borguet[3], Goran Karapetrov[2], Xiaoxing X. Xi[1], Maria Iavarone[1]
[1]Physics, Temple U., [2]Physics, Drexel U., [3]Chemistry, Temple U., [4]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Berlin, Germany

P-E-4: DEFECT INTERACTIONS AND THEIR EFFECTS ON DEFECT POPULATIONS IN GA_2O_3

[CNGMD] Laura Schelhas[5], David Ginley[1], Stephan Lany[1], John Perkins[1], Lauren Garten[1], Paul Ndione[1], Alexie Kolpak[2], Spencer Wyant[2], Tonio Buonassisi[2], Riley Brandt[2], Roy Gordon[3], Danny Chua[3], Brian Gorman[4], John Mangum[4], Kipil Lim[5], Michael Toney[5], William Tumas[1]
[1]National Renewable Energy Laboratory, [2]Massachusetts Institute of Technology, [3]Harvard University, [4]Colorado School of Mines, [5]SLAC National Accelerator Laboratory

P-E-6: 2D TRANSITION METAL CARBIDES (MXENES) AS ENERGY STORAGE MATERIALS: A COMBINED VIEW FROM FIRST-PRINCIPLES SIMULATIONS AND EXPERIMENTS

[FIRST] Yu Xie[1], Michael Naguib[1], Hsiu-Wen Wang[1], Jeremy Come[1], Jennifer Black[1], Babak Anasori[2], Nina Balke[1], Yury Gogotsi[2], Paul R. Kent[1]
[1]Oak Ridge National Laboratory, [2]Drexel University

P-E-8: ATOMIC LAYER DEPOSITION IN METAL-ORGANIC FRAMEWORKS (AIM) AND GAS-PHASE CATALYSIS

[ICDC] Zhanyong Li[1], Varinia Bernales[2], Aaron B. League[2], Neil M. Schweitzer[1], Manuel A. Ortuño[2], Dale R. Pahls[2], Aaron W. Peters[1], Andrew "Bean" Getsoian[3], Aleksei Vjunov[4], Ana E. Platero-Prats[5] , Timothy C. Wang[1], Karena W. Chapman[5], Jeffrey T. Miller[3,6], Johannes A. Lercher[4], Christopher J. Cramer[2], Laura Gagliardi[2], Joseph T. Hupp[1], Omar K. Farha[1,7]

[1]Dept. Chemistry, and Chemical and Biological Engineering, Northwestern University; [2]Dept. Chemistry, Supercomputing Institute, and Chemical Theory Center, University of Minnesota; [3]Chemical Science and Engineering Division, Advanced Photon Source, Argonne National Laboratory; [4]Institute for Integrated Catalysis, Pacific Northwest National Laboratory; [5]X-ray Science Division, Advanced Photon Source, Argonne National Laboratory; [6]School of Chemical Engineering, Purdue University; [7]Dept.Chemistry, Faculty of Science, King Abdulaziz University, Saudi Arabia

P-E-10: CALORIMETRIC STUDY OF ACTINIDE MATERIALS

[MSA] Lei Zhang[1], Anna Shelyug[2], Alexandra Navrotsky[2], Peter C. Burns[1]

[1] Department of Civil and Environmental Engineering and Earth Sciences, University of Notre Dame

[2] Peter A. Rock Thermochemistry Laboratory and NEAT ORU, and Department of Chemical Engineering and Materials Science, University of California, Davis

P-E-12: SOLID-STATE (AND GAS-PHASE) NMR: A WINDOW INTO MATERIALS FOR ACID GAS CAPTURE

[UNCAGE-ME] Robert Marti[1], Erika Sesti[1], Sophia E. Hayes[1]

[1]Department of Chemistry, Washington University, Saint Louis

P-E-14: CHARGE DENSITY WAVES IN A FEW LAYERS OF TiSe$_2$

[CCDM] Maria Iavarone[1], T. Polakovic[2], Marian Precner[2], G. Plummer[2], James Curtis[2], S. Ciocys[2], Qiao Qiao[3], Yimei Zhu[3], Samantha L. Shumlas[4], Daniel Strongin[4], Goran Karapetrov[2]

[1]Physics, Temple U., [2]Physics, Drexel U., [3]BNL, [4]Chemistry, Temple U.

P-E-16: NU-1000 AND RELATED MOF-BASED MATERIALS AS PLATFORMS FOR CATALYST DESIGN

[ICDC] Steven Pellizzeri[1], Anthony B. Thompson[2], Camille D. Malonzo[2], Thomas Webber[2], Timothy Wang[3], Pere Miró[4], Peilin Liao[4], Melissa Barona[4], Omar Farha[3], Joseph T. Hupp[3], Lee Penn[2], Andreas Stein[2], Randall Q. Snurr[4], Laura Gagliardi[2], Rachel Getman[1], Connie C. Lu[2]

[1]Dept. Chemical Engineering and Biomolecular Engineering, Clemson University; [2]Dept. Chemistry, Chemical Theory Center, and Supercomputing Institute, University of Minnesota; [3]Dept. Chemistry, Northwestern University; [4]Dept. Chemical and Biological Engineering, Northwestern University

