Science for our Nation's Energy Future

Energy Frontier Research Centers
Principal Investigators' Meeting

July 18 - 19, 2013
Washington, D.C.

Washington Marriott
Wardman Park

U.S. DEPARTMENT OF ENERGY | Office of Science

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Agenda Day 1

Thursday, July 18, 2013
8:30 AM – 6:30 PM

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

8:30 – 10:10 AM **Perspectives on Frontiers in Energy Research, *Salon 2***

8:30 AM **Welcome**
Patricia Dehmer, Acting Director, DOE Office of Science

8:40 AM **Keynote Address: "From Quanta to the Continuum: Opportunities for Mesoscale Science"**
George Crabtree, Argonne National Laboratory and University of Illinois at Chicago

9:20 AM **Keynote Address: "A New Industrial Revolution for a Sustainable Energy Future"**
Arun Majumdar, Google

10:00 AM **Announce winners of *EFRC Science Using Only Ten-Hundred and One Words* Challenge; introduce Graduate Student and Postdoctoral Researcher speakers**

10:10 AM **Break**

10:30 AM **Parallel Technology Talks**

A. **Bioenergy Technologies**, *Delaware Suite A*
Valerie Reed, Acting Program Director for the Bioenergy Technologies Office, DOE Energy Efficiency and Renewable Energy
B. **Vehicle Technologies – Energy Storage**, *Delaware Suite B*
David Howell, Team Lead for Hybrid Electric Systems, DOE Energy Efficiency and Renewable Energy, Vehicle Technologies Office
C. **Solar Energy Technologies**, *Virginia Suite C*
Minh Le, Program Director for the Solar Energy Technologies Office, DOE Energy Efficiency and Renewable Energy
E. **ARPA-E**, *Virginia Suite B*
Eric Rohlfing, Acting Deputy Director for Technology, DOE ARPA-E
F. **Nuclear Energy***, Salon 3*
Monica Regalbuto, Deputy Assistant Secretary for Fuel Cycle Technologies, DOE Office of Nuclear Energy

10:50 AM **Parallel Scientific Sessions I**

A. Solar fuels and biomass, *Delaware Suite A*
B. Energy storage, *Delaware Suite B*
C. Organic photovoltaics, *Virginia Suite C*
E. Energy conservation and conversion, *Virginia Suite B*
F. Materials and chemistry for nuclear energy applications, *Salon 3*
H. Catalysis, *Virginia Suite A*

12:10 – 1:40 PM	**Lunch (buffet lunch provided)**

12:30 – 1:30 PM **“Bring Your Own Lunch” Sessions**

1. **Science Policy and Communication**, *Virginia Suite A*
   Benjamin L. Brown, Senior Science and Technology Advisor, DOE Office of Science
2. **Transitioning Science to Technology,** *Delaware Suite A*
   - Harry Atwater, Director of the Light-Material Interactions in Energy Conversion (LMI) EFRC at the California Institute of Technology
   - Gang Chen, Director of the Solid-State Solar Thermal Energy Conversion Center (S3TEC) EFRC at the Massachusetts Institute of Technology
   - Paul Mutolo, Director External Partnerships for the Energy Materials Center at Cornell (emc^2) EFRC at Cornell University
   - Dion Vlachos, Director of the Catalysis Center for Energy Innovation (CCEI) EFRC at the University of Delaware
3. **The Materials Genome Initiative**, *Delaware Suite B*
   Cyrus Wadia, Assistant Director for Clean Energy & Materials R&D, White House Office of Science and Technology Policy

1:40 PM **Parallel Scientific Sessions II**

A. Solar fuels and biomass, *Delaware Suite A*
B. Energy storage, *Delaware Suite B*
C. Organic photovoltaics, *Virginia Suite C*
E. Energy conservation and conversion, *Virginia Suite B*
F. Materials and chemistry for nuclear energy applications, *Salon 3*
G. Carbon Capture and Sequestration, *Virginia Suite A*

3:20 PM **Break**

3:40 PM **Parallel Scientific Sessions III**

A. Solar fuels and biomass, *Delaware Suite A*
B. Energy storage, *Delaware Suite B*
C. Organic photovoltaics, *Virginia Suite C*
D. Inorganic photovoltaics, *Salon 3*
E. Energy conservation and conversion, *Virginia Suite B*
H. Catalysis, *Virginia Suite A*

5:00 PM **Poster Session I, *Salon 3***

6:30 PM **Adjourn**

Agenda Day 2

Friday, July 19, 2013
8:30 AM – 12:00 PM

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

8:30 AM **Parallel Scientific Sessions IV**

A. Solar fuels and biomass, *Delaware Suite A*
B. Energy storage, *Delaware Suite B*
D. Inorganic photovoltaics, *Salon 3*
F. Materials and chemistry for nuclear energy applications, *Virginia Suite C* (ROOM CHANGE)
Ia. Predictive Theory and Modeling, *Virginia Suite A*
Ib. Predictive Theory and Modeling, *Virginia Suite B*

9:30 AM **Poster Session II and announce winners of the *Graduate Student and Postdoctoral Researcher Competition, Salon 3***

11:00 AM **Parallel Scientific Sessions V**

A. Solar fuels and biomass, *Delaware Suite A*
C. Organic photovoltaics, *Virginia Suite C*
D. Inorganic photovoltaics, *Salon 3*
G. Carbon Capture and Sequestration, *Delaware Suite B* (ROOM CHANGE)
Ia. Predictive Theory and Modeling, *Virginia Suite A*
Ib. Predictive Theory and Modeling, *Virginia Suite B*

12:00 PM **Adjourn**

2013 EFRC PI Meeting – Graphic Agenda for Thursday, July 18, 2013

		A. Solar fuels and biomass	**B. Energy storage**	**C. Organic photovoltaics**	**E. Energy conservation and conversion**	**F. Materials and Chemistry for Nuclear Energy Applications**	**H. Catalysis**
Room		*Delaware Suite A*	*Delaware Suite B*	*Virginia Suite C*	*Virginia Suite B*	*Salon 3*	*Virginia Suite A*
Chair		*Robert Stack*	*Tim Fitzsimmons*	*Mark Spitler*	*Craig Henderson*	*John Vetrano*	*Raul Miranda*
Tech Talks	**10:30**	Bioenergy Technologies	Vehicle Technologies – Energy Storage	Solar Energy Technologies	ARPA-E	Nuclear Energy	N/A
I-1	**10:50**	[**CLSF**] Yaraslova Yingling *NC State* Three Dimensional Model of a Plant Cellulose Synthase	[**MEEM**] Bruce Dunn *UCLA* Capacitive Energy Storage	[**CISSEM**] Neal R. Armstrong, Antoine Kahn *Arizona, Princeton* Energetics of Key Interfaces Relevant to Hybrid Photovoltaics	[**CES**] Mao Zheng** *UI-UC* Growth of Novel Superconductors by Atomic Layer by Layer Molecular Beam Epitaxy	[**CMSNF**] Lingfeng He $^{\#}$ *Wisconsin* Microstructural investigation of Kr and Xe irradiated UO_2	[**IACT**] Peter C. Stair *Northwestern* ALD Overcoats: A New Tool for High Performance Catalyst Design
I-2	**11:10**	[**C3Bio**] Lee Makowski *Northeastern* Molecular mechanisms of cellulose synthesis, assembly and deconstruction	[**FIRST**] Sheng Dai *ORNL* Novel Carbon Materials for Electrical Energy Storage and Catalysis	[**ANSER**] Brett Savoie** *Northwestern* Concerted Processes in Organic Photovoltaics: The Related Challenges of Generating and Collecting Charge in a Disorder Environment	[**CES**] J. C. Séamus Davis *BNL, Cornell* Iron-based Superconductors – Rosetta Stone of Room Temperature Superconductivity	[**CMIME**] Michael J Demkowicz *MIT* Creating radiation-resistant materials by tailoring interfaces	[**CALCD**] Challa S. S. R. Kumar *Louisiana State* A step towards synthesis and in situ characterization of catalysts with atomic-precision
I-3	**11:30**	[**CLSF**] Christopher Lee** *Penn State* Understanding Crystalline Cellulose Microfibrils Assembly in Plant Cell Walls Using Sum-Frequency-Generation (SFG) Vibration Spectroscopy	[**NEES**] A. Alec Talin *SNL* The Performance and Stability of Li-ion Batteries with Ultra-Thin Solid Electrolyte	[**CST**] David A. Vanden Bout *UT-Austin* Model Systems for Studying Conjugated Polymer Interactions	[**NERC**] Bartosz A. Grzybowski *Northwestern* Nanoparticle Electronics without Semiconductors	[**CDP**] Don Nicholson *ORNL* First principles and model Hamiltonians working in concert to understand defects in iron and iron based alloys	[**CME**] Monte Helm *PNNL* Rational Design of Molecular Electrocatalysts for Oxidation and Production of H_2 Using First Row Transition Metals
I-4	**11:50**	[**CLSF**] Janna Maranas *Penn State* Cellulose and Hemicellulose Structure in Plant Cell Walls	[**MEEM**] Veronica Augustyn** *UCLA* High-Rate Electrochemical Energy Storage with Nb_2O_5	[**CEEM**] Alan Heeger *UCSB* Organic Photovoltaic Device Performance	[**CES**] Peter Abbamonte *UI-UC* Materials Discovery Effort in the Center for Emergent Superconductivity	[**CMSNF**] Anter El-Azab *Purdue* Defect Disorder and Electrochemical Effects of Voids in UO_2	[**CALCD**] Gareth S. Parkinson $^{\#}$ *Vienna U. of Technology* Adsorbate induced adatom mobility in a model catalyst: Pd/Fe_3O_4

12:30 – 1:30 Bring Your Own Lunch Sessions

4. Science Policy and Communication, *Virginia Suite A*
5. Transitioning Science to Technology, *Delaware Suite A*
6. The Materials Genome Initiative, *Delaware Suite B*

** Graduate Student Finalist; # Postdoctoral Researcher Finalist

2013 EFRC PI Meeting – Graphic Agenda for Thursday, July 18, 2013

		A. Solar fuels and biomass	**B. Energy storage**	**C. Organic photovoltaics**	**E. Energy conservation and conversion**	**F. Materials and Chemistry for Nuclear Energy Applications**	**G. Carbon capture and sequestration**
Room		*Delaware Suite A*	*Delaware Suite B*	*Virginia Suite C*	*Virginia Suite B*	*Salon 3*	*Virginia Suite A*
Chair		*Mike Markowitz*	*Michael Sennett*	*Craig Henderson*	*Refik Kortan*	*Philip Wilk*	*Thiyaga P. Thiyagarajan*
II-1	**1:40**	[**CNEEC**] Joseph Montoya** *Stanford* Electrocatalysis of Total Water Splitting On Perovskite Oxides and Oxynitrides	[**CST**] Keith J. Stevenson *UT-Austin* Elucidation of Lithium-ion Coupled Electron Transfer Mechanisms at Transition Metal Phosphate Interfaces via Spectro-electrochemical Raman Experiments and Theory	[**CE**] Marc Baldo *MIT* More than one electron per photon in a solar cell	[**RMSSEC**] Vinayak P. Dravid *Northwestern* Achieving High Thermoelectric Performance in PbTe Using All-scale Hierarchical Architecture	[**MSA**] Peter C. Burns *Notre Dame* Properties of Nanoscale Uranium Cage Clusters in Aqueous Solution	[**CFSES**] Sanjay Srinivasan *UT-Austin* Emergent Behavior during CO_2 Transport within Faults – Observations based on the Crystal Geyser Analog
II-2	**2:00**	[**UNC**] Thomas J. Meyer *UNC Chapel Hill* From Catalysis to Devices	[**NECCES**] M. Stanley Whittingham *Binghamton* The LIFEPO4 Story: Theory, Experiment and Characterization	[**RPEMSC**] David Reichman *Columbia* Understanding MEG for Photovoltaic Opportunities	[**S3TEC**] Maria Luckyanova** *MIT* Coherent Phonon Heat Conduction in Superlattices	[**Efree**] Thomas C. Fitzgibbons *Penn State* Carbon Nanomaterials From High Pressure Reactions of Benzene	[**NCGC**] Jonathan B. Ajo-Franklin *LBNL* Synchrotron Observations of 3D $scCO_2$ Distribution in Reservoir Materials: Implications for Modeling & Site Characterization
II-3	**2:20**	[**BISfuel**] Dong-Kyun Seo *Arizona State* Synthetic development of nanoporous transparent conducting metal oxides and their inorganic/bio hybrids	[**emc2**] David Muller *Cornell* Operando Electron Microscopy of Energy Conversion and Energy Storage Materials	[**CE**] Shane Yost[#] *MIT* Understanding and Predicting the Singlet Fission Rate: A Combined Theoretical and Experimental Effort	[**RMSSEC**] Joseph P Heremans *Ohio State* Anharmonicity Engineering: a New Way to Reduce the Lattice Thermal Conductivity	[**MSA**] Rene Johnson** *UC Davis* Reaction Dynamics of a Nanometer-sized Uranyl Cluster in Solution	[**CFSES**] Thomas Dewers *SNL* Geomechanics of Geologic Carbon Storage: Hazards, Long-Term Sealing, and Storage Security
II-4	**2:40**	[**UNC**] John M. Papanikolas *UNC Chapel Hill* Dynamics of Chromophore-Catalyst Assemblies at Interfaces	[**HeteroFoaM**] Wilson K. S. Chiu *Connecticut* A Rapid 3-D Micro-structural Assessment Tool for the Rational Design of Complex HeteroFoaM Electrodes	[**CEN**] Mark E. Thompson *U. of Southern California* Exciton Management in Organic Photovoltaics	[**S3TEC**] Gang Chen *MIT* Probing and Engineering Phonons and Electrons Transport In nanostructured thermoelectric materials	[**CMIME**] Irene J Beyerlein *LANL* Criteria for Interfacial Stability in Bulk Nanocomposites subjected to Extreme Mechanical Strains	[**NCGC**] Shuo Zhang** *UC Berkeley* Controls on Mineralization in Volcanogenic Reservoir Rocks
II-5	**3:00**	[**PARC**] Jerilyn Timlin *SNL* Shedding Light on the Global Pigment Localization and Adaptation of Photosystems in Living Organisms	[**emc2**] Ulrich Wiesner *Cornell* Block Copolymer Directed Nanostructured Materials for Energy Conversion and Storage	[**CE**] Alan Aspuru-Guzik *Harvard* Rethinking spectroscopy - unraveling coherent exciton dynamics with ultrafast quantum process tomography	[**CSTEC**] Pramod Reddy *Michigan* Energy Dissipation in Atomic-Scale Devices	[**MSA**] Alexandra Navrotsky *UC Davis* Energetics of Complex Actinide Materials - Calorimetric and Computational Studies	[**CGS**] Zoey R. Herm** *UC Berkeley* Solid, Porous Material for Improved Efficiency of Gasoline Production and Low-Cost and Non-Toxic Enhancement of Gasoline Quality

** Graduate Student Finalist; # Postdoctoral Researcher Finalist

3:20 – 3:40 Break

		A. Solar fuels and biomass	**B. Energy storage**	**C. Organic photovoltaics**	**D. Inorganic photovoltaics**	**E. Energy conservation and conversion**	**H. Catalysis**
Room		*Delaware Suite A*	*Delaware Suite B*	*Virginia Suite C*	*Salon 3*	*Virginia Suite B*	*Virginia Suite A*
Chair		*Dawn Adin*	*Lane Wilson*	*Bonnie Gersten*	*George Maracas*	*Christopher Fecko*	*Paul Maupin*
III-1	**3:40**	[**PARC**] Robert Blankenship *Washington U.* Phycobilisomes Feed Both Photosystems in One Megacomplex in Synechocystis sp. PCC 6803, a cyanobacterium	[**NEES**] Khim Karki** *Maryland* Nano-engineering of silicon nanostructures for lithium-ion batteries and energy storage devices	[**MEEM**] Sarah Tolbert *UCLA* Control of Nanoscale Architecture in Solution-Processed Polymer-Based Photovoltaics	[**RPEMSC**] Tony F. Heinz *Columbia* Optical Properties of Novel Atomically Thin Materials	[**CEEM**] Daniel Steiauf# *UCSB* Role of Auger Recombination in the Efficiency Droop of Nitride Light Emitting Diodes	[**CCHF**] T. Brent Gunnoe *U. Virginia* Development of Well Defined Single-Site Catalysts Supported on Mesoporous Silica Nanoparticles: Application Toward Hydrocarbon Functionnalization
III-2	**4:00**	[**CABS**] Richard T. Sayre *New Mexico Consortium/LANL* Targeted Alterations in Plastoquinone Pool Size Substantially Increases Biomass Productivity in Microalgae	[**CEES**] Paul Fenter *ANL* Understanding and Controlling Silicon Lithiation	[**PHaSE**] Thomas P. Russell *UMass Amherst* Multi-length Scale Morphologies in Polymer-based Organic Photovoltaic Active Layers	[**LMI**] Bryce Sadtler# *Caltech* Phototropic Growth Control of Nanoscale Pattern Formation in Photoelectrodeposited Se – Te films	[**SSLS**] George T. Wang *SNL* Nanowires for Solid-State Lighting	[**CALCD**] John Flake *Louisiana State* Product selectivity in the electrochemical reduction of CO$_2$ at Cu electrodes
III-3	**4:20**	[**PARC**] Michelle Liberton# *Washington U.* Probing Light Harvesting and Photosynthetic Productivity in Cyanobacteria	[**NECCES**] Clare P. Grey *Stony Brook* Design and Applications of In-situ Metrologies in Chemical Energy Storage	[**CSTEC**] Jinsang Kim *Michigan* Lyotropic Liquid Crystalline Conjugated Polymer with Directed Alignment Capability for Plastic Electronics	[**CNEEC**] Mark Brongersma *Stanford* Tailoring Optical and Quantum Confinement to Enhance the Performance of PEC Devices	[**CEEM**] Claude Weisbuch *UCSB* Direct Measurement of Auger Electrons Emitted from a Semiconductor Light-Emitting Diode under Electrical Injection	[**CCHF**] John T. Groves *Princeton* Hydrocarbon Oxygenation and Halogenation with Manganese Catalysts
III-4	**4:40**	[**CABS**] Xuemin (Sam) Wang *U. Missouri, St. Louis/Donald Danforth Plant Science Center* Metabolite Sensing and Phospholipid Turnover in Seed Oil Production	[**NEES**] YuHuang Wang *Maryland* Heterostructured Si-CNT electrodes with chemically tailored interface	[**RPEMSC**] Xavier Roy# *Columbia* Nanoscale Atoms in Solid-State Chemistry	[**LMI**] Harry Atwater *Caltech* Maximizing Light Absorption in Nanostructures	[**SSLS**] Andrew M. Armstrong *SNL* Optical and Electrical Characterization of Defects in Nanoscale InGaN/GaN Heterostructures	[**IACT**] Brandon J. O'Neill** *Wisconsin* Stabilization by Atomic Layer Deposition of Copper Catalysts for Liquid Phase Reactions

5:00 – 6:30 Poster Session I (odd # posters), Salon 3

2013 EFRC PI MEETING – GRAPHIC AGENDA FOR FRIDAY, JULY 19, 2013

		A. Solar fuels and biomass	**B. Energy storage**	**D. Inorganic photovoltaics**	**F. Materials and Chemistry for Nuclear Energy Applications**	**Ia. Predictive theory and modeling**	**Ib. Predictive theory and modeling**
Room		*Delaware Suite A*	*Delaware Suite B*	*Salon 3*	*Virginia Suite C*	*Virginia Suite A*	*Virginia Suite B*
Chair		*Christopher Fecko*	*Jane Zhu*	*Mark Spitler*	*Jim Rhyne*	*Wade Sisk*	*Jim Davenport*
IV-1	**8:30**	[**CNEEC**] Xiaolin Zheng *Stanford University* Atomic-Scale Engineering of Water-Splitting Catalysts	[**CETM**] Mark Doherty *GE Global Research* Toward Molecular Electrocatalysts for Reversible Dehydrogenation-Hydrogenation of Alcohols	[**CASP**] Lance M. Wheeler** *Minnesota* Hypervalent Surface Interactions for Colloidal Stability and Doping of Silicon Nanocrystals	[**CMSNF**] Judy Pang *ORNL* Investigations of Anharmonic Phonon Properties and Thermal Transport of UO_2 by Inelastic Neutron Scattering and First-principles Simulation	[**CEFRC**] William H. Green *MIT* Predicting the Performance of Alternative Fuels	[**CID**] Romain Gautier# *Northwestern* New Ternary Materials Discovered by Inverse Design
IV-2	**8:50**	[**BISfuel**] Anne K. Jones *Arizona State* Fast and efficient hydrogen production catalysis via a bio-inspired [NiFe] coordination complex	[**CEES**] Andrew Gewirth *UI-UC* Examining the Solid Electrolyte Interphase at Li-Ion Battery Electrodes	[**CEN**] P. Daniel Dapkus *U. Southern California* Solar Cells and LEDs based on nanostructured semiconductors	[**CDP**] H. Xu *ORNL* Cascade-induced defect formation and evolution in iron: A comparison of computational and experimental results	[**IACT**] Jeffrey Greeley *Purdue* Mechanistic Analysis and Design of Heterogeneous Catalysts for Biomass Conversion	[**CMIME**] Abishek Kashinath** *MIT* Preventing helium-induced damage through interface engineering
IV-3	**9:10**	[**ANSER**] Michael Wasielewski *Northwestern* Interrogating the Photogenerated Ir(IV) State of a Water Oxidation Catalyst using Ultrafast Optical and X-ray Absorption Spectroscopy	[**NECCES**] Nicole Trease# *Stony Brook* Development of In situ Magnetic Resonance Techniques to Study Li Metal Batteries and Supercapacitors in Real Time	[**CASP**] Victor I. Klimov *LANL* Making the Most of a Solar Photon: Semiconductor Nanocrystals and Solar Energy Conversion	[**Efree**] Malcolm Guthrie *Carnegie Institution of Washington* High Pressure Neutron Diffraction With Diamonds	[**CEFRC**] Jacqueline H. Chen *SNL* High-Fidelity Simulations of Turbulence-Chemistry Interactions Towards Predictive Models for Energy Conversion Devices with Alternative Fuels	[**CID**] Alex Zunger *U. Colorado* Predictive Theory and Modeling of New Materials and New Functionalities via Inverse Design

9:30 – 11:00 Poster Session II (even # posters), Salon 3
10:30 Announce winners of the *Graduate Student and Postdoctoral Researcher Competition*

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

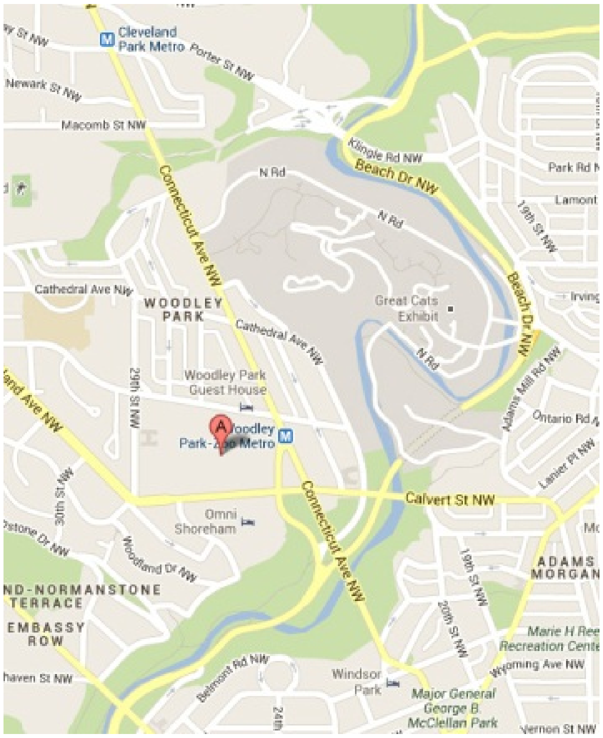
2013 EFRC PI MEETING – GRAPHIC AGENDA FOR FRIDAY, JULY 19, 2013

		A. Solar fuels and biomass	**C. Organic photovoltaics**	**D. Inorganic photovoltaics**	**G. Carbon capture and sequestration**	**Ia. Predictive theory and modeling**	**Ib. Predictive theory and modeling**
Room		*Delaware Suite A*	*Virginia Suite C*	*Salon 3*	*Delaware Suite B*	*Virginia Suite A*	*Virginia Suite B*
Chair		*Jeffrey Krause*	*Gregory Fiechtner*	*Christopher Fecko*	*Larry Rahn*	*Mark Pederson*	*Robin Hayes*
V-1	**11:00**	[**CCEI**] Dion G. Vlachos *Delaware* Transformation of Aldose Sugars to Platform Furans using $CrCl_3$ with HCl in Aqueous Media	[**CISSEM**] Jeanne E. Pemberton, David S. Ginger *Arizona, U. Washington* The Science Behind Molecular Interface Modifiers: From Molecular Structure to Solar Cell Performance	[**CASP**] Joseph M. Luther *NREL* Recent Progress in Quantum-Dot Solar Cells: Achieving Quantum Efficiencies Greater than Unity	[**CGS**] Wendy L. Queen *LBNL* Drawing Correlations Between Structure and Gas-Adsorption/ Separation Properties of Metal-Organic Frameworks	[**NERC**] Sharon Glotzer *Michigan* Emergent phenomena in driven systems of active colloids	[**S3TEC**] Marin Soljacic *MIT* Nanophotonics for energy-conversion applications
V-2	**11:20**	[**C3Bio**] Hilkka I. Kenttämaa *Purdue* Exploring the mechanisms of fast pyrolysis of cellulose by pyroprobe/ tandem mass spectrometry, isotope labeling, model compound studies and quantum chemical calculations	[**ANSER**] Tobin Marks *Northwestern* Interface Science of Organic Photovoltaics	[**CID**] David Ginley *NREL* Combining Theory and Experiment to Understand Optical Properties and Carrier Generation in P-Type Oxides	[**NCGC**] Andrew G. Stack *ORNL* Upscaling Carbonate Mineral Growth Rates from the Nano- to Pore-Scales	[**CETM**] Ingolf Warnke *Yale* Electronic Structure in the CETM-EFRC: Towards a Fundamental Understanding of Electrocatalytic (De-) Hydrogenation	[**HeteroFoaM**] Andreas Heyden *U. South Carolina* Design and Discovery of Novel Electrode Materials for Solid Oxide Fuel Cells
V-3	**11:40**	[**CCEI**] Jacob S. Kruger *Delaware* Elucidating the Roles of an H-BEA Zeolite in Aqueous-Phase Fructose Dehydration	[**PHaSE**] Todd Emrick *UMass Amherst* Functional Conjugated Polymers: Organized Nanocomposites and Interlayer Materials	[**LMI**] Paul Alivisatos *LBNL* Luminescent Concentration with Semiconductor Quantum Rods	[**CGS**] Berend Smit *UC Berkeley* Computational Approaches in Gas Separation	[**CME**] Simone Raugei *PNNL* First-Principles Design of Electrocatalysts for Energy Storage and Production: H_2 Oxidation and H_2 Production	[**FIRST**] Paul R.C. Kent *ORNL* Experimentally guided model development and predictive theory in the FIRST Center

12:00 **Adjourn**

Talk ID: Letter of Technical Session – Session Block – Number
(e.g. B-I-1 is an Energy Storage talk on Thursday at 10:50 am in Delaware Suite B)

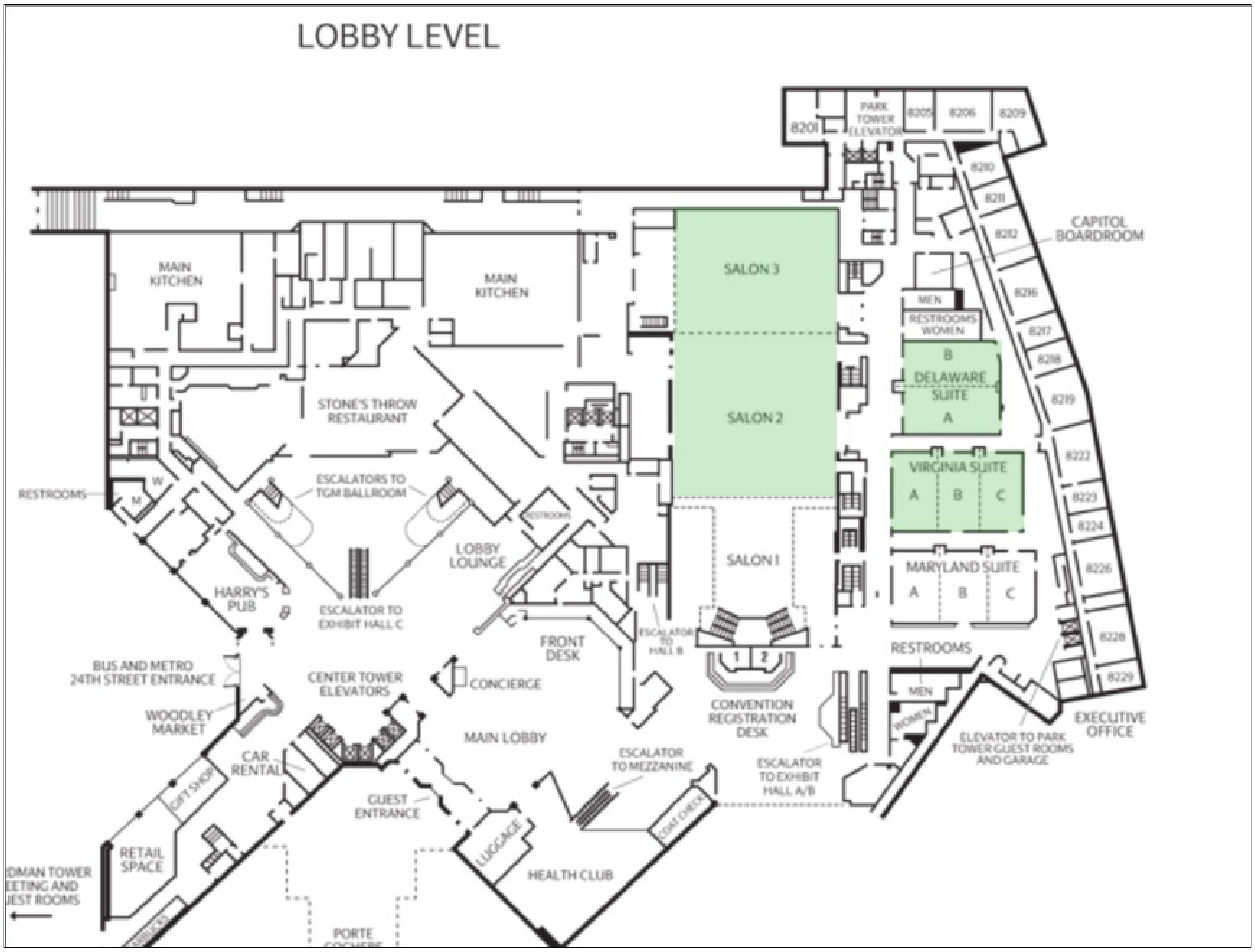
Poster ID: P – Letter of Technical Session – Number
(e.g. P-C-1 is an Organic Photovoltaics poster on Thursday at 5:00 – 6:30 pm)



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:
Salon 2, Salon 3
Delaware Suite A and B
Virginia Suite A, B, and C



Talk Abstracts

A. SOLAR FUELS AND BIOMASS

Session I: Thursday, July 18, 2013, 10:30 – 12:10; Delaware Suite A

10:50 AM

A-I-1: THREE DIMENSIONAL MODEL OF A PLANT CELLULOSE SYNTHASE

[CLSF] L. Sethaphong[1], C. H. Haigler[2], J. D. Kubicki[3], J. Zimmer[4], Yaraslava G. Yingling[1]

[1]Department of Materials Science and Engineering and [2]Department of Plant Biology, North Carolina State University; [3]Deparment of Geosciences, Pennsylvania State University; [4]School of Medicine, University of Virginia

Cellulose fibrils within plant cell walls provide the foundation for plant structure and are renewable biomaterials that account for most of the world's biomass. A three-dimensional model of a plant cellulose synthase (CESA) has remained elusive despite over forty years of experimental effort. Here the computational prediction of an all-atom structure of cellulose synthase will be described. All CESA models possess a conserved catalytic region which contains a ß-sheet and conserved amino acid motifs similar to those required for catalysis in other GT-2 glycosyltransferases (i.e. DD, DCD, ED, and QVLRW). Most interestingly, plant specific modules (termed the 'plant conserved region', P-CR, and the 'class specific region', CSR) folded into distinct subdomains remote from the catalytic region; their locations suggest that they might be involved with CESA oligomerization to form the larger 28-nm cellulose synthesis complex seen in plant membranes. The modeling of P-CR and CSR regions from Arabidopsis indicated that the P-CR region is a candidate for intermolecular protein-protein interactions while CSR may be responsible for CESA insertion and positioning within the cellulose synthesis complex. The comparison of our model with the recently determined crystal structure of a bacterial cellulose synthase indicated important differences and similarities. Differences in the trans-membrane region imply fundamentally distinct mechanisms for organizing the glucan chain, while the essential structures for the catalytic polymerization of cellulose seem conserved within prokaryotes and eukaryotes. Looking to the future, the predicted tertiary structure provides a platform for the biochemical engineering of plant CESAs.

11:10 AM

A-I-2: MOLECULAR MECHANISMS OF CELLULOSE SYNTHESIS, ASSEMBLY AND DECONSTRUCTION

[C3Bio] Bryon S. Donohoe[1], Peter N. Ciesielski[1], James F. Mathews[1], Michael F. Crowley[1], Michael E. Himmel[1], Melvin P. Tucker[1], Hideyo Inouye[2], Jiliang Liu[2], Yan Zhang[2], Anna T. Olek[3], Catherine J. Rayon[3], Nicholas C. Carpita[3], and Lee Makowski[2]

[1]National Renewable Energy Laboratory, Golden, C; [2]Department of Electrical & Computer Engineering, Northeastern University, Boston, M; [3]Department of Botany and Plant Pathology, Purdue University, West Lafayette, IN

The structure of the cellulose microfibril, its size, crystallinity and potential aggregation in macrofibrils in plant cell walls, is a major factor in its recalcitrance to deconstruction. We study molecular mechanisms of cellulose synthesis and assembly in order to gain control over microfibril structure and properties together with the development of catalytic deoxygenation chemistry and selective bond breaking to enable efficient transformations of polysaccharides to useful products. An extensive array of tools for simulation, imaging and analysis has been applied to map the evolution of nanoscale and mesoscale architecture that occurs during treatment of biomass with iron catalysts. Structural studies of corn stover over length scales from microns to Ångstroms indicate that cellulose fibrils follow one of two pathways during treatment with iron ions: (i) Disintegration through slippage of molecular sheets in the crystalline cellulose fibrils generates amorphous fragments with sufficient flexibility that their glycosidic bonds become susceptible to hydrolytic attack. (ii) Twisting of intact fibrils released from the cell wall matrix by cleavage of hemicellulosic cross-links. Significantly, the twisted fibrils cannot undergo planar slippage that appears to be an obligate first step in deconstruction. These results suggest strategies for modification of microfibril structure by genetic control of the biosynthetic apparatus. Small-angle (SAXS) and wide-angle (WAXS) x-ray scattering studies have provided the first snapshot of the 3-D contour structure of a cellulose synthase catalytic domain and evidence for dimerization of the two-domain structure of the protein tail-to-tail to form the fundamental functional unit of synthesis.

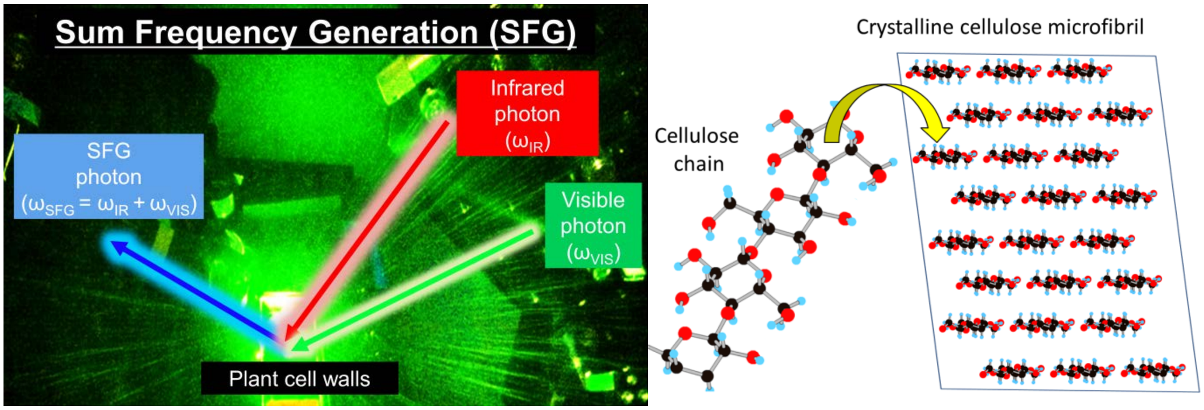
11:30 AM - Graduate Student Finalist

A-I-3: UNDERSTANDING CRYSTALLINE CELLULOSE MICROFIBRILS ASSEMBLY IN PLANT CELL WALLS USING SUM-FREQUENCY-GENERATION (SFG) VIBRATION SPECTROSCOPY

[CLSF] Christopher M. Lee[1], Kabindra Kafle[1], Yong Bum Park[2], James D. Kubicki[3], Daniel Cosgrove[2], Candace Haigler[4] and Seong H. Kim[1]

Departments of [1] Chemical Engineering, [2]Biology, and [3]Geosciences, Pennsylvania State University. [4]Department of Crop Science and Plant Biology, North Carolina State University

Plant cell walls constitute the most abundant biomass usable for production of chemicals and transportation fuels, but they are highly recalcitrant to biochemical transformation processes. This is in part due to the crystalline nature of cellulose and its interactions with other matrix polymers in cell walls. The organization or assembly of crystalline cellulose with matrix polymers also varies depending on developmental stages of the plant as well as plant species. Thus, understanding the crystalline structure and hierarchical organization of cellulose in plant cell walls could greatly advance science-based efforts to economical transportation fuels from biorenewable sources. We use sum-frequency-generation (SFG) vibration spectroscopy to probe crystalline cellulose in intact cell walls and provide the structural information of cellulose microfibril arrangements over a length scale of 100s of nm. In this talk, we show the changes in cellulose ordering in intact young (primary) and mature (secondary) plant cell walls from *A. thaliana* and *G. hirsutum* (cotton). The SFG analysis of these plant samples revealed that crystalline cellulose microfibrils are organized differently in plant cell walls at different growth stages. When the samples were treated by standard methods of purify cellulose from plant cell walls, which has been the main approach for structural analysis of cellulose in biomass, cellulose organization in the wall was disturbed. Thus, SFG offers unprecedented opportunity to reveal important organizational features of cellulose within cell walls at different developmental stages and in lignocellulosic biomass harvested from different sources and pretreated for more efficient biochemical conversion to sugars and other chemicals.