P-E-18: TPD AND SEM INVESTIGATION OF ACID GAS INTERACTIONS WITH CERIUM AND TITANIUM MOFS AND MOF-DERIVED OXIDES

[UNCAGE-ME] William P. Mounfield, III[1], Uma Tumuluri[2], Yang Jiao[1], Zili Wu[2], Krista S. Walton[1]

[1]School of Chemical & Biomolecular Engineering, Georgia Institute of Technology

[2]Chemical Science Division and Center for Nanophase Materials Sciences, Oak Ridge National Laboratory

P-E-20: INCORPORATING POLYMORPHS INTO MATERIALS BY DESIGN: TARGETED SYNTHESIS OF METAL OXIDE POLYMORPHS

[CNGMD] Zamyla Chan[4], David Ginley[1], Vladan Stevanovic[1,5], John Perkins[1], Lauren Garten[1], Paul Ndione[1], Kristin Persson[2,8], Gerbrand Ceder[2,8], Daniil Kitchaev[3], Daniel Nocera[4], Roy Gordon[4], Lu Sun[4], Brian Gorman[5], John Mangum[5], Ann Deml[5], Prashun Gorai[5], Janet Tate[6], James Haggerty[6], Chiyuki Sato[6], Laura Schelhas[7], Kevin Stone[7], Johanna Nelson Weker[7], Michael Toney[7], Hong Kevin Ding[8], Wenhao Sun[8], William Tumas[1]

[1]National Renewable Energy Laboratory, [2]UC-Berkeley, [3]Massachusetts Institute of Technology, [4]Harvard University, [5]Colorado School of Mines, [6]Oregon State University, [7]SLAC National Accelerator Laboratory, [8]Lawrence Berkeley National Laboratory

P-E-22: IRRADIATION INDUCED POINT DEFECT EVOLUTION IN NI-BASED CONCENTRATED SOLID SOLUTION ALLOYS

[EDDE] Mohammad W. Ullah[1], Dilpuneet S. Aidhy[1], Chenyang Lu[2], Hongbin Bei[1], Ke Jin[1], Lumin Wang[2], Yanwen Zhang[1], William J. Weber[1,3]

[1]Oak Ridge National Laboratory; [2]University of Michigan; [3]University of Tennessee

P-E-24: TETRAVALENT AND HEXAVALENT URANIUM CLUSTERS: SYNTHESIS AND CHARACTERIZATION IN SOLUTION

[MSA] Clement Falaise[1] and May Nyman[1]

[1] Department of Chemistry, Oregon State University

P-E-26: THERMOELECTRIC SKUTTERUDITES – WHY AND HOW HIGH zT CAN BE ACHIEVED

[S^{3}TEC] Yinglu Tang*[1,2], Zachary M. Gibbs*[3], Luis A. Agapito[4,5], Riley Hanus, Guodong Li[1,2,6], Hyun-Sik Kim[1,2,7], Marco Buongiorno Nardelli[4], Stefano Curtarolo[5], Sinn-wen Chen[8], G. Jeffrey Snyder[1,2]

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P-E-28: MIXED-LINKER ZIFS: STRUCTURE DETERMINATION AND CONTROL OF GAS AND VAPOR ADSORPTION AND DIFFUSION PROPERTIES

[UNCAGE-ME] Juan Hazbon[1], Souryadeep Bhattacharyya[1], Krishna Jayachandrababu[1], Ross Verploegh[1], Rebecca Han[1], David S. Sholl[1], Sankar Nair[1]

[1]School of Chemical & Biomolecular Engineering, Georgia Institute of Technology

P-E-30: URANYL PEROXIDE NANO-CAGE FULLERENE: U60, AT ELEVATED PRESSURES

[MSA] Katlyn M. Turner[1], Yu Lin[1], Fuxiang Zhang[2], Brendan T. McGrail[3], Wendy L. Mao[1], Peter C. Burns[3], Rodney C. Ewing[1]

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F. CATALYSIS

P-F-2: ATOMICALLY WELL-DEFINED CATALYSTS AND PHOTOCATALYSTS FOR SOLAR FUELS

[ANSER] Dong Wook Kim[1,2], Idan Hod[1], Chung-Wei Kung[1], William Hoffeditz[1], Michael R. Wasielewski[1], Michael J. Pellin[1,2], Omar K. Farha[1], Alex B. F. Martinson[2], Joseph T. Hupp[1,2]

[1] Dept. Chemistry, Northwestern University; [2] Materials Science Division, Argonne National Laboratory

P-F-4: MECHANISM OF CO(SALOPHEN)-CATALYZED AEROBIC OXIDATION OF *P*-HYDROQUINONE

[CME] Colin W. Anson[1], Soumya Ghosh[2], Sharon Hammes-Schiffer[2], Shannon S. Stahl[1]

[1]University of Wisconsin-Madison; [2]University of Illinois at Urbana-Champaign

P-F-6: TURNING A CHEAP, POOR CATALYST INTO A CHEAP, EXCELLENT CATALYST: MODIFICATION OF THE LAYERED WATER OXIDATION CATALYST NIRNESSITE

[CCDM] Akila C. Thenuwara[1], Samantha L. Shumlas[1], Nuwan H. Attanayake[1], Elizabeth Cerkez [1], Ian G.McKendry[1], Laszlo Fraser[1], Eric Borguet[1], Qing Kang[1], Michael Zdilla[1], Jianwei Sun[2] and Daniel R.Strongin[1]

[1]Chemistry, Temple U., [2]Physics, Temple U.

P-F-8: HOW DOES NANOPOROUS AU DISSOCIATE O_2?

[IMASC] Matthew M. Montemore[1], Lucun Wang[2], Cynthia M. Friend[2], Robert J. Madix[2], Efthimios Kaxiras[1,3]

[1] School of Engineering and Applied Sciences, Harvard University; [2] Department of Chemistry and Chemical Biology, Harvard University; [3] Department of Physics, Harvard University

P-F-10: STUDIES TOWARDS COBALT-CATALYZED CONVERSION OF BIOREFINERY LIGNIN TO VALUE-ADDED CHEMICALS AND FUELS

[C3Bio] Joseph J. Bozell, Berenger Biannic, Rebecca E. Key, William T. Hartwig, Costyl N. Ngnouomeuchi, Ernesto C. Zuleta

Center for Renewable Carbon, University of Tennessee.

P-F-12: A MECHANISTIC UNDERSTANDING FOR WHY PTCO NANOCRYSTALS ARE SELECTIVE FOR HYDRODEOXYGENATION OF HMF

[CCEI] Jing Luo[1], Hongseok Yun[2], Vassili Vorotnikov[3], Vicky Doan-Nguyen[4], Dionisios G. Vlachos[3], Christopher B. Murray[2,4], Raymond J. Gorte[1]

[1]Department of Chemical and Biomolecular Engineering, University of Pennsylvania; [2]Department of Chemistry, University of Pennsylvania; [3]Department of Chemical and Biomolecular Engineering, University of Delaware; [4]Department of Materials Science and Engineering, University of Pennsylvania

P-F-14: OXYGEN-ASSISTED FUNDAMENTAL REACTIONS AND COMPETITION FOR ACTIVE SITES ON MODEL GOLD SINGLE-CRYSTAL CATALYST SURFACES

[IMASC] Fanny Hiebel[1], Stavros Karakalos[1], Fairoja Cheenicode Kabeer[2], Alexandre Tkatchenko[2], Cynthia M. Friend[1], Robert J. Madix[1]

[1] Department of Chemistry and Chemical Biology, Harvard University; [2] Fritz-Haber Institute, Germany

P-F-16: Bio-Inspired Molecular Iron Electrocatalysts for Hydrogen Oxidation: The Evolution of a Hydrogenase Functional Mimic

[CME] Jonathan M. Darmon, Aaron M. Appel, Neeraj Kumar, Simone Raugei, R. Morris Bullock, Monte L. Helm
Pacific Northwest National Laboratory

P-F-18: Molecular Catalysts for Solar Fuels Processes: Design, Synthesis and Analysis

[UNC] Andrew G. Walden, Christopher J. Dares, Matthew V. Sheridan, Benjamin D. Sherman, Matthew T. Campbell, Gary L. Glish, Thomas J. Meyer, Alexander J. M. Miller
Department of Chemistry, University of North Carolina at Chapel Hill

P-F-20: Development of Lewis Acid Zeolite Catalysts for Biomass Conversion

[CCEI] Hong Je Cho[1], Chun-Chih Chang[1], Paul Dornath[1], Paul J. Dauenhauer[2], Wei Fan[1]
[1]*Department of Chemical Engineering, University of Massachusetts Amherst*
[2]*Department of Chemical Engineering and Materials Science, University of Minnesota*

P-F-22: Overpotential is an Important Factor Governing Electrocatalytic O_2 Reduction Rates with Iron Porphyrins

[CME] Michael L. Pegis[1], John A.S. Roberts[2,3], Neeraj Kumar[2], Derek J. Wasylenko[4,5], Simone Raugei[2], Aaron M. Appel[2], James M. Mayer[1]
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P-F-24: Development and Characterization of Molecular Iridium Complexes Supported on Metal Nodes of Metal-Organic Frameworks

[ICDC] Samuel O. Odoh[1], Dong Yang[2], Martino Rimoldi[3], Joshua Borycz[1], Timothy C. Wang[3], In Soo Kim[4], Alex B. F. Martinson[4], Omar K. Farha[3], Joseph T. Hupp[3], Christopher J. Cramer[1], Laura Gagliardi[1], Bruce C. Gates[2]
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G. Synthesis of Functional Matter

P-G-2: The Design, Preparation and Characterization of PbE/CdE (E=S, Se, Te) Heterostructured Nanocrystals for Advanced Solar Energy Conversion

[CASP] Boris D. Chernomordik[1], Qianglu Lin[2], Samuel Keene[3], Nikolay S. Makarov[2], Kirill A. Velizhanin[4], Justin C. Johnson[1], Matt Law[3], Victor I. Klimov[2], Jeffrey M. Pietryga[2], Matthew C. Beard[1]
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P-G-4: Molecular Simulation of Complex Materials for Electrochemical Supercapacitors