Images: SFG signals generated by plant cell walls is based upon spectral addition (left) occurring in ordered arrangements of crystalline cellulose microfibrils (right).

11:50 AM

A-I-4 - CELLULOSE AND HEMICELLULOSE STRUCTURE IN PLANT CELL WALLS

[CLSF] Shih-Chun Huang[1], Yong Bum Park[2], Tian Zhang[3], Daniel J. Cosgrove[2], Janna K. Maranas[1]
[1]Department of Chemical Engineering, [2]Department of Biology, [3]Cell & Developmental Biology Graduate Program, Pennsylvania State University

Hemicelluloses are important structural components of plant cell walls, but their nanoscale distribution and conformation are unknown. Measurement of hemicellulose conformation by scattering methods is challenging because the atomic compositions of hemicellulose and cellulose are similar. We provide the missing conformational information using small angle neutron scattering in combination with D_2O contrast matching. Measurements were made with depectinated, primary walls of wildtype and xyloglucan-deficient [*xxt1xxt2*] *Arabidopsis thaliana*, with cellulose and hemicellulose highlighted in different samples. The cellulose microfibril diameter of ~3 nm and microfibril spacing [20-40 nm in wildtype] are consistent with available data. Interfibril spacing in the mutant is wider [10-70 nm], which we interpret as the formation of loose bundles lacking preferential orientation relative to one another, an interpretation supported by atomic force microscopy. Hemicellulose (primarily xyloglucan) in wildtype forms extended coils and short [49 nm] coatings on microfibrils. One third of the xyloglucan is in this configuration, coating 16-35% of the cellulose surface. A recent study concluded that only a tiny fraction of the xyloglucan contributes to wall biomechanics [Plant Physiology 158:1933]. We suggest that the xyloglucan-mediated strength arises from tight contact between two coated microfibrils; we estimate 0.64-3.1% of the xyloglucan to be in this configuration, assuming random contact of microfibrils. Negligible coating is observed in the mutant, consistent with its reduced mechanical strength and absence of xyloglucan connectors.

Session II: Thursday, July 18, 2013, 1:40 – 3:20; Delaware Suite A

1:40 PM – Graduate Student Finalist

A-II-1: ELECTROCATALYSIS OF TOTAL WATER SPLITTING ON PEROVSKITE OXIDES AND OXYNITRIDES

[CNEEC] Joseph H. Montoya[1], Aleksandra Vojvodic[2], Jens K. Norskov[1,2]
[1]Department of Chemical Engineering, Stanford University, Stanford, CA 94305; [2]SLAC National Accelerator Laboratory, 2575 Sand Hill Rd, Menlo Park, CA 94025

Perovskite oxides and oxynitrides have recently been the subject of multiple screening studies to determine which materials have bandstructures conducive to overall water splitting [1,2]. However, such screening studies neglect the effect of kinetic overpotentials for oxygen evolution (OER) and hydrogen evolution (HER). In the present work, we use density functional theory (DFT) calculations to describe the limiting potentials for both OER and HER on various perovskite materials. From our results, we derive scaling relations for the binding energies of H_2O oxidation intermediates that are compatible with well-established theoretical descriptions of oxide materials for OER [3]. Using this approach, we comment on the stability and surface structure of perovskites in the electrochemical environment. Most importantly, we demonstrate that perovskite photoelectrocatalysts with bandgaps suitable for total water splitting may have kinetic limitations that make co-catalysts necessary, as shown in Figure 1. We also determine the theoretical overpotentials of a larger dataset of perovskite compounds for both OER and HER in order to identify trends in activity for these electrodes in water splitting devices.

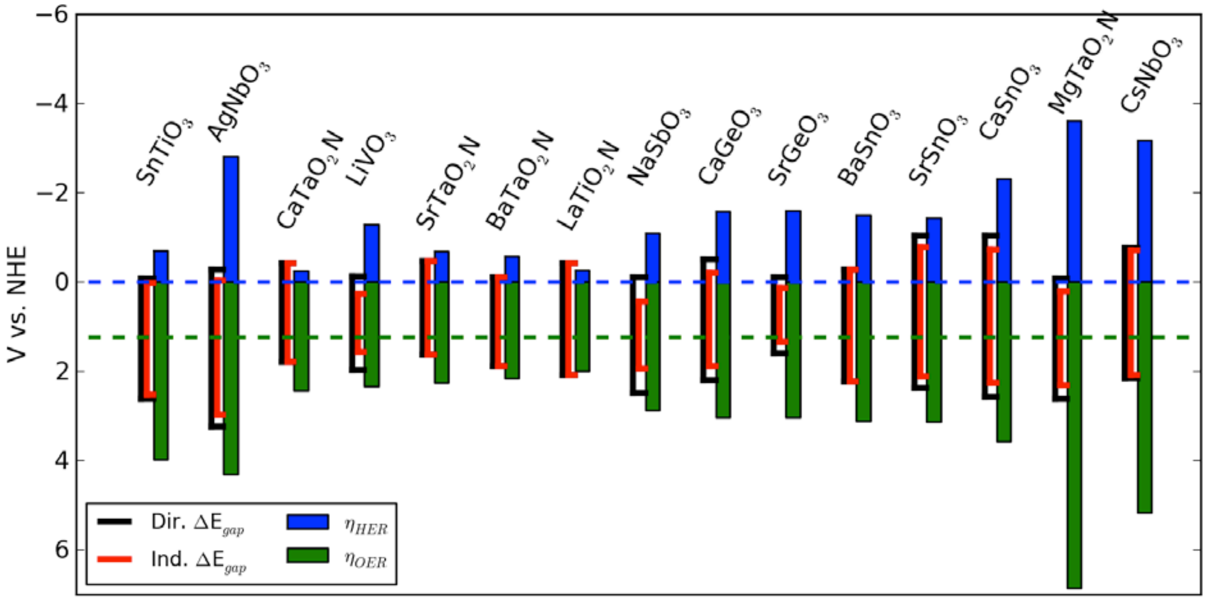


Figure 1 - Theoretical overpotentials and bandgaps for HER and OER on screened materials [1]

[1] I. E. Castelli, T. Olsen, S. Datta, D. D. Landis, S. Dahl, K. S. Thygesen, K. W. Jacobsen, (2012). *Energy Env Sci*, *5*(2), 5814-5819.

[2] Y. Wu, P. Lazic, G. Hautier, K. Persson, G. Ceder, (2013). *Energy Env Sci*, *6*(1), 157-168.

[3] I. C. Man, H. Y. Su, F. Calle-Vallejo, H. A. Hansen, J. I. Martinez, N. G. Inoglu, J. Kitchin, T. F. Jaramillo, J. K. Nørskov, J. Rossmeisl, *ChemCatChem, 3*(7), 1159-1165

2:00 PM

A-II-2: FROM CATALYSIS TO DEVICES

[UNC] Thomas J. Meyer[1], Javier J. Concepcion[1], Robert A. Binstead[1], Michael R. Norris[1], MingTian Zhang[1], Aaron K. Vannucci[1], Maurice S. Brookhart[1], Peng Kang[1], Zuofeng Chen[2].

[1] *Department of Chemistry, University of North Carolina at Chapel Hill, Chapel Hill, NC 27599-3290*

Dye Sensitized Photoelectrosynthesis Cells (DSPEC) offer a hybrid approach to Artificial Photosynthesis and solar fuels, combining important elements of semiconductor devices with molecular assemblies for integrated light absorption and catalysis. Catalysis of the multi-electron/multi-proton half-reactions for water oxidation or water/carbon dioxide reduction at sufficient rates and adequate longevity is a formidable challenge, but significant progress has been made in the UNC EFRC. In water oxidation, a family of single site polypyridyl Ru complexes has been investigated, both in solution and, as phosphonic acid derivatives, on the surfaces of transparent conducting oxides and oxide semiconductors. In acidic solution, surface bound catalysts have been shown to undergo water oxidation with pH dependent rates, with high Faradaic efficiencies through 1,000's of turnovers without decomposition. Water oxidation reactivity has been extended to a family of chromophore-catalyst assemblies linked chemically, in oligoproline assemblies, to assemblies prepared by a layer-by-layer procedure, to complexes of Cu(II), and to fluoride-doped tin oxide surfaces doped with Co(II) by solution-surface exchange. In a recent extension, solar water oxidation is being investigated in a chemically linked assembly on TiO_2 in a core shell configuration.

Electrocatalytic reduction of carbon dioxide to CO and formate has also been investigated, based on a series of polypyridyl complexes of Ru for reduction to CO, and Ir pincer catalysts for reduction to formate. A single site Ru catalyst has been shown to catalyze both water oxidation and CO_2 reduction, and a water soluble Ir pincer complex catalyzes reduction of CO_2 selectively to formate in water.

2:20 PM

A-II-3: SYNTHETIC DEVELOPMENT OF NANOPOROUS TRANSPARENT CONDUCTING METAL OXIDES AND THEIR INORGANIC/BIO HYBRIDS

[BISFuel] Alex Volosin, Daniel Mieritz, Barun Das, Sudhanshu Sharma, Dominik Schmidt, Dong-Kyun Seo
Department of Chemistry and Biochemistry, Center for Bio-Inspired Solar Fuel Production Arizona State University, Tempe, AZ 85287-1604, USA

Nanoporous transparent conducting oxides (TCOs) can be fabricated as high surface-area electrodes, which are one critical component of photoelectrochemical devices that convert sunlight into electrical or chemical energy. The accessible nanopores and high surface areas of these materials are important for achieving a high loading of desired electroactive species directly onto the electrode surface while maintaining a high crystallinity of the metal oxides for efficient electron transport throughout the material. However, it has been quite challenging to produce high-porosity high surface-area TCO materials while maintaining the electrical conductivity and optical transparency. A synthetic method is presented for the production of nanoporous particles and thin films of the TCOs which is based on a sol-gel method modified to induce a sequential formation of interpenetrating inorganic and organic networks. Nanoporous antimony-doped tin oxide (ATO) coatings with high surface area, optical transparency and good electron transport properties have been prepared using the new method. Biological molecules such as self-assembled DNA structures, cytochrome-*c* protein and customized peptide catalysts have been successfully incorporated into the nanopores of the ATO film, and their stability and (photo)electrochemical activity have been successfully demonstrated. Further studies have indicated that the synthetic method can be extended to produce other important TCOs such as tin oxide (SnO_2), zirconium-doped titanium oxide ($Ti_{1-x}Zr_xO_2$) and the *p*-type semiconductor $CuAlO_2$ in desirable nanoporous forms.

2:40 PM

A-II-4: DYNAMICS OF CHROMOPHORE-CATALYST ASSEMBLIES AT INTERFACES

[UNC] John M. Papanikolas[1], Stephanie E. Bettis, Li Wang, Erik M. Grumstrup, Robert J. Brown, Zachary A. Morseth, Stephen A. Miller, Paul G. Giokas, Ian J. McNeil, Robin R. Knauf, M. Kyle Brennaman, Kenneth Hanson, Dennis L. Ashford, Michael R. Norris, Derek M. Ryan, Marcey L. Waters, Christopher J. Fecko, Jillian L. Dempsey, Andrew M. Moran, Thomas J. Meyer
[1] *Department of Chemistry, University of North Carolina at Chapel Hill, Chapel Hill, NC 27599-3290*

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 interfacial electron transfer dynamics that take place following the photoexcitation of chromophore-catalyst assemblies anchored to TiO_2. Three different architectures have been examined with chromophores and catalyst chemically linked, both bound to a peptide scaffold, and by a layer-by-layer technique. Transient spectroscopy provides a detailed picture of

the dynamic processes that underpin the initial photoactivation of the water oxidation catalyst. In particular, metal-to-ligand charge transfer (MLCT) excitation of a Ru(II) chromophore is followed by efficient electron injection into the TiO_2 on time scales ranging from tens of femtoseconds to hundreds of picoseconds. Injection is followed by electron transfer from the catalyst to the oxidized chromophore on the picosecond time scale. Once formed, the photo-oxidized catalyst is reduced by back electron transfer from the surface on the microsecond to millisecond timescale.

3:00 PM

A-II-5: SHEDDING LIGHT ON THE GLOBAL PIGMENT LOCALIZATION AND ADAPTATION OF PHOTOSYSTEMS IN LIVING ORGANISMS

[PARC] Aaron M. Collins[1], Michelle Liberton[2], Sangeeta Negi[3], Volker Urban[4], Hugh O'Neill[4], Brad O'Dell[4], Richard Sayre[3,5], Himadri B. Pakrasi[2], Jerilyn A. Timlin[1]

[1]Department of Bioenergy and Defense Technologies, Sandia National Laboratories, Albuquerque, NM; [2]Department of Biology, Washington University in St. Louis, St. Louis, MO; [3]New Mexico Consortium, Los Alamos, NM; [4]Oak Ridge National Laboratory, Oak Ridge, TN; [5]Los Alamos National Laboratory, Los Alamos, NM

The structure and function of the individual constituents of the light-harvesting antenna and two photosystems oxygenic phototrophs are well known for some organisms however, how these complexes are globally organized and distributed within the thylakoid membranes is not known in detail. Here, we present hyperspectral confocal fluorescence microscopy coupled with multivariate spectral image analysis as an enabling technology to investigate the organisms-wide distribution of pigments among several diverse photosynthetic organisms. Our results reveal a reoccurring theme of global pigment heterogeneity and dynamic adaptation under light-limiting conditions unattainable with other methods. When complemented with electron microscopy and small angle neutron scattering, this work provides a more complete picture of the flexibility photosynthetic organisms have to alter light harvesting in response to changes in environmental conditions.

Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

Session III: Thursday, July 18, 2013, 3:40 – 5:00; Delaware Suite A

3:40 PM

A-III-1: PHYCOBILISOMES FEED BOTH PHOTOSYSTEMS IN ONE MEGACOMPLEX IN *SYNECHOCYSTIS* SP. PCC 6803, A CYANOBACTERIUM

[PARC] Haijun Liu[1,2], Hao Zhang[2,3], Dariusz Niedzwiedzki[2,3], Mindy Prado[1,2], Michael L. Gross[3], Robert E. Blankenship[1,2,3]

[1]Department of Biology, Washington University in St. Louis, St. Louis, MO 63130; [2]Photosynthetic Antenna Research Center, Washington University in St. Louis, St. Louis, MO 63130; [3]Department of Chemistry, Washington University in St. Louis, St. Louis, MO 63130

In photosynthetic organisms, photons are harvested by light harvesting complexes and transferred to reaction centers where photochemistry takes place, leading to long-term energy storage. We have isolated and characterized a megacomplex composed of a phycobilisome (PBS) and its energy acceptors, Photosystem II (PSII) and Photosystem I (PSI) in the cyanobacterium *Synechocystis*

PCC6803. The two terminal energy emitters of the PBS, ApcE and ApcD, are closely associated with components of PSII and PSI respectively. The PBS core fully covers PSII, but only overlaps partially with PSI. Time-resolved spectroscopy indicated efficient energy transfer between the PBS and two photosystems in the megacomplex. The structural information on the proteins and cofactors and their interactions within the megacomplex provides a basis for understanding how phycobilisomes transmit excitation energy to reaction centers and how the energy balance of two photosystems is achieved, to adapt organisms to varying ecophysiological conditions and operate at maximum efficiency.

4:00 PM

A-III-2: TARGETED ALTERATIONS IN PLASTOQUINONE POOL SIZE SUBSTANTIALLY INCREASES BIOMASS PRODUCTIVITY IN MICROALGAE

[CABS] Sowmya Subramanian[1], Kelly M Gillespie[2], Ellen Marsh[2], Edgar B. Cahoon[3] and Richard T. Sayre[1]
[1]New Mexico Consortium/Los Alamos National Laboratory, 4200 W Jemez Rd, Los Alamos, NM 87544, USA; [2]Donald Danforth Plant Science Center, 975 N Warson Road, St. Louis, MO 63132, USA;
[3]Department of Biochemistry at University of Nebraska-Lincoln, Lincoln, NE 68588, USA.

Improving biomass production is one of the many approaches crucial to the development of economical and environmentally sustainable biofuels. One of the bottlenecks in the efficient conversion of sunlight into chemical energy is the oxidation of reduced plastoquinone (PQ) by the cytochrome b_6f complex. PQH_2 oxidation is the rate-limiting step in photosynthetic electron transfer. We hypothesized that buffering the fast rate of PQ reduction and slow rate of PQH_2 oxidation by increasing the PQ pool size would improve photosynthetic efficiency and reduce photoinhibition. To accomplish this goal, we have engineered transgenic algae to over-express in plastids enzymes in the plastoquinone biosynthetic pathway that may be limiting including: yeast Prephenate dehydrogenase (PDH) and *A. thaliana* Homogentisate solanesyltransferase (HST). PDH converts prephenate directly into homogentisate circumventing competing endogenous reactions for tyrosine synthesis, while HST catalyzes the prenylation of homogentisate with solanesyl diphosphate, and subsequent decarboxylation. Preliminary chlorophyll fluorescence kinetics analyses indicate that the transgenics expressing PDH and HST genes exhibit lower F_0 values due to non-photochemical quenching and accelerated quinone reduction kinetics due to increased PQ reduction at the Q_B site of photosystem II, consistent with an increased PQ pool size. Significantly, the PDH transgenics have substantially enhanced growth rates and accumulate 5-fold more biomass than wild-type algae when grown in fluctuating light conditions. These results will be discussed in the context of possible mechanisms by which elevated PQ levels could impact biomass productivity.

4:20 PM – Postdoctoral Researcher Finalist

A-III-3: PROBING LIGHT HARVESTING AND PHOTOSYNTHETIC PRODUCTIVITY IN CYANOBACTERIA

[PARC] Michelle Liberton[1], Lawrence Page[1*], Aaron M. Collins[2], William B. O'Dell[3], Hugh O'Neill[3], Volker S. Urban[3], Jerilyn A. Timlin[2], and Himadri B. Pakrasi[1]
[1]Department of Biology, Washington University, St. Louis, MO 63130; [2]Department of Bioenergy and Defense Technologies, Sandia National Laboratories, Albuquerque, NM 87185; [3]Biology and Soft Matter Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831
**Current address: Terra Biologics, St. Louis, MO 63132*

Photosynthetic antenna systems function in the process of converting sunlight into cellular fuel, a topic of considerable interest in bioenergy research. In the cyanobacterium *Synechocystis* sp. PCC 6803, light harvesting is accomplished by a combination of membrane intrinsic pigment-proteins and large extrinsic

phycobilisome complexes. The phycobilisomes associate with the cytoplasmic surface of thylakoid membranes, and studies have shown that modulation of phycobilisome size results in changes to the membrane spacing (1). We have used a combination of approaches to explore the consequences of antenna modification in terms of physiology and membrane morphology and dynamics in wild-type *Synechocystis* 6803 and a series of mutants with varying degrees of phycobilisome truncation. Our work using transmission electron microscopy (TEM), hyperspectral confocal fluorescence microscopy (HCFM), small angle neutron scattering (SANS), and an optimized photobioreactor system have revealed the adaptive strategies that cells employ to compensate for antenna reduction. As the phycobilisome antenna was truncated, large-scale changes in thylakoid morphology were observed, accompanied by increased physical segregation of the two photosystems (2). Repeating distances between thylakoid membranes measured by SANS were correlated with TEM data, and corresponded to the degree of phycobilisome truncation (3). We found that cyanobacterial membranes have a high degree of structural flexibility, and that changes in the membrane system upon illumination are rapid and reversible (3). Phycobilisome truncation in *Synechocystis* 6803 did not confer an advantage in growth or biomass accumulation, in contrast to predictions from algal models (4). These results highlight the dynamic nature of the intracellular membrane system in cyanobacterial cells and suggest an adaptive strategy that allows cells to compensate for decreased light harvesting capability.

(1) Olive J, Ajlani G, Astier C, Recouvreur M, Vernotte C. (1997) Biochim Biophys Acta 1319: 275–282.
(2) Collins AM, Liberton M, Jones HD, Garcia OF, Pakrasi HB, Timlin JA. (2012) Plant Physiol 158: 1600-09.
(3) Liberton M, Page LE, O'Dell WB, O'Neill H, Urban VS, Pakrasi HB. (2013) J Biol Chem 288: 3632-40.
(4) Page LE, Liberton M, Pakrasi HB. (2012) Appl Environ Microbiol: 78: 6349-51.

This material is based upon work supported as part of the Photosynthetic Antenna Research Center (PARC), 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-SC 0001035. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000. The Bio-SANS instrument is a resource of the Center for Structural Molecular Biology at Oak Ridge National Laboratory that is supported by the U.S. Department of Energy, Office of Science, Office of Biological and Environmental Research Project ERKP291. Bio-SANS is located at the Oak Ridge National Laboratory's High Flux Isotope Reactor. The neutron source is sponsored by the Scientific User Facilities Division, Office of Basic Energy Sciences, U.S. Department of Energy.

4:40 PM

A-III-4: METABOLITE SENSING AND PHOSPHOLIPID TURNOVER IN SEED OIL PRODUCTION

[CABS] Sangchul Kim[1,2], Maoyin Li[1,2], Liang Guo[1,2], Yu Liu[1,2], Jia Li[2], Jan Jaworski[2], Xuemin Wang[1,2]
[1]Department of Biology, University of Missouri-St. Louis, MO 63121, USA; [2]Donald Danforth Plant Science Center, St. Louis, MO 63132, USA.

Phospholipids play pivotal roles in triacylglycerol (TAG) biosynthesis and accumulation. The most common phospholipid phosphatidylcholine (PC) serves as a substrate for fatty acid desaturation and other modifications and can also provide diacylglycerol (DAG) directly for TAG synthesis. The simplest, minor phopsholipid phosphatidic acid (PA) provides DAG for PC and TAG biosynthesis. PA also plays a role in acyl trafficking from the endoplasmic reticulum to plastids, where TAG and fatty acids are produced. Furthermore, PA is a class of important mediators in cell signaling and metabolic regulation. PA binds to transcriptional factors and central metabolic enzymes and such interaction

serves to coordinate and modulate lipid and carbohydrate metabolism. The turnover of PC by phospholipases affects the production of PA, lipid metabolism, and TAG accumulation. The results suggest two new mechanisms of cellular regulation of lipid metabolism and novel avenues to improve storage lipid production.

Session IV: Friday, July 19, 2013, 8:30 – 9:30

8:30 AM

A-IV-1: ATOMIC-SCALE ENGINEERING OF WATER SPLITTING CATALYSTS

[CNEEC] Stacey Bent[1], Bruce Clemens[2], Arthur Grossman[3], Thomas Jaramillo[1], Jens Norskov[1], Friedrich Prinz[4], Robert Sinclair[2], and Xiaolin Zheng[4]

[1]Department of Chemical Engineering, Stanford University, California 94305, United States; [2]Department of Materials Science and Engineering, Stanford University, California 94305, United States; [3]Carnegie Institute, Stanford University, California 94305, United States; [4]Department of Mechanical Engineering, Stanford University, California 94305, United States

A major effort in CNEEC is focused on a critical aspect of solar fuels science: developing active, stable, non-precious metal catalysts for the hydrogen evolution reaction (HER) and the oxygen evolution reaction (OER). This presentation will describe our accomplishments with emphasis on theory-based catalyst design. We utilize electronic structure calculations to guide the development of promising catalysts and concepts. With theory as the basis, we synthesize candidate materials with atomic-scale control and study their functionality for the HER and OER. Advanced microscopy and spectroscopy are crucial in this endeavor, as we have shown that nanostructured features play a significant role in catalysis. The talk will focus on MoS_2 nanomaterials for the HER and metal oxide nanomaterials for the OER. Some of these catalysts developed within CNEEC are among the most active and most stable non-precious metal catalysts ever reported.

More recently, we have been integrating these materials with commonly known semiconductors (e.g. silicon and $BiVO_4$) to produce working photocathodes and photoanodes. Preliminary work is underway to further integrate the HER catalysts developed in this project with the advanced semiconductor systems currently under development in at CNEEC. As the photocathodes developed in this project are rapidly approaching theoretical limits, our future goals will be more centered on photocathode development both in terms of OER catalysis and photoanodic semiconductors. The ultimate long-term goal of CNEEC is the pairing of appropriate photocathodes with photoanodes to produce a system capable of unassisted water-splitting that is stable and efficient.

8:50 AM

A-IV-2: FAST AND EFFICIENT HYDROGEN PRODUCTION CATALYSIS VIA A BIO-INSPIRED [NIFE] COORDINATION COMPLEX

[BISFuel] Lu Gan[1,2], Souvik Roy[1,2], Thomas L. Groy[1], Anne K. Jones[1,2]

[1]Department of Chemistry and Biochemistry, [2]Center for Bio-Inspired Solar Fuel Production, Arizona State University, Tempe, Arizona 85287

The primary barrier to wide scale electrocatalytic production of hydrogen from water is development of efficient catalysts for this transformation using only abundant transition metals. Although the biological catalysts for hydrogen production, hydrogenases, use only the first row transition metals nickel and iron, no functional models of these enzymes match their exquisite

combination of high turnover frequencies and low activation energies. Here we report characterization of a functional model of [NiFe]-hydrogenases, the complex [Ni(bdt)(dppf)] for bdt=1,2-benzenedithiol and dppf=1,1’-Bis(diphenylphosphino)ferrocene. This [NiFe] complex reduces protons at high efficiency with fast rates (1240 s^{-1}). The catalytic properties of this complex are better than those of any other synthetic [NiFe] complex reported to date despite the fact that many of the chemical features largely thought to be essential for effective catalysis are not present in this compound. The properties of this complex will be compared to other novel models including redox non-innocent ligands, and the mechanism of catalysis by this complex will be considered.

9:10 AM

A-IV-3: Interrogating the Photogenerated Ir(IV) State of a Water Oxidation Catalyst using Ultrafast Optical and X-ray Absorption Spectroscopy

[ANSER] Michael T. Vagnini[1], Michael W. Mara[1,2], Michael R. Harpham[2], Jier Huang[2], Megan L. Shelby[1,2], Lin X. Chen[1,2], and Michael R. Wasielewski[1]
[1]Northwestern University, [2]Argonne National Laboratory

Photodriven molecular water oxidation catalysts for fuel formation requires understanding the single electron transfer events involved in catalyst activation. In an effort to photogenerate and characterize the highly reactive Ir(IV) state of the Ir(III)-based water oxidation catalyst Cp*Ir(ppy)Cl (ppy = 2-phenylpyridine), we have incorporated the complex into a covalent electron acceptor–chromophore–Cp*Ir(ppy)Cl triad, in which naphthalene-1,8:4,5-bis(dicarboximide) (NDI) is the electron acceptor and perylene-3,4-dicarboximide (PMI) is the chromophore. Photoexcitation of the PMI chromophore in dichloromethane results in two competitive reactions: NDI–^{1*}PMI–Ir(III) $\rightarrow$ NDI–PMI$^{\bullet-}$–Ir(IV) and NDI–^{1*}PMI–Ir(III) $\rightarrow$ NDI$^{\bullet-}$–PMI$^{\bullet+}$–Ir(III) that each proceed with $\tau < 5$ ps, as determined by femtosecond transient absorption spectroscopy. Both intermediate ion pairs undergo charge shift reactions to produce NDI$^{\bullet-}$–PMI–Ir(IV). The fully charge-separated ion pair has a lifetime of 17.2 ± 0.1 ns, and its photophysical behavior is similar in the more polar solvent benzonitrile. Time-resolved X-ray absorption measurements on the triad at 100 ps following PMI photoexcitation show a new absorption feature at the L_{III}-edge of Ir and a blue-shifted white-line peak, which provides direct evidence of a change in the Ir oxidation state from Ir(III) to Ir(IV), consistent with the photophysical measurements. Our work underscores the utility of ultrafast spectroscopy performed on covalent assemblies of electron donor-acceptor systems with solar fuels catalysts to generate and probe their higher valence states in ways that complement chemical or electrochemical oxidation and establish the nature of key intermediates implicated in their catalytic mechanisms.

Session V: Friday, July 19, 2013, 11:00 – 12:00; Delaware Suite A

11:00 AM

A-V-1: Transformation of Aldose Sugars to Platform Furans using CrCl3 with HCl in Aqueous Media

[CCEI] Vinit Choudhary[1], Samir Mushrif[1], Chris Ho[1], Cory Mackintosh[1], Michael Orella[1], Andre Anderko[2], Vladimiros Nikolakis[1], Nebojsa Marinkovic[3], Anatoly Frenkel[3], Dionisios G. Vlachos[1], Stanley I. Sandler[1]
[1]University of Delaware, [2]OLI Systems Inc., [3]Yeshiva University

An approach to utilize biomass requires its conversion to various furan derivatives, which can potentially substitute petroleum precursors in producing chemicals, polymers and fuels. The objective of this work is to gain mechanistic understanding into the aldose conversion to platform furan derivatives using a combination of Lewis and Brønsted acids.

In particular, we combined Lewis acid ($CrCl_3$) with a Brønsted acid (HCl) in water to catalyze aldose sugar (glucose and xylose) transformation to 5-(hydroxymethyl)furfural (HMF) and furfural, respectively. For the first time, we employed kinetics experiments in conjunction with speciation modeling of $CrCl_3$ in aqueous media and revealed that among the various metal ions generated in aqueous media, partially hydrolyzed ions, such as $CrOH^{2+}$, are the most active for the metal salt catalyzed aldose-to-ketose isomerization. Additionally, complex interactions between the two catalysts were explained: Brønsted acidity retards aldose-to-ketose isomerization by decreasing the equilibrium concentration of $CrOH^{2+}$. In contrast, Lewis acidity promotes side reactions during fructose dehydration and HMF rehydration reactions. Thus, an optimization between the Lewis and Brønsted acidities along with reaction conditions is required. Additionally, spectroscopic studies (NMR and EXAFS) revealed strong catalytic and mechanistic similarities among $CrCl_3$, $AlCl_3$ and Sn-beta catalyzed aldose-ketose isomerization. Furthermore, the reaction pathway for aldose-to-ketose isomerization using $CrCl_3$ as a catalyst is deciphered from isotopic labeling NMR experiments. Finally, a strong interaction between the glucose molecule and the Cr ion is indicated in EXAFS experiments and CPMD simulations.

11:20 AM

A-V-2: EXPLORING THE MECHANISMS OF FAST PYROLYSIS OF CELLULOSE BY PYROPROBE/TANDEM MASS SPECTROMETRY, ISOTOPE LABELING, MODEL COMPOUND STUDIES AND QUANTUM CHEMICAL CALCULATIONS

[C3Bio] John C. Degenstein[1], Matthew R. Hurt[2], Mckay W. Easton[1], Priya Murria[2], Vinod K. Venkatakrishnan[1], Linan Yang[2], Huaming Sheng[2], Guannan Li[2], John J. Nash[2], Rakesh Agrawal[1], W. Nicholas Delgass[1], Fabio H. Ribeiro[1], Hilkka I. Kenttamaa[2]
[1]School of Chemical Engineering and [2]Department of Chemistry, Purdue University, West Lafayette, IN

Fast pyrolysis is a potentially viable approach to produce fuels and valuable chemicals from lignocellulosic biomass. Rational design of fast-pyrolysis reactors requires knowledge of the mechanisms and reaction pathways from biomass to bio-oil. Cellulose, a polymer of glucose, is the most abundant component of biomass and a logical starting point for fundamental studies. The mechanisms of fast pyrolysis of cellulose and model compounds (e.g., cellobiose) were explored by constructing two pyroprobe/mass spectrometry systems - one to determine the primary products, and one to study the reactions of the primary products in order to simulate a pyrolysis reactor. The rapidly quenched products were immediately ionized by atmospheric pressure chemical ionization and characterized by collision-activated dissociation in multi-stage tandem mass spectrometry experiments at high resolution (to determine elemental compositions). Only a few primary products formed from cellobiose: predominantly glucose, cellobiosan, and a molecule with elemental composition $C_8H_{14}O_7$. These molecules concurrently polymerize to form anhydro-oligosaccharides. Similar findings were observed for cellulose. A handful of primary products, some fairly large in size, react to predominantly form just three molecules: cellobiosan, cellotriosan and a molecule with elemental composition $C_{14}H_{24}O_{12}$. These results are in stark contrast to the complex bio-oils produced in many pyrolysis reactors, and that levoglucosan is the major final product. Examination of model compounds and dopants, isotope labeling, proton affinity measurements, and high-level quantum chemical calculations on reaction energetics and transition states suggest specific acid-catalyzed mechanisms for the formation of the primary products of cellobiose.

11:40 AM

A-V-3: ELUCIDATING THE ROLES OF AN H-BEA ZEOLITE IN AQUEOUS-PHASE FRUCTOSE DEHYDRATION

[CCEI] Jacob S. Kruger, Marta León, Vladimiros Nikolakis, Dionisios G. Vlachos
University of Delaware

The main paths by which zeolites catalyze the dehydration of fructose to 5-Hydroymethylfurfural (HMF) and the rehydration of HMF to levulinic acid in aqueous solutions are elucidated using an H-BEA zeolite with SiO_2/Al_2O_3 = 18 (H-BEA-18) as a representative solid acid catalyst. Specifically, the relative roles of zeolite-induced homogeneous chemistry, external surface acid sites, and adsorption of products and reactants on the catalyst for these reactions are delineated. H-BEA-18 increases the conversion of fructose and HMF in part by catalyzing fructose isomerization to glucose and HMF rehydration to formic and levulinic acids, respectively. Octahedral aluminum, which is formed during calcination of the zeolite, catalyzes both fructose isomerization and reactions to unknown products from both fructose and HMF. The zeolite is susceptible to partial dissolution under reaction conditions, producing homogeneous species that catalyze undesired side reactions. These zeolite-derived homogeneous species contain both Si and Al, and characterization by FTIR, NMR, and comparative studies suggests that the dissolved species are small fragments of dissolved zeolite. H-BEA-18 more readily converts HMF, furfural, and levulinic acid compared to sugars, likely due to the relatively strong adsorption of furans and levulinic acid. In contrast, changes in the initial pH due to the addition of the zeolite and catalysis by sites on the external surface of the zeolite contribute negligibly to the chemistry under the conditions investigated. Cumulatively, these experiments provide significant insights into catalyst behavior in aqueous-phase carbohydrate transformations and can help in the design of solid acid catalysts in the future.

B. ENERGY STORAGE

Session I: Thursday, July 18, 2013, 10:30 – 12:10; Delaware Suite B

10:50 AM

B-I-1: CAPACITIVE ENERGY STORAGE

[MEEM] Mark Asta[1], Bruce Dunn[2], Brian Laird[3], Yunfeng Lu[2], Vidvuds Ozolins[2], Laurent Pilon[2], Sarah H. Tolbert[2]
[1]*University of California, Berkeley;* [2]*University of California, Los Angeles,* [3]*University of Kansas*

Our research program on capacitive energy storage combines experimental and computational components to achieve fundamental understanding of charge storage processes in redox-based materials. Efforts include atomic and multiscale modeling, materials synthesis and characterization, and electrochemical studies. Because of pseudocapacitance mechanisms, these materials offer much higher energy densities than traditional double-layer capacitors. We have developed synthetic routes to materials architectures optimized for pseudocapacitive charge storage. Our kinetic studies of Nb_2O_5 further provide considerable insight regarding the pseudocapacitance associated with ion insertion. We have identified the electrochemical features associated with intercalation pseudocapacitance, a process based on facile 2D ion diffusion. The principal benefit of this mechanism is that high levels of charge storage are achieved within short periods of time because of fast solid-state diffusion and the fact that materials do not undergo phase transformations upon lithium ion insertion. Current studies with WO_3 show that intercalation pseudocapacitance can be extended to aqueous systems. Another active research area has been in the use of first-principle and continuum level computational methods. Our DFT studies on hydrous ruthenia provide fundamental understanding of how interfacial energies and reversible proton adsorption influence its charge storage properties. At the continuum level, we have continued to improve our simulation tools and have now extended our initial studies of electrical double layer systems to include redox-based materials. We also initiated an effort that combines first-principles and classical molecular dynamics simulations of electrolytes and electrolyte/oxide interfaces. Studies focus on $LiClO_4$ in acetonitrile-and combine design with experimental validation.