[FIRST] Matthew W. Thompson[1], Yu Zhang[1], Guang Feng[2], Christoph Klein[1], Boris Dyatkin[3], Hsiu-Wen Wang[4], Jennifer Black[4], Cheng Zhan[5], Peter T. Cummings[1]
[1]*Vanderbilt University,* [2]*Huazhong University of Science and Technology, China,* [3]*Drexel University,* [4]*Oak Ridge National Laboratory,* [5]*University of California at Riverside*

P-G-6: MANIPULATING LIGHT USING OPTICAL METASURFACES

[LMI] Seyedeh Mahsa Kamali[1], Di Wu[2], Soo Jin Kim[2], Amir Arbabi[1], Ehsan Arbabi[1], Yu Horie[1], Gururaj Naik[2], Pengyu Fan[2], Ju-Hyung Kang[2], Jennifer A. Dionne[2], Mark L. Brongersma[2], Andrei Faraon[1]
[1]California Institute of Technology, [2]Stanford University

P-G-8: THE ENGINEERING OF QUANTUM DOTS FOR APPLICATION IN SINGLE- AND MULTI-LAYER LUMINESCENT SOLAR CONCENTRATORS

[CASP] Thomas A. Baker[1], Samantha Ehrenberg[2], Jaehoon Lim[1], Kirill A. Velizhanin[3], Hunter McDaniel[1,4], Hongbo Li[1], Hyung Jun Song[1], Jeffrey M. Pietryga[1], Uwe Kortshagen[2], Victor I. Klimov[1]
[1] Chemistry Division, Los Alamos National Laboratory; [2] Department of Mechanical Engineering, University of Minnesota; [3] Theory Division, Los Alamos National Laboratory; [4] UbiQD

P-G-10: PERFORMANCE ENHANCEMENTS IN VISIBLE AND INFRARED QUANTUM-DOT LIGHT EMITTING DEVICES

[CE] Geoffrey J Supran[1], Katherine W Song[1], Gyu Weon Hwang[1], Raoul E Correa[1], Jennifer Scherer[1], Eric A Dauler[1], Yasuhiro Shirasaki[1], William A Tisdale[1], Moungi G Bawendi[1], Vladimir Bulović[1].
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P-G-12: IMPROVING SOLAR POWERED THERMOPHOTOVOLTAIC DEVICES WITH NANOPHOTONIC FEATURES

[S^{3}TEC] David M. Bierman[1], Veronika Stelmakh[2], Andrej Lenert[1], Bikram Bhatia[1], Walker Chan[2], Ivan Celanovic[2], Marin Soljacic[3], Evelyn N. Wang[1]
[1] Dept. Mechanical Engineering, Massachusetts Institute of Technology; *[2] Dept. Electrical Engineering and Computer Science, Massachusetts Institute of Technology*; *[3] Dept. Physics, Massachusetts Institute of Technology*

P-G-14: COMBINATORIAL GROWTH OF NOVEL SUPERCONDUCTING MATERIALS

[CES] Alexandra Cote[1], Samantha Rubeck[1], Thomas Neulinger[1], Ankita Bhutani[1], Julia Zuo[1], Duck Young Chung[2], Mercouri Kanatzidis[2,3], Laura Greene[1,4], Daniel Shoemaker[1], Jian-Min Zuo[1], James Eckstein[1]
[1]Fredrick Seitz Materials Research Laboratory, University of Illinois; [2]Argonne National Laboratory; [3]Department of Chemistry, Northwestern University; [4]Department of Physics, Florida State University

P-G-16: SELECTIVE AND TUNABLE O_2 BINDING IN COBALT METAL-ORGANIC FRAMEWORKS

[CGS] Dianne J. Xiao[1], Miguel I. Gonzalez[1], Lucy E. Darago[1], Jeffrey R. Long[1,2]
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H. BIOSCIENCE

P-H-2: CHARACTERIZING SHORT-LIVED FLAVIN OXIDATION-REDUCTION INTERMEDIATES BY TRANSIENT ABSORPTION SPECTROSCOPY

[BETCy] Cara Lubner[1], John Hoben[2], Michael Ratzloff[1], Anne-Frances Miller[2], Paul King[1]
[1]National Renewable Energy Laboratory, [2]University of Kentucky

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

[PARC] Xun Lu, Sudipa Ghimire-Rijal, Christoper Stanley, Dean A. Myles and Matthew J. Cuneo
Biology and Biomedical Sciences Group, Oak Ridge National Laboratory

P-H-6: HYDRATION CONTROL OF THE MECHANICAL AND DYNAMICAL PROPERTIES OF CELLULOSE

[CLSF] Loukas Petridis[1], Bingxin Fan[2], Janna Maranas[2], Hugh M. O'Neil[1]
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[2]Department of Chemical Engineering, Pennsylvania State University

P-H-8: MEASURING AND MODELING CHANGES IN BIOMASS STRUCTURE DURING CATALYTIC CONVERSION

[C3Bio] Jiliang Liu[1], Yan Zheng[1], Lee Makowski[1], Bryon S. Donohoe[2], Mike Himmel[2], Mike Crowley[2], Peter N. Ciesielski[2]
[1]Department of Bioengineering and Department of Chemistry and Chemical Biology, Northeastern University, [2]Biosciences Center, National Renewable Energy Laboratory

P-H-10: HOW CELLULOSE ELONGATES - A QM/MM STUDY OF THE MOLECULAR MECHANISM OF CELLULOSE POLYMERIZATION IN BACTERIAL CESA

[CLSF] Hui Yang[1], Jochen Zimmer[2], Yaroslava Yingling[3], James D. Kubicki[1]
[1]Department of Geosciences, The Pennsylvania State University; [2]Center for Membrane Biology and Department of Molecular Physiology and Biological Physics, University of Virginia School of Medicine; [3]Department of Materials Science and Engineering, North Carolina State University

P-H-12: EXPANDING THE SPECTRAL RANGE OF PHOTOSYNTHESIS

[PARC] Benjamin M. Wolf[1,2], Jeremy D. King[1,2], Dariusz Niedzwiedzki[1,2,10], Haijun Liu[1,2], Hao Zhang[1,2], Gregory S. Orf[1,2], Nancy Y. Kiang[4,6,9], Mary Nicole Parenteau[4,5], Kathy Ann Miller[7], Cameron Hearne[4], Ron Lindeman[8], Min Chen[11], Robert E. Blankenship[1,2,3,9]
[1]Dept. Biology, Washington University in St. Louis; [2]Photosynthetic Antenna Research Center, Washington University in St. Louis; [3]Dept. Chemistry, Washington University in St. Louis; [4]NASA Ames Research Center; [5]SETI Institute; [6]NASA Goddard Institute for Space Studies; [7]University and Jepson Herbaria; [8]Retired; [9]NASA Astrobiology Institute Virtual Planetary Laboratory; [10]PARC Ultrafast Laser Facility; [11]University of Sydney

P-H-14: MANAGING THE PARTITIONING OF PYRIDINE NUCLEOTIDE-BASED REDOX EQUIVALENTS IN DIRECTING ELECTRON FLOW TO CHEMICAL BOND FORMATION

[BETCy] Diep Nguyen[1], John Hoben[2], Oleg Zadvornyy[3], Gerti Schut[1], David Jennings[4], Anne K. Jones[4], John W. Peters[3], Anne-Frances Miller[2], Michael Adams[1]
[1]University of Georgia, [2]University of Kentucky, [3]Montana State University, [4]Arizona State University

P-H-16: VISUALIZING THE MOLECULAR STRUCTURE OF STATIC AND DYNAMICALLY STRETCHED PRIMARY PLANT CELL WALLS BY AFM AND FESEM

[CLSF] Tian Zhang[1], Daniel Durachko[1], Lei Lei[2], Yunzhen Zheng[1], Charles T. Anderson[1], Ying Gu[2], Bernhard Tittmann[3], Daniel Cosgrove[1]
[1]Department of Biology, [2] Department of Biochemistry and Molecular Biology, [3]Department of Engineering Science and Mechanics, Pennsylvania State University

P-H-18: COMMUNICATING BIOCATALYTIC SYSTEMS

[CBES] John F. Edelbrock[1], Benjamin G. Jones[1], Victor V. Yashin[2], Armando Hernandez-Garcia[3], Job Boekhoven[3], Monica Olvera de la Cruz[1,4,5], Anna C. Balazs[2], Samuel I. Stupp[1,3,4,6]
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J. MESOSCALE SCIENCE

P-J-2: EXCITON-POLARITON BOSE-EINSTEIN CONDENSATES: THERMALIZATION, INTERACTION, AND COHERENT CONTROL

[CE] Yongbao Sun[1], Yoseob Yoon[1], Mark Steger[2], Gangqiang Liu[2], Saeed A. Khan[3], Ge Li[3,4],
Loren N. Pfieffer[3], Ken West[3], Hakan E. Tureci[3], David W. Snoke[2], Keith A. Nelson[1]

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P-J-4: CUPRATE SUPERCONDUCTORS AND THE IMPACT OF OUT-OF-PLANE ATOMIC MOTION

[CES] John M. Tranquada[1], E. Bozin[1], B. Shen[2], W. K. Kwok[2], J. D. Rameau[1], P. D. Johnson[1], S. Vig[3], V. Mishra[2], G. D. Gu[1], M. R. Norman[2], P. Abbamonte[3]

[1]Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory
[2]Materials Science Division, Argonne National Laboratory
[3]Department of Physics and Materials Research Laboratory, University of Illinois

P-J-6: THE SYNTHESIS OF NANOPOLYCRYSTALLINE DIAMOND AND DIAMOND NANOWIRES FROM PERIODIC MESOPOROUS CARBON

[EFree] Cong Liu[1], Shah Najiba[1], Manik Manda[1]l, Jihua Chen[2], Yingwei Fei[3], Kai Landskron[1]

[1] Department of Chemistry, Lehigh University; [2] Department of Mechanical and Materials Engineering, Florida International University; [3] Geophysical Laboratory, Carnegie Institution of Washington

P-J-8: UNDERSTANDING ION TRANSPORT FOR MODEL NANOSCALE ELECTRODE SYSTEMS

[NEES] Timothy S. Plett[1], Trevor Gamble[1], Eleanor Gillette[2], William Mann[3], Wenqing Shi[4], Yuhan Zeng[4], Ivan Vlassiouk[5], Lane Baker[4], Sang Bok Lee[2], Zuzanna Siwy[1,6]