11:10 AM

B-I-2: NOVEL CARBON MATERIALS FOR ELECTRICAL ENERGY STORAGE

[FIRST] Sheng Dai[1], Pasquale Fulvio[1], John M. McDonough[2], Majid Beidaghi[2], Yury Gogotsi[2]
[1]*Chemical Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831;* [2]*Department of Materials Science and Engineering, Drexel University, Philadelphia, PA 19104*

Key interactions of importance in energy technologies, such as electrical energy storage devices and mesoporous catalyst substrates, involve nanoscale textures, fluid nanoconfinement, and reactive interfaces. For example, enhancements in electrochemical energy storage using supercapacitors resides in the enormous increase in electrode surface area and the tailored nanotextures resulting from making the surface hierarchically nanoporous. The complex interplay of solvent and solute structure and dynamics at the charged interface, the transport of electrolyte ions into and out of the pores, the solvation/desolvation processes occurring in pores approaching bare-ion dimensions, and formation of interfaces via chemical reactions are all important parameters. New fundamental science of fluid-solid interfaces is related to whether "new" phenomena emerge when the interface has nanoscale texture (angstrom-submicron pores, slits, roughness, curvature, steps, pits, etc.),

rather than an infinite planar geometry, as it interacts with electrolyte ions with distinct molecular sizes and shapes. Nanotextured carbon materials with well-defined geometries, surface properties and pore sizes provide an ideal model system for investigating these interfacial and nanoconfined fluid properties. Recent breakthroughs in synthesizing carbon-related materials for elucidating fundamental chemistry in nanotextured interfaces will be discussed.

11:30 AM

B-I-3: THE PERFORMANCE AND STABILITY OF LI-ION BATTERIES WITH ULTRA-THIN SOLID ELECTROLYTE

[NEES] A. A. Talin[1,2], D. Ruzmetov[2], P. M. Haney[2], V. P. Oleshko[2], K. Karki[3], K. H. Baloch[3], and J. E. Cumings[3]

[1]Sandia National Laboratories, Livermore, CA 94551, [2]Center for Nanoscale Science and Technology, National Institute of Standards and Technology, Gaithersburg, MD 20899, [3]Dept. of Materials Science and Engineering, University of Maryland, College Park, MD 20742

Thin film solid state Li-ion batteries (LIBs) employing inorganic, non-flammable electrolytes are inherently safe, have negligible self-discharge rates and have demonstrated extremely long cycle life. However, compared to batteries utilizing porous electrodes and liquid electrolytes, thin film LIBs have low energy and power densities, limited by the active electrode film thickness and low electrolyte conductivity. Increasing the electrode thickness to store more energy further reduces power and is ultimately limited by the fracture toughness of the active materials. Various 3D-Li ion battery (3D-LIB) designs based on trenches, inverse opals, vertical rods, and periodic 'sponges' have been proposed to improve power by arranging the anode and cathode sub-structures in close proximity, so that the Li-ion diffusion length during cycling remains short. The success of all of these designs depends on an ultra-thin, conformal electrolyte layer to electrically isolate the anode and cathode while allowing Li-ions to pass through. However, at sufficiently reduced thickness solid electrolytes can become electronically conductive and breakdown at potentials <5 V. In our presentation we will demonstrate fully operational, stable solid state LiBs with electrolyte thickness less than 100 nm. We will discuss the factors that affect electrolyte stability and how battery performance scales with electrolyte thickness.

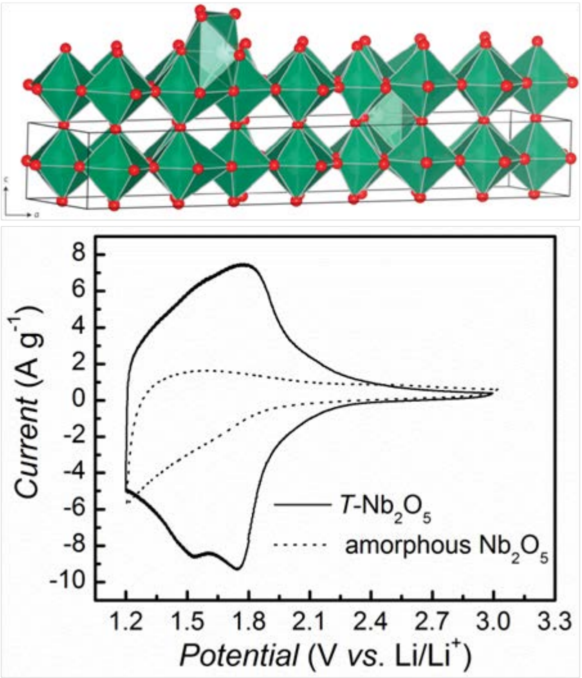
11:50 AM – Graduate Student Finalist

B-I-4: HIGH-RATE ELECTROCHEMICAL ENERGY STORAGE WITH Nb_2O_5

[MEEM] Veronica Augustyn[1], Jeremy Come[2], Michael A. Lowe[3], Jong Wuong Kim[1], Pierre-Louis Taberna[2], Sarah H. Tolbert[4], Hector D. Abruña[3], Patrice Simon[2], and Bruce Dunn[1]

[1]Department of Materials Science and Engineering, University of California, Los Angeles, California 90095, USA; [2]Department of Materials Science, Université Paul Sabatier, CIRIMAT UMR CNRS 5085, Toulouse 31062, France; [3]Department of Chemistry and Chemical Biology, Cornell University, Ithaca, New York 14853, USA; [4]Department of Chemistry and Biochemistry, University of California, Los Angeles, California 90095, USA

The need for more abundant, clean, efficient, and secure energy is opening up applications for electrochemical energy storage (EES) beyond portable electronics. While the opportunities for EES are very promising, these devices still suffer in performance due to material limitations. One challenge for EES is to design electrode materials that can provide high power and high energy densities simultaneously. The research presented here will examine how such electrode materials are possible through the use of pseudocapacitive energy storage. Pseudocapacitance was first noted in 1971 in hydrous RuO_2; research over the past several decades has focused on identifying materials that exhibit the same properties as RuO_2 but at a lower cost. In hydrous RuO_2, protons from the electrolyte adsorb onto the inner and outer surface areas of the material. Here, a different pseudocapacitive mechanism is identified in orthorhombic T-Nb_2O_5, termed intercalation pseudocapacitance. This mechanism leads to the same type of rapid kinetic behavior expected for capacitive charge storage but it occurs due to the intercalation of Li^+ into the bulk of T-Nb_2O_5. For charging times up to 60 seconds, no diffusion limitations are observed and this is what results in the high-rate capability of the material. The intercalation pseudocapacitance mechanism is beneficial for device applications because it does not require materials with ultrahigh surface areas that need to be exposed to the electrolyte. In addition, a set of analytical tools is presented for the facile identification of such rapid energy storage reactions and these can be applied to other materials of interest. This work has been recently published in *Nature Materials (V. Augustyn et. Al., "High Rate Electrochemical Energy Storage via Li+ Intercalation Pseudocapacitance" Nature Materials, 12, 518-522 (2013)* [DOI: 10.1038/NMAT3601]).



Top: Crystal structure of T-Nb_2O_5 stacked along the *c* axis demonstrates the layered arrangement of oxygen (red) and niobium (within polyhedra) atoms along the *a*-*b* plane. This structure accounts for the rapid Li^+ charge storage kinetics in this material. **Bottom**: Cyclic voltammetry at 10 mV s^{-1} of amorphous and T-Nb_2O_5 in a non-aqueous Li^+ electrolyte. While the surface area of the amorphous material is more than 2X higher than that of the crystalline material, the T-Nb_2O_5 exhibits both higher and faster charge storage. This result indicates that charge storage is not limited to the surface in Nb_2O_5.

Session II: Thursday, July 18, 2013, 1:40 – 3:20; Delaware Suite B

1:40 PM

B-II-1: ELUCIDATION OF LITHIUM-ION COUPLED ELECTRON TRANSFER MECHANISMS AT TRANSITION METAL PHOSPHATE INTERFACES VIA SPECTROELECTROCHEMICAL RAMAN EXPERIMENTS AND THEORY

[CST] Keith J. Stevenson,[1,2,3] Anthony G. Dylla,[1] Penghao Xiao,[1] Kyu-Sung Park,[2] Arumugam Manthiram,[2,3] Graeme Henkelman,[1] John B. Goodenough[2,3]
[1]Department of Chemistry, The University of Texas at Austin; [2]Texas Materials Institute, The University of Texas at Austin; [3]Materials Science and Engineering Program, The University of Texas at Austin

This presentation will detail the development of *in situ* spectroelectrochemical Raman spectroscopy for studying electrode material interfaces of lithium-ion batteries. This approach provides the high sensitivity necessary to detect changes in crystal symmetry, oxidation states, local phase inhomogeneities and structural order/disorder, especially for analysis of cycled electrodes. This talk will also highlight *in situ* measurements on the surface phase change during electrochemical lithiation/deliathion for three morphologies of $LiFePO_4$: 1) 25 ± 6 nm width nanorods, 2) 225 ± 6 nm width nanorods and 3) ~2 µm porous microspheres. Both the large nanorod and microsphere geometry show incomplete delithiation at the end of charge, which is most likely caused by anti-site defects along the 1-D diffusion channels in the bulk of the larger particles. Based on the *in situ* Raman measurements, all of the morphologies studied exhibit self-discharge (spontaneous lithiation) with time. Among them, the smallest particles self-discharged (lithiated) the fastest. This suggests that while nanostructuring can offer advantages in terms of lowering anti-site defects within particles, it also creates new problems due to high surface energies that allow self-discharge. The potential dependent Raman vibrational spectra of $LiFePO_4$ as a state of charge to form $FePO_4$ is reported and compared to the theoretical Raman frequencies (wavenumbers) calculated with DFT using the Vienna *ab inito* simulation package (VASP). We demonstrate that by measuring changes in the amplitude and frequency of external modes ($<400\ cm^{-1}$) the lithiation/delithiation related phase change kinetics can be followed directly as a function of the state of charge.

2:00 PM

B-II-2: THE $LiFePO_4$ STORY: THEORY, EXPERIMENT AND CHARACTERIZATION

[NECCES] Fredrick Omenya[1], Natasha A. Chernova[1], Qi Wang[1,2], Kyung-Wan Nam[2], Xiao-Qing Yang[2], Shirley Meng[3], Peter Khalifah[4], Clare P. Grey[4], Aziz Abdellahi[6], Rahul Malik[6], Gerbrand Ceder[6], M. Stanley Whittingham[1,4]
[1]Binghamton University; [2]Brookhaven National Laboratory; [3]University of California at San Diego; [4]Stony Brook University; [5]Cambridge University; [6]MIT

The olivine cathode, $LiFePO_4$, presents a quandary. It is a very good electronic insulator and thought to react by a two-phase mechanism, yet has one of the highest power capabilities of any cathode material. NECCES therefore chose it as a model compound to understand the ultimate limitations of intercalation electrodes. A theoretical model was developed that could explain the high rates, based on a low overpotential being sufficient to drive the reaction mechanism to one involving a single phase, but where only the end members are observed at equilibrium. Single crystal and nano-sized powders were synthesized to provide a range of length-scales and to determine the role of defects, both intrinsic and those brought about by partial substitution of the iron and lithium sites. Ex-situ and in-situ tools were employed to determine the kinetic vs thermodynamic pathways. Vanadium was chosen as an aliovalent substituent, because it has a very different neutron scattering factor to iron, so the positions of the iron and vanadium atoms could be unambiguously determined.

Vanadium substitution was found to increase the single-phase regions and the rate capability consistent with a single-phase mechanism. When V+Fe>1>Li, the iron resides on the Li site not vanadium, and moreover the iron forms clusters, as for example in sarcopside. This keeps the tunnels open so that the lithium ions can still diffuse very rapidly. This combination of theory, experiment and characterization has allowed us to better understand this previously considered "simple" material, and will let us design the material of tomorrow.

2:20 PM

B-II-3: OPERANDO ELECTRON MICROSCOPY OF ENERGY CONVERSION AND ENERGY STORAGE MATERIALS

[emc^2] David A. Muller[1], Megan Holtz[1], Yingchao Yu[2], Jie Gao[2], Kayla Nguyen[1] and Héctor D. Abruña[2]
[1]School of Applied and Engineering Physics, Cornell University, Ithaca, NY; [2]Department of Chemistry and Chemical Biology, Cornell University, Ithaca, NY

Much of what we know about the structure-property relationships of energy conversion and storage materials during their operation is inferred indirectly through bulk measurements or post-mortem studies. To observe electrochemical processes in their native environment on the nanometer scale, we developed a liquid cell incorporating electrodes on the viewing membrane in a transmission electron microscope. This geometry allows us to image the microstructure of an electrode, in liquid and under bias, and further perform spatially-resolved spectroscopy to determine composition and bonding. Using this cell, we have studied the degradation and coarsening of Pt/Co fuel cell cathode electrocatalysts during electrochemical cycling. We also show how valence electron energy-loss spectroscopy (EELS) can be used to observe the lithiation and delithiation dynamics of individual LiFePO4 nanoparticles, as well as the lithium ion distribution in the liquid using energy-filtered transmission electron microscopy (EFTEM). We also consider fundamental limits on this imaging approach imposed by the liquid thickness and maximum allowable beam dose.

These studies are supplemented by an air-operational scanning electron microscope (airSEM) that leaves the sample outside of vacuum – in air or liquid. The sample can be placed on a simple optical microscope slide or even the surface of a liquid. The spatial resolution is 5-10 nm, and the absence of a specimen vacuum chamber simplifies the construction of custom detectors, liquid and electrochemical cells.

2:40 PM

B-II-4: A RAPID 3-D MICROSTRUCTURAL ASSESSMENT TOOL FOR THE RATIONAL DESIGN OF COMPLEX HETEROFOAM ELECTRODES

[HeteroFoaM] George J. Nelson[1], Arata Nakajo[1], Brice N. Cassenti[1], Aldo A. Peracchio[1], Wilson K. S. Chiu[1], Guoliang Xiao[2], Fanglin Chen[2], Steve Wang[3], Anil V. Virkar[4]
[1]University of Connecticut; [2]University of South Carolina; [3]Argonne National Laboratory; [4]University of Utah

An electrode used for electrochemical energy storage is a complex heterogeneous functional material (HeteroFoaM) consisting of multiple porous and solid material phases that are three dimensionally structured and connected at the nanoscale. There is a critical need to rationally design the electrode's structure, morphology, and composition for improved performance. This presentation will describe a rapid assessment tool developed under this EFRC called the "Electrochemical Fin" (ECF) method. ECF accounts for surface electrochemical reactions and ion/electron diffusion due to the 3-D shape of the electrode's microstructure. ECF uses analytical solutions to rapidly predict ion/electron transport and electrochemical reactions in the 3-D microstructure as a 3-D circuit network. To demonstrate this approach, Sr2Fe1.5Mo0.5O6-δ (SFM) electrodes used in reversible electrochemical cells for energy storage are examined to provide fundamental insight into the origins of microstructure-induced transport losses during operation. SFM electrode material is imaged in 3-D and characterized using a synchrotron-based transmission x-ray microscope at the Advanced Photon Source beamline 32-ID-C, and tomographically reconstructed at 30 nm spatial resolution. Detailed 3-D images of the electrode structure is analyzed using the ECF method. Preliminary results indicate that ECF validates well to experimental measurements. Computational time and memory requirements of this analytical ECF method was observed to be up to orders of magnitude less than comparable numerical methods such as finite element or lattice Boltzmann. The prediction of localized heating and overpotential induced by constrictions in the electrode microstructure are used in the rational design of electrodes.

3:00 PM

B-II-5: BLOCK COPOLYMER DIRECTED NANOSTRUCTURED MATERIALS FOR ENERGY CONVERSION AND STORAGE

[emc^2] Ulrich B. Wiesner[1], Francis J. DiSalvo[2], David A. Muller[3], Héctor D. Abruña[2]

[1]Department of Materials Science and Engineering, Cornell University, Ithaca, NY; [2]Department of Chemistry and Chemical Biology, Cornell University, Ithaca, NY; [3]School of Applied and Engineering Physics, Cornell University, Ithaca, NY

The development of energy conversion and storage devices is at the forefront of research geared towards a sustainable future. There are numerous materials based limitations, however, that prevent the widespread use of these technologies including cost, performance and durability. This talk will highlight recent results obtained under the umbrella of the Energy Materials Research Center at Cornell (emc^2) on block copolymers as an emerging and powerful yet affordable tool to direct materials for energy conversion and storage applications into nanostructured electrodes with precise control over structural dimensions, composition and topology. The talk will focus in particular on block copolymer structure-directed nanomaterials for battery and fuel cell electrodes. In each case insights are provided into the various underlying fundamental chemical, thermodynamic and kinetic formation principles enabling general and relatively inexpensive wet-polymer chemistry methodologies for the efficient creation of functional nanomaterials. Examples include nanostructured oxides, oxide-carbon composites, oxide-carbon-metal composites and carbon-sulfur composites with morphologies ranging from hexagonally arranged cylinders to three-dimensionally co-continuous network structures like the double or single gyroid. Rather than Edisonian approaches the talk will emphasize the systematic exploration of fundamental nanostructure – device performance correlations in order to elucidate critical structural characteristics enabling optimized performance.

Session III: Thursday, July 18, 2013, 3:40 – 5:00; Delaware Suite B

3:40 PM – Graduate Student Finalist

B-III-1: NANO-ENGINEERING OF SILICON NANOSTRUCTURES FOR LITHIUM-ION BATTERIES AND ENERGY STORAGE DEVICES

[NEES] Khim Karki[1], Chuanfu Sun[2], Eric Epstein[1], Jeong-Hyun Cho[3], Zheng Jia[4], Yujie Zhu[5] Teng Li[4], Yue Qi[6], Tom Picraux[3], Gary Rubloff[1], Chunsheng Wang[5], YuHuang Wang[2], and John Cumings[1]
[1]Materials Science & Engineering, [2]Chemistry & Biochemistry, [3]Los Alamos National Laboratory, Los Alamos, NM; [4]Mechanical Engineering, [5]General Motors Research, Warren, MI
[6]Chemical & Biomolecular Engineering - University of Maryland, College Park, MD;

The rising demand of energy consumption with virtually depleted natural fuel resources requires the utilization of alternative sources such as solar and wind power. However, the intermittent nature of energy generated from these resources would be unable to meet the threshold of the on and off peak energy demands. Thus, high-performance electrical energy storage technology is desirable to enable clean, efficient and uninterruptible power supply to the consumer. Lithium-ion batteries, among many other storage technologies can store significantly more energy per unit mass (energy density), naturally becoming the best contender to manage renewable resources and achieve economic sustainability.