[1] Dept. Physics, University of California, Irvine; [2] Dept. Chemistry and Biochemistry, University of Maryland; [3] Dept. Physics and Astronomy, California State University; [4] Dept. Chemistry, Indiana University; [5] Oak Ridge National Laboratory; [6] Dept. Chemistry, University of California, Irvine

GRADUATE STUDENT AND POSTDOCTORAL RESEARCHER FINALISTS

Graduate Student

A-II-3: THE EFFECT OF CATION DISORDER ON THE LI INTERCALATION VOLTAGE OF TRANSITION METAL OXIDES

[NECCES] Aziz Abdellahi[1], Alexander Urban[2], Stephen Dacek[1], ShinYoung Kang[1], Pinaki Mukherjee[3], Khim Karki[4], Frederic Cosandey[3], Gerbrand Ceder[2]

[1]Masschusetts Institute of Technology, [2]UC Berkeley [3]Rutgers University, [4]Brookhaven National Laboratory

Postdoctoral Researcher

D-I-5: THE ROLE OF ADVANCED REACTIVE SURFACE AREA CHARACTERIZATION IN IMPROVING PREDICTIONS OF MINERAL REACTION RATES IN SUBSURFACE POROUS MEDIA

[NCGC] Lauren E. Beckingham[1], Elizabeth Mitnick[2], Carl I. Steefel[1], Shuo Zhang[2], Li Yang[1], Marco Voltolini[1], Alexander M. Swift[3], David R. Cole[3], Julie M. Sheets[3], Timothy Kneafsey[1], Gautier Landrot[4], Lawrence Anovitz[5], Saeko Mito[6], Ziqiu Xue[6], Donald DePaolo[1,2], Jonathan Ajo-Franklin[1]

[1]Lawrence Berkeley National Laboratory; [2]University of California, Berkeley; [3]Ohio State University; [4]Synchrotron SOLEIL; [5]Oak Ridge National Laboratory; [6]Research Institute of Innovative Technology for the Earth (RITE)

Graduate Student

A-II-1: PROBING SUPERCAPACITOR CARBON-ELECTROLYTE STRUCTURE AND ION DYNAMICS WITH NEUTRONS

[FIRST] Boris Dyatkin[1], Hsiu-Wen Wang[2], Eugene Mamontov[3], Naresh Osti[3], Katherine Page[3], Ray Unocic[3], Gernot Rother[3], Matthew Thompson[4], Yu Zhang[4], Peter Cummings[4], David Wesolowski[3], Yury Gogotsi[1]

[1]Drexel University; [2]University of Tennessee; [3]Oak Ridge National Laboratory; [4]Vanderbilt University

Graduate Student

H-III-1: EXPANDING THE RANGE OF LIGHT ABSORBERS FOR BACTERIAL PHOTOSYNTHESIS: YFP-ENHANCED CHARGE SEPARATION AT THE RHODOBACTER SPHAEROIDES REACTION CENTRE

[PARC] Kaitlyn M. Faries[1], Katie J. Grayson[2], Pu Qian[2], Preston Dilbeck[1], Elizabeth Martin[2], Jonathan M. Yuen[1], Dariusz M. Niedzwiedzki[3], Dewey Holten[1], Christine Kirmaier[1] and C. Neil Hunter[2]

[1]Dept. Chemistry, Washington University, St. Louis; [2]Dept. Molecular Biology and Biotechnology, University of Sheffield, UK; [3]Photosynthetic Antenna Research Center, Washington University, St. Louis

Postdoctoral Researcher

E-IV-1: PREDICTING AND CONTROLLING POLYMORPHISM IN TRANSITION METAL OXIDES

[CNGMD] Lauren M. Garten[1], Hong Kevin Ding[2], Laura T. Schelhas[3], Kevin Stone[3], Prashun Gorai[1], Paul Ndione[1], Kristin Persson[2], Michael F. Toney[3], Vladan Stevanović[1,4], David S. Ginley[1]

[1]*National Renewable Energy Laboratory;* [2]*Lawrence Berkeley National Laboratory;* [3]*SSRL Materials Science Division, SLAC National Accelerator Laboratory;* [4]*Colorado School of Mines*

Graduate Student

E-I-3: REVEALING THE SUGAR ISOMERIZATION MECHANISM ON HOMOGENEOUS SN-SILICATE CATALYSTS

[CCEI] Tyler Josephson[1], Kramer Brand[2], Jay Labinger[2], Mark Davis[2], Dion Vlachos[1], Stavros Caratzoulas[1]

[1]*University of Delaware;* [2]*California Institute of Technology*

Graduate Student

B-III-3: Incorporation of Perylene-3,4-dicarboximides into Photoanodes and Photocathodes for Solar Fuels

[ANSER] Rebecca J. Lindquist[1], Marek B. Majewski[1], Julianne M. Thomsen[2], William L. Hoffeditz[1], Brian T. Phelan[1], Kelly L. Materna[2], Joseph T. Hupp[1], Gary W. Brudvig[2], Michael R. Wasielewski[1]

[1]*Department of Chemistry, Northwestern University;* [2]*Department of Chemistry, Yale University*