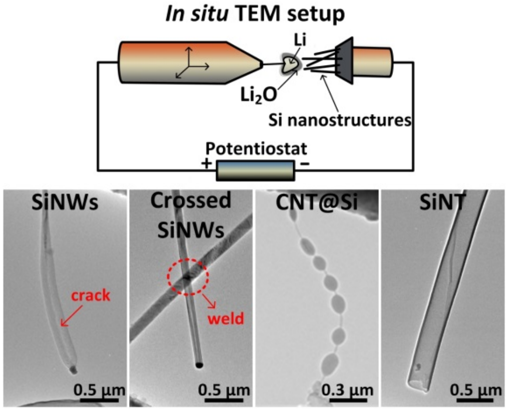


Fig.1: *In situ* TEM setup and silicon nanostructures studied

Recently, it has been proposed that silicon-based nanostructures could be used as lithium storage materials with greatly enhanced storage capacities over that for conventional graphite anodes in the next generation of lithium-ion batteries. However, the studies to date have shown that the nanomaterials, while better, are still not good enough to withstand a large number of lithiation cycles, and moreover, there is insufficient fundamental insight into the science of the improvements or the advances necessary before widespread adoption. Therefore, we conduct real-time investigations of individual silicon nanostructures by fabricating prototype nanoscale electrochemical cells inside a transmission electron microscope (TEM). Using this pioneering technique, we have studied the structural, electrochemical, and mechanical properties of several one-dimensional nanostructures such as silicon nanowires (SiNWs), carbon nanotube@silicon (CNT@Si) heterostructures, and silicon nanotubes (SiNTs) as shown in Fig. 1. While cracking and pulverization are known to be mitigated in part by nanostructured forms of silicon, such as nanowires, several recent studies indicate that cracking can still occur in nanostructures under a variety of conditions. We also observe an opposite effect in which physically distinct SiNWs can become fused through an electrochemically-induced process, which suggests that this welding may lead to self-healing in nanostructured Si-electrodes. Our results show evidence of robust weld strength and facile transport of lithium ions across the welded Si-Si interface, both desirable properties for enhanced battery performance. Similarly, CNT@Si beaded-string heterostructures with chemically tailored carbon–silicon interfaces were designed and synthesized based on a fundamental understanding of carbon surface chemistry and Si nucleation on covalently modified CNT surfaces. *In situ* TEM studies of lithiation propagation reveal that these novel heterostructures can accommodate massive volume changes during lithiation and delithiation without appreciable mechanical failure. These findings thus provide important new insights in the design of high performance Si electrodes, laying a foundation for next-generation lithium ion batteries.

This work was initiated and supported as part of Nanostructures for Electrical Energy Storage (NEES), an Energy Frontier Research Center funded by the U.S. Department of Energy.

4:00 PM

B-III-2: UNDERSTANDING AND CONTROLLING SILICON LITHIATION

[CEES] Paul Fenter,[1] Maria Chan,[2] Tim Fister,[1] Bing Shi,[1] Brandon Long,[1,3] Jason Goldman,[3] Jen Esbenshade,[3] Michael Cason,[3] Ralph Nuzzo,[3] Andrew Gewirth,[3] Xiao Chen,[4] Michael Bedzyk,[4] Christopher Wolverton,[4] Jeffrey Greeley[5]

[1]Chemical Sciences & Engineering Division, Argonne National Laboratory; [2]Center for Nanoscale Materials, Argonne National Laboratory; [3]Department of Chemistry, University of Illinois Urbana-Champaign; [4]Materials Science and Engineering Department, Northwestern University; [5]Chemical Engineering Department, Purdue University

Silicon is widely acknowledged as a possible next-generation anode material for lithium-ion batteries due to its large intrinsic capacity (~4000 mAh/g) relative to graphitic carbon (372 mAh/g). However, silicon's large (~400%) volume change upon lithiation leads to rapid degradation in performance (e.g., due to strain with the current collector, amorphization during lithiation, and pulverization upon repeated cycles). This presentation will review two strategies used in the Center for Electrical Energy Storage (CEES) to understand and control the lithiation of silicon through the use of various architectures. The first strategy uses lithographic microstructures (i.e., pillars) on crystalline silicon surfaces to visualize, control and understand the lithiation process in silicon. The inherent anisotropy of the silicon lithiation process (with preferential lithiation along the [110] directions) is directly manifested in these microstructures, and these observations are understood using first principles calculations. A second strategy draws from studies of the lithiation of amorphous silicon thin films on Cr current collectors. These studies revealed a stratified lithiation process, which is understood in terms of the lithiation of $CrSi_x$ alloys that form discrete layers at $Si/CrSi_x$ interfaces. This observation led to the study of silicon/metal-silicide multilayers that are found to have favorable properties, including a reversible one-dimensional expansion upon lithiation (by >300%) along with promising cycle life and rate capability.

4:20 PM

B-III-3: DESIGN AND APPLICATIONS OF IN-SITU METROLOGIES IN CHEMICAL ENERGY STORAGE

[NECCES] Nicole Trease[1], Andrew Ilott[1,2], Hee Jung Chang[1], Lina Zhou[1,3], Fiona Strobridge[3], Hao Liu[3], Alexej Jerschow[2], Feng Wang[4], Jason Graetz[4], Yimei Zhu[4], Olaf J. Borkiewicz[5], Karena W. Chapman[5], Peter J. Chupas[5], Clare P. Grey[1,4]

[1]Stony Brook University; [2]New York University; [3]University of Cambridge; [4]Brookhaven National Laboratory; [5]Argonne National Laboratory

A full understanding of the operation of a battery and supercapacitor requires that we utilize methods that allow devices or materials to be probed while they are operating (i.e., *in-situ* or *in-operando*). This allows, for example, the transformations of the various cell components to be followed under realistic conditions without having to disassemble and take apart the cell. To this end, the application of new *in* and *ex-situ* Nuclear Magnetic Resonance (NMR), magnetic resonance imaging (MRI), transmission electron microscopy (TEM) and pair distribution function (PDF) analysis of X-ray diffraction (XRD) approaches to correlate structure and dynamics with function in lithium-ion and lithium batteries and supercapacitors will be described. The *in-situ* approach allows processes to be captured, which are very difficult to detect directly by ex-situ methods. New spectroscopic- and diffraction-based approaches allow dynamics and structural transformations to be probed, including sorption processes at the electrolyte-electrode interface, and electrode processes that occur during extremely fast charging and discharging. Via spatial imaging we follow

the formation of interconnected metal nanoparticles on lithiation of conversion materials and the formation of lithium dendrites.

4:40 PM

B-III-4: HETEROSTRUCTURED SI-CNT ELECTRODES WITH CHEMICALLY TAILORED INTERFACES

[NEES] Chuan-Fu Sun,[1] Khim Karki,[2] Shunliu Deng,[1] Hongli Zhu,[2] Edward B. Baker III,[1] Zheng Jia,[3] Alex Brozena,[1] Hongwei Liao,[1] Yin Zhang,[1,4] John Cumings,[2] Liangbing Hu,2 Teng Li,[3] Morihiro Okada,[1] Yue Qi,[5] Gary W. Rubloff,[2] George Schatz,[6] YuHuang Wang[1]

[1]Department of Chemistry and Biochemistry, University of Maryland, College Park, MD 20742, [2]Department of Materials Science and Engineering, University of Maryland, College Park, MD 20742, [3]Department of Mechanical Engineering, University of Maryland, College Park, MD 20742, [4]Department of Physics, Xi'an JiaoTong University, Xi'an, China, [5]General Motors Research, 30500 Mound Rd, Warren, MI, 48090, [6]Department of Chemistry, Northwestern University, Evanston, IL

High-capacity electrode materials have the potential to transform electrical energy storage technologies. Silicon, for instance, can store nearly 10 times more lithium ions per unit weight than do conventional graphite electrodes. However, to harness silicon's potential as an anode for lithium ion batteries, structures must accommodate its huge volume change (~300%) during cycling to maintain mechanical integrity and electrical connection.

In this talk, we will discuss collaborative efforts in addressing this challenge by controlled synthesis and fundamental studies of silicon-carbon heterostructures. We have synthesized electrically connected, non-cracking amorphous silicon beads that are threaded on mechanically robust, electrically conductive carbon nanotube axial supports. The controlled synthesis of this unique beaded-string structure is made possible by a propagative chemistry which creates regular bands of alkylcarboxyl function groups along the nanotubes. The functional bands localize, separate, and anchor the beads. *In situ* transmission electron microscopy combined with atomic and continuum modeling reveal that the chemically tailored Si-C interface plays important roles in constraining the threaded Si beads, such that they exhibit a symmetric "radial breathing" around the CNT string, remaining crack-free and electrically connected throughout lithiation-delithiation cycling. This progress provides some fundamental insights required to control the synthesis of high-capacity heterostructured electrodes.

Session VI: Friday, July 19, 2013, 8:30 – 9:30; Delaware Suite B

8:30 AM

B-IV-1: TOWARD MOLECULAR ELECTROCATALYSTS FOR REVERSIBLE DEHYDROGENATION-HYDROGENATION OF ALCOHOLS

[CETM] Peter J. Bonitatibus Jr., Matthew Rainka, Andrea Peters, Mark Doherty, Oltea Siclovan, and Davide Simone

GE Global Research

Our Energy Frontier Research Center (EFRC) for Electrocatalysis, Transport Phenomena, and Materials for Innovative Energy Storage is focused on fundamental research toward understanding processes in a novel, organic fuel based high-density energy storage system. The key components and focus areas of the system are; (i) organic liquid carriers (LH_n) amenable to electro(de)hydrogenation, (ii) *electrocatalysts*, and (iii) compatible proton exchange membranes

(PEM). We will discuss a strategy and progress toward the development of *transition metal catalysts* for selective and efficient electrodehydrogenation of LH_n to H_2-depleted liquid carriers (L), and to some extent electrohydrogenation of L back to LH_n. The advantage of developing a molecular electrocatalyst is that it (theoretically) allows for an energetically and/or structurally tunable active site and fundamental investigation of a (reversible) reaction mechanism. We have studied the Ir(I)-trop$_2$DACH system, known to catalytically dehydrogenate primary alcohols chemically using benzoquinone as stoichiometric oxidant and base. We transitioned this system to an *electrochemical* setting and replaced the $2e^-/2H^+$ acceptor (benzoquinone) with an electrode and base. We will report our findings in terms of separating proton and electron transfer processes for dehydrogenation, through (a) chemical catalysis results that employed stoichiometric oxidants and base, and (b) evidence for electrocatalysis and electrolysis data. We have observed high selectivity and Faradaic yield using the Ir(I)-trop$_2$DACH system. We will include attempts toward electrocatalytic hydrogenation that use the same catalyst.

8:50 AM

B-IV-2: EXAMINING THE SOLID ELECTROLYTE INTERPHASE AT LI ION BATTERY ELECTRODES

[CEES] Andrew Gewirth,[1] Hadi Tavassol,[1] Joseph Buthker,[1] Glen Ferguson,[1] Larry Curtiss,[2] Maria Chan,[3] Jeffrey Greeley,[3,4] Albert Lipson,[5] Mark Hersam[5]
[1]Department of Chemistry, University of Illinois Urbana-Champaign; [2]Materials Science Division, Argonne National Laboratory; [3]Center for Nanoscale Materials, Argonne National Laboratory; [4]Chemical Engineering Department, Purdue University; [5]Materials Science and Engineering Department, Northwestern University

The Solid Electrolyte Interphase (SEI) is responsible for many important battery properties. At lithium-ion battery electrodes, the SEI can inhibit Li^+ transport to the active electrode and reduce the accessible capacity of the battery. The SEI can also protect the electrode against electrode corrosion and electrolyte decomposition. In CEES, we have developed a number of techniques to examine the SEI at battery electrodes. These techniques, which include scanning ion conductance microscopy (SICM), mass spectrometric, and electrochemical stress, report on the composition and formation of the SEI. For example, we found that at least part of the SEI is formed by solvent oligomerization, yielding a high molecular weight polymer which coats the electrode surface. The degree of polymerization is dependent upon the applied potential, the identity of the solvent, the composition of the electrode surface, and the number of lithiation/delithiation cycles. On model Au anodes, the majority of oligomer formation occurs only after bulk deposition of Li, consistent with the radical-initiated polymerization mechanism predicted from density functional theory (DFT) calculation of the solvent molecules. Electrochemical stress measurements show the presence of compressive stress following lithiation, consistent with detailed calculations. However, while stress measurements obtained from non-oligomerizing solvents, such as the ionic liquid n-buthylmethylimidazolium tetrafluoroborate ($BMIMBF_4$), show little cycle-dependent hysteresis, those from solvents such as EC/DMC and PC reveal the presence of residual tensile stress following delithiation, the origin of which is likely the polymeric SEI.

9:10 AM – Postdoctoral Researcher Finalist

B-IV-3: DEVELOPMENT OF *IN SITU* MAGNETIC RESONANCE TECHNIQUES TO STUDY LI METAL BATTERIES AND SUPERCAPACITORS IN REAL TIME

[NECCES] Nicole M. Trease[1], Hee Jung Chang[1], Andrew J. Ilott[2], S. Chandrashekar[1,2], Hao Wang[1,3], Thomas J.-K. Köster[3], Lin-Shu Du[1], Alexej Jerschow[2], and Clare P. Grey[1,3].
1. Department of Chemistry, Stony Brook University, Stony Brook, NY 11794.
2. Chemistry Department, 100 Washington Square EAStNew York University, New York, NY 10003.
3. Department of Chemistry, Cambridge University, Lensfield Road, Cambridge CB2 1EW, UK.

In situ NMR/ MRI has proven to be a useful tool to probe the structure of Li-ion batteries (LIBs) during real-time charge and discharge[1-4]. *Ex situ* studies of batteries are limited by self-relaxation of the electrode materials before a measurement can be obtained. The application and further development of advanced magnetic resonance techniques *in situ*, such as MRI and complex NMR experiments, has the potential to monitor dynamics and structural changes in functioning electrochemical systems in real time. Here we present *in situ* NMR/ MRI of Li metal batteries and symmetric carbon based supercapacitors.

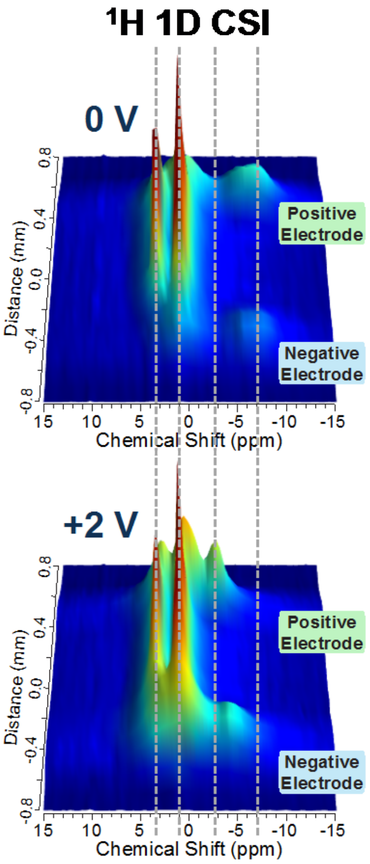


Figure. 1. *In situ* CSI images of an YP17 carbon symmetric supercapacitor at 0V and +2V. Changes in the chemical shift are observed at different voltages indicative of changes in the interaction of the cation with the carbon electrode.

The formation of dendrites on the surface of Li metal poses a serious safety issue and has prevented the mass commercialization of Li metal batteries. To further understand the formation of Li microstructures, *in situ* ^{7}Li NMR/MRI is used. Using chemical shift magnetic resonance imaging (CSI), the spatial information of the MRI image is correlated to the chemical shift information typically associated with NMR allowing both qualitative and quantitative element specific information to be probed *in situ*. This allows the visualization of where specific chemical species are located within the battery. Analysis of the NMR shift and location of the microstructures on the electrodes surface, gives a correlation between the type of microstructure and the NMR shift.

Supercapacitors function based on the separation of the cations and anions of the electrolyte to the negatively and positively charged electrodes, respectively, resulting in the formation of an electrical double layer at the electrode surface. *In situ* NMR studies showed that the anions and cations of the electrolyte in the supercapacitor films are found to be in three different environments[3]. By using CSI we can achieve spatial resolution of each of the different components at the electrode-electrolyte interface providing further insight on the functionality of supercapacitors as depicted in the CSI images in Fig. 1.

REFERENCES

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2. S. Chandrashekar, et al. *Nature Materials.* **2012**, *11*, 311-315.
3. H. Wang, et al. *J. Am. Chem. Soc.*, **2011**, *133*, 19270-19273.
4. N.M. Trease, et al., *Solid State Nucl. Magn. Reson.* **2012**, *42*, 62-70.

C. ORGANIC PHOTOVOLTAICS

Session I: Thursday, July 18, 2013, 10:30 – 12:10; Virginia Suite C

10:50 AM

C-I-1: ENERGETICS OF KEY INTERFACES RELEVANT TO HYBRID PHOTOVOLTAICS

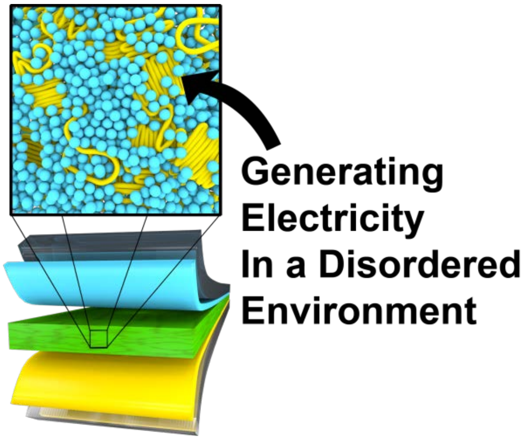
[CISSEM] Neal R. Armstrong,[1] Antoine Kahn[2]
[1]The University of Arizona, [2]Princeton University

We review the fundamental mechanisms of charge carrier extraction in organic bulk heterojunction solar cells, with emphasis placed on the energetics of key interfaces involving transparent metal oxides and other materials of importance for hybrid photovoltaics. We begin with the requirements for high and low work function electrodes for efficient hole and electron extraction contacts, respectively. We review the considerable work done within CISSEM to understand and optimize nickel oxide (NiO_x) as a most promising high work function interlayer, and review evidence that this naturally p-doped large band gap oxide also acts as an efficient electron blocker, and forms interlayers that selectively extract holes while decreasing electron recombination at the anode. We demonstrate how a nm-thin layer of the ultra-high work function molybdenum trioxide (MoO_3) can enhance hole extraction by further p-doping NiO_x, increase its surface conductivity and decrease the hole extraction barrier. Finally, we turn to the “universal” electrode work function-lowering polymer polyethylenimine-ethoxylated (PEIE) and demonstrate how this very versatile, solution processable material can be utilized to enhance built-in fields in organic photovoltaic cells and create effective electron collection electrodes.