Graduate Student

B-I-1: UNDERSTANDING AND IMPROVING THE CHEMISTRY OF LEAD CHALCOGENIDE QUANTUM DOTS FOR PHOTOVOLTAICS

[CASP] Ashley R. Marshall[1,2], Arthur J. Nozik[2], Matthew C. Beard[1], Joseph M. Luther[1]

[1]*National Renewable Energy Laboratory;* [2]*Dept. Chemistry and Biochemistry, University of Colorado*

Postdoctoral Researcher

G-V-1: ULTRAFAST SYNTHESIS METAL-ORGANIC FRAMEWORKS CRITICAL FOR ENERGY-EFFICIENT CO_2 CAPTURE

[CGS] L. Maserati[1], S. M. Meckler[1,2] , C. Li[1,3], J. R. Long[2,4] and B. A. Helms[1]

[1]*The Molecular Foundry, Lawrence Berkeley National Laboratory;* [2]*Department of Chemistry, University of California, Berkeley;* [3]*Department of Chemical Engineering, University of California, Berkeley;* [4]*Materials Sciences Division, Lawrence Berkeley National Laboratory*

Graduate Student

I-III-5: ANOMALOUS SURFACE THERMODYNAMICS OF GAS ADSORPTION ON ZEOLITE-TEMPLATED CARBON

[EFree] Maxwell Murialdo, Nicholas P. Stadie, Channing C. Ahn, Brent Fultz

California Institute of Technology

Postdoctoral Researcher

F-III-3: METAL-ORGANIC FRAMEWORK NODES AS NEARLY IDEAL SUPPORTS FOR MOLECULAR CATALYSTS: NU-1000- AND UIO-66-SUPPORTED IRIDIUM COMPLEXES FOR ETHYLENE HYDROGENATION AND DIMERIZATION

[ICDC] Samuel O. Odoh[1], Dong Yang[2], Timothy Wang[3], Omar K. Farha[3], Joseph T. Hupp[3], Christopher Cramer[1], Bruce C. Gates[2], Laura Gagliardi[1]

[1]Department of Chemistry, Chemical Theory Center, and Supercomputing Institute, University of Minnesota; [2]Department of Chemical Engineering & Materials Science, University of California, Davis; [3]Departments of Chemistry and Chemical and Biological Engineering, Northwestern University

Postdoctoral Researcher

F-III-4: ACID GAS INTERACTION WITH OXIDE NANOSHAPES WITH WELL-DEFINED SURFACE FACETS

[UNCAGE-ME] Uma Tumuluri[1], Meijun Li[1], Brandon Cook[2], William Mounfield[3], Joshua D. Howe[3], Bobby Sumpter[2], Krista S. Walton[3], David S. Sholl[3], Sheng Dai[1], Zili Wu[1,2]

[1]Chemical Science Division, Oak Ridge National Laboratories; [2]Center for Nanophase Material Science, Oak Ridge National Laboratories; [3]School of Chemical & Biomolecular Engineering, Georgia Institute of Technology

Graduate Student

G-II-5: STRUCTURAL EVOLUTION OF URANYL PEROXIDE NANO-CAGE FULLERENE: U60, AT ELEVATED PRESSURES

[MSA] Katlyn M. Turner[1], Yu Lin[1], Fuxiang Zhang[2], Brendan T. McGrail[3], Wendy Mao[1], Peter C. Burns[3], Rodney C. Ewing[1]

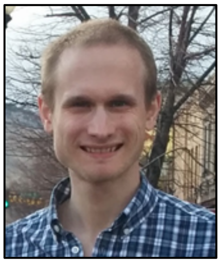
[1]Dept. Geological Sciences, Stanford University; [2]Dept. of Earth & Environmental Sciences, University of Michigan; [3]Dept. Civil & Environmental Engineering & Earth Sciences, University of Notre Dame

Postdoctoral Researcher

H-II-3: STRUCTURAL STUDIES OF PLANT CELLULOSE SYNTHASE SUPPORT 18 SYNTHASES IN THE CELLULOSE SYNTHESIS COMPLEX

[CLSF] Venu Gopal Vandavasi[1], B. Tracy Nixon[2], Daniel K. Putnam[3], Katayoun Mansouri[4], Jung-Goo Lee[4], Abhishek Singh[4], Juan Du[2], Eric M. Roberts[5], Alison W. Roberts[6], Erin Slabaugh[4], Jonathan K. Davis[4], Qiu Zhang[1], Loukas Petridis[1], William T. Heller[1], Udaya Kalluri[1], Leighton Coates[1], Paul Langan[1], Jeremy C. Smith[1], Jens Meiler[3], Yaroslava G. Yingling[4], Candace H. Haigler[4] Hugh O'Neill[1,7]

[1]Oak Ridge National Laboratory; [2]Pennsylvania State University; [3]Vanderbilt University; [4]North Carolina State University; [5]Rhode Island College; [6]University of Rhode Island; [7]University of Tennessee



Graduate Student

C-I-5: CHARACTERIZATION OF THE LOW-ENERGY BOSONIC MODES IN $\mathrm{BI_2SR_2CACU_2O_{8+X}}$ WITH INCIPIENT CHARGE ORDER

[CES] Sean Vig[1], Anshul Kogar[1], Vivek Mishra[2], Luke Venema[1], Melinda S. Rak[1], Ali A. Husain[1], Genda D. Gu[3], Eduardo Fradkin[1], Mike R. Norman[2], Peter Abbamonte[1,2]

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Postdoctoral Researcher

F-II-1: DYNAMIC EVOLUTION OF NANOPOROUS GOLD CATALYSTS DURING ACTIVATION AND SELECTIVE OXIDATION REACTIONS

[IMASC] Branko Zugic[1], Lucun Wang[1], Michelle L. Personick[1], Matthew Montemore[2], Christian Heine[3], Luan Nguyen[4], Nare Janvelyan[1], Dmitri Zakharov[5], Eric Stach[5], Miquel Salmeron[3], Monika M. Biener[6], Juergen Biener[6], Franklin (Feng) Tao[4], Efthimios Kaxiras[2], Robert J. Madix[2], Cynthia M. Friend[1,2]

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2015 EFRC PI MEETING – ACRONYMS AND IDS

Talk ID: **Letter of Technical Session – Session Block – Number**
(e.g. A-I-1 is an Energy Storage talk on Monday at 1:10 pm)

Poster ID: **P – Letter of Technical Session – Number**
(odd # on Mon/even # on Tue. e.g. P-F-1 is a Catalysis poster on Mon at 5:00 – 6:30 pm)

ENERGY FRONTIER RESEARCH CENTERS

[ANSER] Argonne-Northwestern Solar Energy Research Center
Michael Wasielewski, Northwestern University

[BETCy] Center for Biological Electron Transfer and Catalysis
John Peters, Montana State University

[C3Bio] Center for Direct Catalytic Conversion of Biomass to Biofuels
Maureen McCann; Purdue University

[CASP] Center for Advanced Solar Photophysics
Victor Klimov, Los Alamos National Laboratory

[CBES] Center for Bio-Inspired Energy Science
Samuel Stupp, Northwestern University

[CCDM] Center for the Computational Design of Functional Layered Materials
John Perdew, Temple University

[CCEI] Catalysis Center for Energy Innovation
Dionisios Vlachos, University of Delaware

[CE] Center for Excitonics
Marc Baldo, Massachusetts Institute of Technology

[CEES] Center for Electrochemical Energy Science
Paul Fenter, Argonne National Laboratory

[CES] Center for Emergent Superconductivity
Peter Johnson, Brookhaven National Laboratory

[CFSES] Center for Frontiers of Subsurface Energy Security
Larry Lake, University of Texas at Austin

[CGS] Center for Gas Separations Relevant to Clean Energy Technologies
Jeffrey Long, University of California, Berkeley

[CLSF] Center for Lignocellulose Structure and Formation
Daniel Cosgrove, Pennsylvania State University

[CME] Center for Molecular Electrocatalysis
R. Morris Bullock, Pacific Northwest National Laboratory

[CNGMD] Center for Next Generation of Materials by Design: Incorporating Metastability
William Tumas, National Renewable Energy Laboratory

[EDDE] Energy Dissipation to Defect Evolution
Yanwen Zhang, Oak Ridge National Laboratory

[EFree] Energy Frontier Research in Extreme Environments
Russell Hemley, Carnegie Institution of Washington

[FIRST] Fluid Interface Reactions, Structures and Transport Center
David Wesolowski, Oak Ridge National Laboratory

[GSCO2] Center for Geologic Storage of CO_2
Scott M. Frailey, University of Illinois at Urbana-Champaign

[ICDC] Inorganometallic Catalyst Design Center
Laura Gagliardi, University of Minnesota

[IMASC] Integrated Mesoscale Architectures for Sustainable Catalysis
Cynthia Friend, Harvard University

[LMI] Light-Material Interactions in Energy Conversion
Ralph Nuzzo, California Institute of Technology

[m2M] Center for Mesoscale Transport Properties
Esther Takeuchi, Stony Brook University

[MSA] Materials Science of Actinides
Peter Burns, University of Notre Dame

[NCGC] Center for Nanoscale Controls on Geologic CO_2
Donald DePaolo, Lawrence Berkeley National Laboratory

[NECCES] NorthEast Center for Chemical Energy Storage
M. Stanley Whittingham, Binghamton University

[NEES] Nanostructures for Electrical Energy Storage
Gary Rubloff, University of Maryland

[PARC] Photosynthetic Antenna Research Center
Robert Blankenship, Washington University in St. Louis

[S3TEC] Solid-State Solar-Thermal Energy Conversion Center
Gang Chen, Massachusetts Institute of Technology

[SHINES] Spins and Heat in Nanoscale Electronic Systems
Jing Shi, University of California, Riverside

[UNC] Center for Solar Fuels
Thomas Meyer, University of North Carolina

[UNCAGE-ME] Center for Understanding and Control of Acid Gas-induced Evolution of Materials for Energy
Krista Walton, Georgia Institute of Technology

NATIONAL LABORATORIES

ANL	Argonne National Laboratory
BNL	Brookhaven National Laboratory
LBNL	Lawrence Berkeley National Laboratory
LANL	Los Alamos National Laboratory
NREL	National Renewable Energy Laboratory
NRL	Naval Research Laboratory
ORLN	Oak Ridge National Laboratory
PNNL	Pacific Northwest National Laboratory
SNL	Sandia National Laboratories