11:10 AM – Graduate Student Finalist

C-I-2: CONCERTED PROCESSES IN ORGANIC PHOTOVOLTAICS: THE RELATED CHALLENGES OF GENERATING AND COLLECTING CHARGE IN A DISORDER ENVIRONMENT.

[ANSER] Brett M. Savoie[1]; Henry Heitzer[1]; Brian S. Rolczynszki[1]; Bijan Movaghar[1]; Stephen Loser[1]; Sylvia Lou[1]; Luping Yu[1,2]; Lin X. Chen[1,3]; Tobin J. Marks[1]; Mark A. Ratner[1]
[1]*Northwestern University;* [2]*University of Chicago;* [3]*Argonne National Laboratory*



Remarkable progress has been made towards increasing the efficiencies of organic photovoltaic cells (OPVs) in the past few years, with cells based on solution-processed blends of conjugated polymers and fullerenes routinely showing near unity quantum efficiencies. However, the question of how such high efficiencies can be achieved in disordered materials with low dielectric constants remains unanswered. Existing models based on the Marcus and Onsager frameworks fail to explain many of the experimental results on charge generation, lack predictive power, and offer no insight into the origin of the fullerene's success as an electron acceptor in these systems.

Using a joint theoretical and experimental approach, uniquely achievable through the ANSER Center and involving four center principal investigators, I show that the crucial ingredient for efficient charge generation is the participation of many molecules in the process. Using ultrafast optoelectronic experiments and large-scale many-molecule modeling, we find that aggregates of organic semiconductors, like fullerenes, can sustain delocalized states over several molecules. Critically, these states are robust to disorder, owing to the unique spherical topology of the fullerene component and its degenerate unoccupied electronic levels. Proceeding from this discovery we find that several experimentally observed, but unexplained, features of charge generation can be understood by moving away from single molecule descriptions and considering the emergent properties of ordered arrays of molecules.

These insights into charge generation are complemented by recent work on charge collection from the ANSER Center. Unity quantum efficiencies also imply perfect collection efficiency of the generated charge. However, under operating conditions and away from short circuit, we often observe that collection efficiency drops, resulting in low FF. From recent modeling work and an examination of small molecule systems developed within ANSER, I trace the connection between increased disorder and why many optimized device thicknesses are less than the absorption length of the active materials.

Emphasis is placed throughout on the discovered overlaps between challenges facing both problems, the means for overcoming disorder, and the unique opportunities the collaborations fostered by the ANSER Center have provided.

11:30 AM

C-I-3: MODEL SYSTEMS FOR STUDYING CONJUGATED POLYMER INTERACTIONS

[CST] Zhongjian Hu,[1] Ryan T. Haws,[1] Benjamin Hanson,[2] Robert J. Ono,[1] Michael Tauber,[3] Venkat Ganesan,[2] Christopher W. Bielawski,[1] Peter J. Rossky,[1,2] and David A. Vanden Bout[1]
[1]*Department of Chemistry, The University of Texas at Austin* ; [2]*Department of Chemical Engineering, The University of Texas at Austin*; [3]*Department of Chemistry, University of California, San Diego*

Despite the promise of conjugated polymers for the realization of organic photovoltaics (OPVs), the morphological heterogeneity for films significantly complicates the relationship between their structural and photophysical properties. We have developed two model systems to study isolated interchain interactions in conjugated polymers. The first is a triblock copolymer system consisting of two poly(3-hexylthiophene) (P3HT) chains connected by a flexible linker. The second are small polymer aggregates assembled from single chains. Interactions between the triblock segments can be controlled using solvent quality to create a solution system whose spectroscopy mimics that of a film. Changing the dielectric of the solvent shows that the interacting system has an excited state dominated by charge transfer (CT) character. This state is responsible for quenching the emission in solid-state P3HT and important for understanding charge separation and recombination in OPVs. This is supported by theoretical modeling of two interacting P3HT chains in a variety of dielectric media. Molecular dynamics simulations of the triblock copolymer reveal that two interacting chains are insufficient to reproduce the experimental data. To examine larger systems small polymer aggregates are controllably assembled through solvent vapor annealing of individual polymer chains. Spectroscopy on single thiophene aggregates reveals that excitonic properties evolve from intrachain to interchain characteristic with increasing number of chains in the aggregates. Increasing the packing distance of polymers notably confines the excitonic energy to individual chains. Energy transfer within the aggregates is found to be a function of both alignment of the backbones and length of the sidechains.

11:50 AM

C-I-4: ORGANIC PHOTOVOLTAIC DEVICE PERFORMANCE

[CEEM] Loren G. Kaake[1,2], Yanming Sun[5], Thomas Van der Poll[1,2], Guillermo C. Bazan[1,2], and Alan J. Heeger[1,3,4]
[1]*Center for Energy Efficient Materials, University of California Santa Barbara, Santa Barbara, California 93106-5090, USA;* [2]*Department of Chemistry, University of California Santa Barbara, Santa Barbara, California 93106-9510;* [3]*Department of Physics, University of California Santa Barbara, Santa Barbara, California 93106-9530;* [4]*Materials Department, University of California Santa Barbara, Santa Barbara, California 93106-5050;* [5]*Center for Polymers and Organic Solids, University of California Santa Barbara, Santa Barbara, California 93106-5090, USA*

I will describe recent progress on solution processed organic photovoltaic devices, including a description of the mechanism for ultrafast charge transfer over 10-20 nm in the phase separated nano-morphology. During the absorption process, the momentum of the photon is uncertain. This results in an uncertainty regarding the location of the photoexcitation, which in turn corresponds to an uncertainty in the position of the photoexcitation. Thus, a delocalized wavefunction (a coherent state described as a superposition of the eigenstates of the Hamiltonian of the disordered BHJ material) is created initially, and this transient delocalized wavefunction provides a mechanism for ultrafast charge transfer over relatively long distances. Improving overall device performance requires the formation of interpenetrating percolated networks for both electrons and holes that enable efficient charge extraction. The need for pure materials within the phase –separated

domains will be emphasized, as increased recombination can result from even dilute synthetic by-products. Higher currents and fill factors result from changes brought about by solvent additives, which alter both the initial charge transfer and the transport of the mobile carriers to the electrodes, thus enabling sweep-out of the carriers prior to recombination.

Session II: Thursday, July 18, 2013, 1:40 – 3:20; Virginia Suite C

1:40 PM

C-II-1: MORE THAN ONE ELECTRON PER PHOTON IN A SOLAR CELL

[CE] Dan Congreve, Jiye Lee, Nick Thompson, Eric Hontz, Shane Yost, Troy Van Voorhis, Marc Baldo
Center for Excitonics, Massachusetts Institute of Technology, Cambridge, MA

Singlet exciton fission can be used to split a molecular excited state in two. In solar cells, it promises to double the photocurrent from high energy photons, thereby breaking the single junction efficiency limit. We demonstrate organic solar cells that exploit singlet exciton fission in pentacene to generate more than one electron per incident photon in the visible spectrum. Using a fullerene acceptor, a poly(3-hexylthiophene) exciton confinement layer, and a conventional optical trapping scheme, the peak external quantum efficiency is (109+/-1)% at 670 nm for a 15-nm-thick pentacene film. The corresponding internal quantum efficiency is (160+/-10)%. Independent confirmation of the high internal efficiency is obtained by analysis of the magnetic field effect on photocurrent, which determines that the triplet yield approaches 200% for pentacene films thicker than 5 nm. To our knowledge, this is the first solar cell to generate quantum efficiencies above 100% in the visible spectrum. Alternative multiple exciton generation approaches have been demonstrated previously in the ultraviolet, where there is relatively little sunlight. Singlet exciton fission differs from these other mechanisms because spin conservation disallows the usual dominant loss process: a thermal relaxation of the high-energy exciton into a single low-energy exciton. Consequently, pentacene is efficient in the visible spectrum at 670 nm because only the collapse of the singlet exciton into *two* triplets is spin-allowed.

2:00 PM

C-II-2: UNDERSTANDING MEG FOR PHOTOVOLTAIC OPPORTUNITIES

[RPEMSC] David Reichman
Department of Chemistry, Columbia University

Multiple exciton generation (MEG), a process whereby a single photon may be converted into multiple electron-hole pairs, has been proposed as a means of circumventing the Shockley-Queisser (SQ) limit and thereby increasing the efficiency of photovoltaic devices. In this talk I will discuss progress towards understanding and harnessing variants of the MEG process in organic crystals as well as layered inorganic materials.

2:20 PM – Postdoctoral Researcher Finalist

C-II-3: PREDICTING AND UNDERSTANDING THE SINGLET FISSION RATE: A COMBINED THEORETICAL AND EXPERIMENTAL EFFORT

[CE] Shane R. Yost[1], Jiye Lee[2], Mark W. B. Wilson[1], David P. McMahon[1], Rebecca R. Parkhurst[1], Nicholas J. Thompson[2], Akshay Rao[3], Kerr Johnson[3], Matthew Y. Sfeir[4], Moungi Bawendi[1], Timothy M. Swager[1], Richard H. Friend[3], Marc A. Baldo[2], and Troy Van Voorhis[1]

[1]Department of Chemistry and [2]Department of Electrical Engineering and Computer Science, Massachusetts Institute of Technology, 77 Massachusetts Ave. Cambridge, MA 02139; [3]Cavendish laboratory, University of Cambridge, JJ Thomson Avenue, Cambridge CB30HE, UK. [4]Center for Functional Nanomaterials, Brookhaven National Laboratory, Building 735, Upton, New York 11973

Exciton fission is a process whereby one singlet exciton splits into two independent triplets. Because fission generates two triplet excitons from a single high energy photon, fission-based solar cells could lead to single junction photovoltaics with power conversion efficiencies above 40%[1]. Here, we measure fission dynamics using ultrafast photoinduced absorption and derive a first principles expression for the singlet fission rate. Our results show that the experimental rates are consistent with a nonadiabatic Marcus-like mechanism in weakly interacting systems and an adiabatic, coupling independent pathway at larger interaction strengths. For a range of electronic couplings covering three orders of magnitude, we predict near unit fission efficiency in any material where fission is energetically favored. This is confirmed experimentally, as we observe high fission yields even in materials where molecules are orthogonally oriented at large separations (>5 Å). We conclude that singlet exciton fission in thin films is robust against variations in molecular structure. The success of this kinetic model simplifies the rational design of fission materials. Crucial molecular properties such as solubility and energy level alignment can be safely tailored by functionalizing an active core while maintaining a high quantum yield.

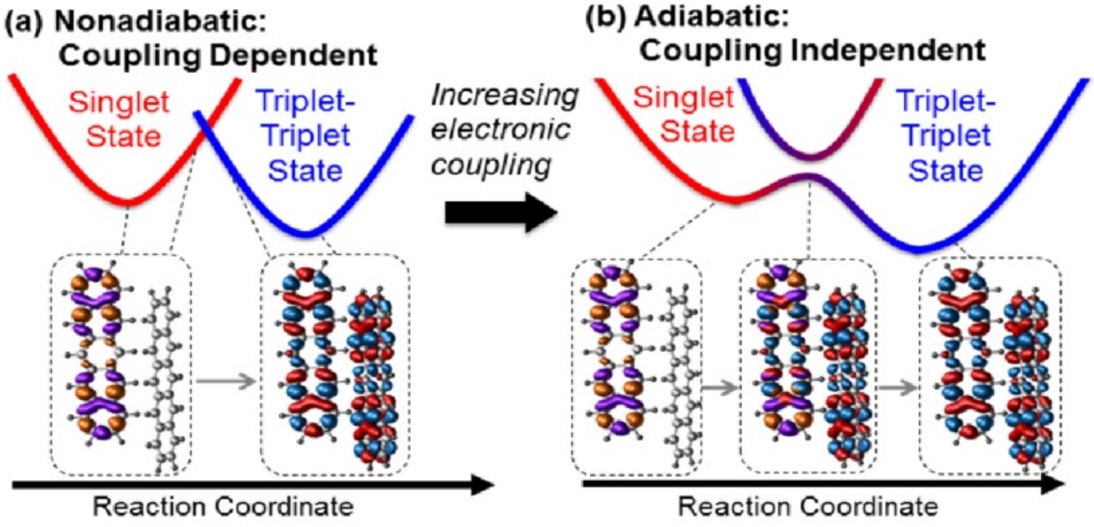


Figure 1. As the coupling between the singlet and triplet-triplet states increases the fission process transitions from nonadiabatic (a) to adiabatic (b) energy transfer. In the nonadiabatic regime transitions between electronic states is abrupt, and the rate is coupling dependent. In the adiabatic case the electronic state changes continuously from singlet to triplet-triplet, and the rate becomes coupling independent.

1. Smith, M. B. & Michl, J. Singlet Fission. *Chemical Reviews* **110**, 6891-6936 (2010).

2:40 PM

C-II-4: EXCITON MANAGEMENT IN ORGANIC PHOTOVOLTAICS

[CEN] Mark E. Thompson, Stephen E. Bradforth, Sean Roberts, Robert McAnally, Joseph Mastron
University of Southern California

A key aspect in controlling the efficiency of organic photovoltaics (OPVs) is managing the energy and spin of the excitons formed on optical excitation of the donor and acceptor materials. Our studies take several important directions, including both the efficient and broadband absorption of solar energy and the use of singlet fission to enhance exciton formation. This talk will focus on our work with singlet fission materials. We have used ultrafast transient absorption and time resolved emission experiments performed on 5,12-diphenyltetracene (DPT), 5,12-dinaphtyltetracene (DNT) and 6,13-bis-diethylphenylpentacene (DPP) to investigate singlet fission in these materials. Unlike tetracene, which tends to form polycrystalline films when vapor deposited, the pendant phenyl groups of DPT, DNT and DPP frustrate crystal growth, yielding amorphous films. Despite the high level of disorder in these films, we find that DPT and DNT exhibit a surprisingly high singlet fission yield, with 1.2 triplets being created per excited singlet. This triplet production occurs over two principal time scales, with ~50% of the triplets appear within 1 ps after photoexcitation followed by a slower phase of triplet growth over a few hundred picoseconds. To fit these kinetics, we have developed a model that assumes that due to molecular disorder, only a subset of DPT or DNT dimer pairs adopt configurations that promote fission. Singlet excitons directly excited at these sites can undergo fission rapidly, while singlet excitons created elsewhere in the film must diffuse to these sites to fission. We will discuss OPVs with these materials and supplemental absorbers.

3:00 PM

C-II-5: RETHINKING SPECTROSCOPY – UNRAVELING COHERENT EXCITON DYNAMICS WITH ULTRAFAST QUANTUM PROCESS TOMOGRAPHY

[CE] Alan Aspuru-Guzik,[1] Moungi Bawendi[2] and Keith Nelson[2]
[1]Dept of Chemistry, Harvard University, Cambridge, MA, [2]Center for Excitonics, Massachusetts Institute of Technology, Cambridge, MA

Recently, long-lived room-temperature exciton coherences have been observed in photosynthetic complexes by means of non-linear ultrafast optical spectroscopy. These observations pose a challenge for the synthesis of artificial condensed-phase systems that support this long-lived coherences. In addition, more advanced tools for the characterization and detection of coherent oscillations in these systems are necessary. Typical ultrafast experiments only report on specific projections of the optical response of the material to the electric field, which yield only partial information about the coherent and incoherent exciton dynamics in the systems. Ambiguity in the measured signals has led to many arguments in the literature about the source of quantum coherence. We propose a quantum process tomopgraphy (QPT) protocol amenable for the limited control of current nonlinear optical settings. We apply this protocol to fully characterize the quantum dynamics of a system consisting of the inner and outer walls of a self-assembled double-walled cynanine nanotube at room tempreature. For achieving this, we processed the data stemming from eight transient grating experiments with different pulse spectrum configurations. The quantitative analysis of the data reveals unidirectional energy transfer from the outer to the inner wall exciton bands, as well as an unexpected electronic coherence between those two states which lasts for about 200 femtoseconds, indicating substantial electronic coupling between the walls. The accurate characterization of the exciton dynamics for this system constitutes a crucial step for its rational incorporation into engineered light-harvesting architectures. Our work constitutes the first experimental QPT in a condensed molecular system, and provides a simple protocol to adapt and extend standard spectroscopic experiments so that they provide the largest amount of information possible about molecular systems.

Session III: Thursday, July 18, 2013, 3:40 – 5:00; Virginia Suite C

3:40 PM

C-III-1: CONTROL OF NANOSCALE ARCHITECTURE IN SOLUTION-PROCESSED POLYMER-BASED PHOTOVOLTAICS

[MEEM] Samson A. Jenekhe[1], Nikos Kopidakis[2], Daniel Neuhauser[3], Yves Rubin[3], Benjamin J. Schwartz[3], and Sarah H. Tolbert[3]

[1]University of Washington, Seattle; [2]National Renewable Energy Laboratory; [3]University of California, Los Angeles

In this work, we combine materials synthesis and self-assembly, spectroscopy, device fabrication, and quantum chemistry to understand how control over nanoscale architecture can be used to tune performance in solution-processed polymer-fullerene photovoltaics. Our work on novel fullerene derivatives has focused on understanding how the interplay between fullerene energy level and polymer/fullerene intermolecular interactions controls device performance. We have also been examining 'shuttlecock' fullerenes that self-assemble into well-defined one-dimensional stacks in devices. To understand how stacking affects device performance, we have used a combination of time-resolved microwave conductivity and theoretical calculations to examine the local versus global mobility of carriers. We have shown that in polymer/fullerene devices, both local and macroscopic carrier mobility need to be optimized to produce high power conversion efficiencies, and we have developed design rules for new fullerene derivatives that should achieve this goal. We also have been controlling nm-scale architecture using sequential processing, where the polymer is first deposited and fullerene is then infiltrated into the polymer network from an orthogonal solvent. This method avoids the pitfalls of processing kinetics that can lead to irreproducibility in BHJs, and we are exploring a range of new polymers to understand how crystallinity controls fullerene incorporation. Finally, we have been exploring water-soluble polymers and fullerenes, using amphiphilic assembly to create well defined nanoscale architectures. While device work is still in progress, we have shown that we can create systems with architectures optimized to rapidly separate electrons and holes and keeps those carriers apart on the hours to days time-scale.

4:00 PM

C-III-2: MULTI-LENGTH SCALE MORPHOLOGIES IN POLYMER-BASED ORGANIC PHOTOVOLTAIC ACTIVE LAYERS

[PHaSE] Thomas P. Russell

Department of Polymer Science and Engineering, University of Massachusetts, Amherst, MA 01003, USA

Single layer organic photovoltaic devices have now reached efficiencies in excess of 10%, with tandem devices achieving efficiencies of 12% and performance that is comparable to, if not better, than amorphous silicon. Key to these advances have been gaining an understanding of the morphology of the active layers and developing new strategies to tailor the morphology to optimize performance. For simple, spin-coated active layers, we have quantitatively demonstrated that bulk heterojunctions arise from the ordering of photoactive polymer. With low bandgap polymers, on the other hand, we have shown that the use of an additive that selectively solubilizes the fullerene-based based component leads to a multi-length scale morphology. A fibrillar network structures is generated in solution that establishes a framework within which a finer texture is produced. An

alternate strategy that is being pursued for active layer fabrication is based on the co-assembly of hole- and electron-transporting nanoparticles (NPs) where, by spray and water-based coating processes, the interactions between the NPs gives rise to a bicontinuous, multi-length scale morphology, suitable for PV applications. This approach offers the distinct advantage of affording the opportunity to tailor the hole-conducting polymer to optimize performance.

Research was done in collaboration with M. Barnes, A. Briseño, A. Dinsmore, T. Emrick, J. Hsu (UT Dallas), W. H.Jo (Seoul National U), D. Maroudas, R. Hayward, D. Venkataraman

4:20 PM

C-III-3: LYOTROPIC LIQUID CRYSTALLINE CONJUGATED POLYMER WITH DIRECTED ALIGNMENT CAPABILITY FOR PLASTIC ELECTRONICS

[CSTEC] Bong-Gi Kim[1], Eun J. Jeong[2], Sungbaek Seo[1], John Kieffer[2], Emmanouil Kioupakis[2], Jinsang Kim[1,2,3]
[1]Macromoelcular Science and Engineering, University of Michigan, Ann Arbor, MI 48109; [2]Materials Science and Engineering, University of Michigan, Ann Arbor, MI 48109; [3]Chemical Engineering, University of Michigan, Ann Arbor, MI 48109

Conjugated polymers (CPs) are emerging active materials for various optoelectronic applications, such as organic solar cells, thin film transistors, light emitting diodes, as well as optical and amperometric sensors. Their optical and electronic properties, such as absorption, emission, and conductivity, are highly anisotropic due to the 1-dimensional p-orbital overlap along the CP backbone. In consequence, unless conjugated polymers are molecularly and macroscopically assembled and aligned with a well-defined structure, their interesting properties cannot be fully realized in their device applications. In reality, however, the directed assembly and particularly macroscopic alignment of CPs is a challenging task.

We systematically investigated and established a molecular design principle of CPs to achieve concentration-regulated chain planarization, self-assembly, liquid crystal-like good mobility, non-interdigitated side chains, and ensuing chain alignment along an applied flow field. A thin film transistor built on highly aligned CP films showed more than three orders of magnitude faster carrier mobility along the CP alignment direction than the perpendicular direction. The established molecular design principle for directed alignment of CPs is readily applicable to many useful CP developments for various optoelectronic devices and to achieve the full realization of the anisotropic properties of CPs in devices such as photovoltaic cells. Strategic combination of the developed lyotropic liquid crystalline CP design rules, rationally devised chemical structures of CP for an intrinsic intramolecular high hole mobility, and a novel fabrication scheme may open the door to wet-processable high performance plastic electronics. CSTEC researchers have been collaborating to head toward such organic photovoltaics.

Reference: Bong-Gi Kim, Eun Jeong Jeong, Jong Won Chung, Sungbaek Seo, Bonwon Koo, Jinsang Kim "A Molecular Design Principle of Lyotropic Liquid-Crystalline Conjugated Polymers with Directed Alignment Capability for Plastic Electronics" ***Nature Materials*** **2013** DOI:10.1038/nmat3595.

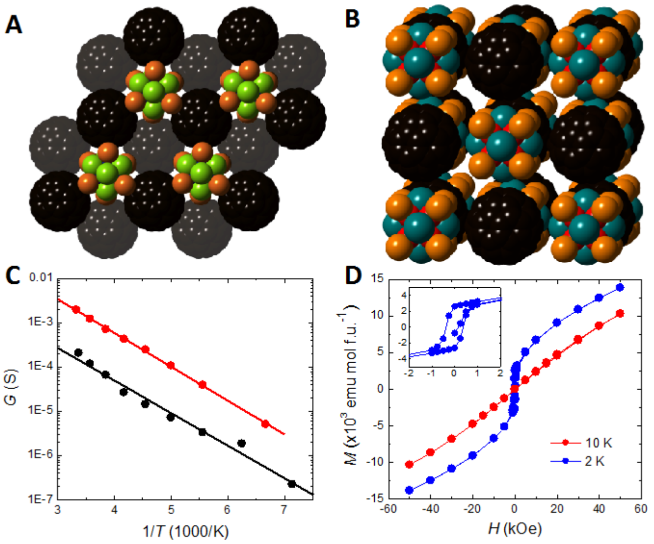
4:40 PM – Postdoctoral Researcher Finalist

C-III-4: NANOSCALE ATOMS IN SOLID-STATE CHEMISTRY

[RPEMSC] Xavier Roy[1], Chul-Ho Lee[1,2], Andrew C. Crowther[3], Christine L. Schenck[1], Tiglet Besara[4], Roger A. Lalancette[6], Theo Siegrist[4,5], Peter W. Stephens[7], Louis E. Brus[1], Philip Kim[2], Michael L. Steigerwald[1], Colin Nuckolls[1]

[1]Department of Chemistry, Columbia University, New York, NY 10027 (USA) *http://nuckolls.chem.columbia.edu/*; *[2]Department of Physics, Columbia University, New York, NY 10027 (USA); [3]Department of Chemistry,* Barnard *College, New York, NY 10027 (USA); [4]National High Magnetic Field Laboratory, FSU, Tallahassee, FL 32310 (USA); [5]Department of Chemical and Biomedical Engineering, FAMU-FSU College of Engineering, Tallahassee, FL 32310 (USA); [6]Department of Chemistry, Rutgers State University, Newark, NJ 07102 (USA); [7]Department of Physics and Astronomy, SUNY Stony Brook, Stony Brook, NY 11794 (USA)*

Conventional binary solid-state compounds, A_xB_y, are infinite, crystalline arrays of atoms A and B. In this work, we describe analogous binary solids in which the 'atomic' building blocks are pseudo-spherical molecular clusters rather than simply atoms. We combine independently prepared electronically and structurally complementary molecular cluster building blocks to form atomically precise binary solid-state compounds. When the building blocks are atoms (ions), binary solids assemble into simple crystalline arrays such as the rock-salt and CdI_2 lattices. We show that when similarly-sized clusters combine the same lattice results, albeit at the dramatically increased length scale of nanometers rather than Angstroms. The internal structures of the constituent clusters remain unchanged, but charge is transferred between them, forming ionic solids analogous to NaCl. We show that we can tune the structural, electronic, and magnetic properties of our artificial atoms and assemble crystalline solids that exhibit collective physical properties. In these materials, the constituent clusters are able to interact electronically and the assemblies show activated electrical transport with activation energies of 100 to 150 meV and spontaneous magnetic ordering at low temperature, akin to atoms in a solid-state compound. These results chart a clear path to creating whole families of multi-functional solid-state materials whose electronic and magnetic properties can be tuned by varying the constitution of the superatom building blocks.



Space filling molecular structure of (A) $Co_6Se_8(PEt_3)_6 \bullet 2C_{60}$ showing the crystal packing looking down the *ab* plane and of (B) $Ni_9Te_6(PEt_3)_8 \bullet C_{60}$. Carbon, black; nickel, red; cobalt, blue; phosphorus, orange; tellurium, teal; selenium, green. The ethyl groups on the phosphines were removed to clarify the view. (C) Plot of the conductance (*G*) vs. 1/*T* for $Co_6Se_8(PEt_3)_6 \bullet 2C_{60}$. The four probes conductance measurements were done on a single crystal (black) and a pressed pellet (red). The Arrhenius fits are shown as solid lines. (D) Magnetization (*M*) as a function of applied field (*H*) at 10 K and 2 K for $Ni_9Te_6(PEt_3)_8 \bullet C_{60}$. The inset shows the enlarged magnetic hysteresis at 2 K.

Session V: Friday, July 19, 2013, 11:00 – 12:00; Virginia Suite C

11:00 AM

C-V-1: THE SCIENCE BEHIND MOLECULAR INTERFACE MODIFIERS: FROM MOLECULAR STRUCTURE TO SOLAR CELL PERFORMANCE

[CISSEM] David S. Ginger,[1] Jeanne E. Pemberton[2]
[1]University of Washington, [2]The University of Arizona

We describe the development and application of a unique set of experimental and theoretical tools to understand how molecular interface modifiers control performance in thin film organic solar cells. At the device level, molecular interface modifiers can be used to improve the performance of solution-processed organic photovoltaics by modifying contact wettability, work function, and carrier selectivity. From the molecular perspective, we present highly-integrated, foundational studies of molecular binding modes of contact surface modifiers that show good agreement between molecular attachment geometries predicted by theory, measured using laboratory-scale surface spectroscopy, and measured using synchrotron experiments conducted at U.S. DOE user facilities. We vertically integrate these studies with a device-level perspective using model photodiodes to elucidate the changes in internal electric fields brought about by interface modification and demonstrate the modified contacts' unexpected deviation from the Schottky-Mott limit. Finally, we show how we are using these materials to validate new tools to look for variations in recombination losses due to nanoscale heterogeneity in widely used transparent conductive oxides.

11:20 AM

C-V-2: INTERFACE SCIENCE OF ORGANIC PHOTOVOLTAICS

[ANSER] Brett M. Savioe[1], Nanjia Zhou[1], Sylvia J. Lou[1], Xugang Guo[1], Amod Talmisina[1], Matthew R. Leonardi[1], Charles K. Song[1], Jodi M. Szarko[1], Brian S. Rolczynski[1], Hui Lin[1], Kyle A. Luck[1], Sylvia J. Lou[1], Xinge Yu[1], Peijun Guo[1], Hui Huang[1], Nicholas Jackson[1], Tobias Harschneck[1], Patrick Hartnett[1], Tao Xu[2], Tejas A. Shastry[1], Erika E. Swartz[1], Joseph Strzalka[3], Benjamin J. Leever[4], Richard H. Friend[5], Juan Bisquert[6], Lin X. Chen[1,3], Mark A. Ratner[1], Robert P.H. Chang[1], Mark C. Hersam[1], Luping Yu[2], Michael R. Wasielewski[1], Antonio Facchetti[1], Tobin J. Marks[1]
[1]Northwestern University, [2]University of Chicago, [3]Argonne National Laboratory, [4]Air Force Research Laboratory, [5]Cambridge University, [6]Universitat Jaume I

The ability to fabricate molecularly tailored interfaces with nanoscale precision can 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 decohesion. For soft matter-soft matter interfaces, it can facilitate exciton scission and photocurrent generation in such cells. In this lecture, challenges and opportunities in organic photovoltaic interface science are illustrated for three 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 orientational organization at electrodes, 3) controlling exciton dynamics and carrier generation at donor-acceptor interfaces in the active layer. It will be seen that such rational interface engineering along with improved bulk-heterojunction polymer structures guided by

theoretical/computational analysis affords solar power conversion efficiencies greater than 9% along with far greater cell durability.

11:40 AM

C-V-3: FUNCTIONAL CONJUGATED POLYMERS: ORGANIZED NANOCOMPOSITES AND INTERLAYER MATERIALS

[PHaSE] Todd Emrick

Department of Polymer Science and Engineering, University of Massachusetts, Amherst, MA 01003, USA

This presentation will describe efforts to prepare new functional conjugated polymers for improving solar cell performance. In one example, conjugated polymers are equipped with chain-end functionality for coordination to semiconductor nanoparticles and nanorods. The polymer component is hole transporting, and the nanoparticle component is electron transporting, such that the organized combination of these two materials has the potential for improving charge transport and solar cell efficiency. In a second example, conjugated polymers are decorated with pendent dipoles, making them suitable to serve as interlayer materials at the active layer/cathode interface. The orthogonal solubility of these interlayer polymers, relative to the active layer polymer, enables sequential deposition by spin-coating and gives large improvements in solar cell efficiency.

D. INORGANIC PHOTOVOLTAICS

Session III: Thursday, July 18, 2013, 3:40 – 5:00; Salon 3

3:40 PM

D-III-1: OPTICAL PROPERTIES OF NOVEL ATOMICALLY THIN MATERIALS

[RPEMSC] Tony F. Heinz

Departments of Physics and Electrical Engineering, Columbia University

The fascinating properties of graphene have inspired the research community to examine the broader class of stable, atomically thin materials. There is particular interest in novel semiconducting materials. Here we discuss recent advances in the study of atomically thin layers of MoS_2 as representative of the broader class transition metal dichalcogenides. These materials can be produced by exfoliation of bulk crystals, but can also be synthesized using chemical vapor deposition methods. We will describe the properties of such films and of the structure and influence of grain boundaries. Although the physical structure of the monolayer of MoS_2 is similar to that of graphene from the point of view of symmetry, the A and B sublattices in MoS_2 are distinct. This difference allows MoS_2 to be a semiconductor with a significant band gap. Through characterization of the optical properties of the material as a function of thickness, we show that quantum confinement effects lead to a crossover in MoS2 from an indirect gap semiconductor in the bulk to a direct gap semiconductor at monolayer thickness. As expected for lower-dimensional materials, we show that excitonic effects are strong in monolayer MoS_2. This leads to charged excitons that are stable even at room temperature. The mechanical integrity of ultrathin films of these materials permits the fabrication of novel heterostructures. We will discuss the distinctive properties of two components systems formed from pairs of transition metal dichalcogenides and from a single transition metal dichalcogenide in contact with a graphene monolayer.

4:00 PM – Postdoctoral Researcher Finalist

D-III-2: PHOTOTROPIC GROWTH CONTROL OF NANOSCALE PATTERN FORMATION IN PHOTOELECTRODEPOSITED SE–TE FILMS

[LMI] Bryce Sadtler[1]; Stanley P. Burgos[2]; Nicolas A. Batara[2]; Joseph A. Beardslee[1]; Harry A. Atwater[2,3]; Nathan S. Lewis[1,3,4]

[1] Division of Chemistry and Chemical Engineering; [2] Applied Physics and Materials Science Department;
[3] Kavli Nanoscience Institute; [4] Beckman Institute, California Institute of Technology, Pasadena CA 91125

Photoresponsive materials that adapt their growth rates dynamically to the local incident electromagnetic field would provide a remarkable route to the synthesis of complex three-dimensional mesoscale structures. Such light-mediated growth processes could enable the design of a variety of energy conversion materials such as self-assembled photonic devices, 3-D electrode architectures, chiral and negative index metamaterials, as well as optoelectronic devices that exhibit wavelength- and polarization-selective photoconductivity. We report the observation of light-mediated growth in an inorganic system and consequently demonstrate the ability to create complex, nanostructured materials via feedback between illumination and the morphology that develops in response to optical excitation. Ordered nanoscale lamellar patterns developed spontaneously in electrodeposited selenium–tellurium (Se–Te) alloy films grown under uniform illumination on unpatterned substrates in an isotropic electrolyte solution. These inorganic nanostructures exhibited phototropic growth in which the lamellar stripes grew towards the incident light source, adopted an orientation parallel to the light polarization direction, and showed an increased growth rate with increasing light intensity (see Figure 1). The illumination wavelength controlled the lamellar period, which varied from 130 nm for ultraviolet light to 412 nm for near-infrared light. Furthermore, the patterns responded dynamically to changes during growth in the polarization, wavelength, and angle of the incident light, enabling the template-free and pattern-free synthesis of woodpile, spiral, branched, or zigzag structures. Full-wave electromagnetic simulations were used to model the absorption profile of nanostructured Se–Te films. To simulate feedback between the local absorption and film growth, an iterative model was used in which the photocarrier generation rate calculated from the electromagnetic simulations controlled the local deposition rate in Monte Carlo simulations of the evolution of the surface. This model reproduced the experimentally observed nanoscale lamellar patterns and also reproduced their dependence on the wavelength and polarization of the incident illumination. The simulations and experiments indicate that phototropic growth is an emergent resonant phenomena that occurs dynamically during film growth in response to the incident illumination conditions, providing the ability to grow structures of entirely different geometries, periods, and directions abruptly on top of one another, and the ability to change the physical growth direction of the material by changing the direction of the incident light beam.

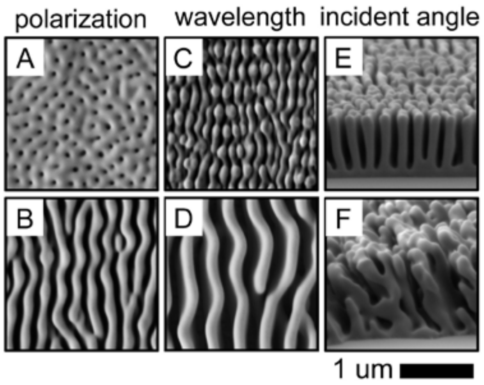


Figure 1. Phototropic growth control of selenium–tellurium films. Nanoscale patterns grown under (A) randomly polarized and (B) linearly polarized, 625 nm illumination. Patterns grown under (C) 405 nm and (D) 940 nm, linearly polarized illumination. Cross-sectional images of patterns grown under (E) normal incident, 625 nm illumination and (F) 625 nm illumination at an angle of 60° from normal.

4:20 PM

D-III-3: TAILORING OPTICAL AND QUANTUM CONFINEMENT TO ENHANCE THE PERFORMANCE OF PEC DEVICES

[CNEEC] Stacey Bent[1], Mark Brongersma[2], Bruce Clemens[2], Shanhui Fan[3], David Goldhaber-Gordon[4], Thomas Jaramillo[1], Friedrich Prinz[5], Robert Sinclair[2], Xiaolin Zhang[5]

[1]Department of Chemical Engineering, Stanford University, California 94305, United States; [2]Department of Materials Science and Engineering, Stanford University, California 94305, United States; [3]Department of Electrical Engineering, Stanford University, California 94305, United States; [4]Department of Physics, Stanford University, California 94305, United States; [5]Department of Mechanical Engineering, Stanford University, California 94305, United States

In solar energy harvesting devices, one is often faced by the challenge of whether one should realize devices featuring a high-efficiency-at-high-cost or a low-efficiency-at-low-cost. This dichotomy can be overcome if high-efficiency thin-film devices can be made a reality. The only plausible route to achieve such devices is by exploiting physical phenomena capable of a) dramatically enhancing the light absorption per unit volume of active semiconductor material and b) facilitating a new level of control over where the light is absorbed in a solar energy harvesting device. Whereas optical and quantum confinement effects are well-established as physical phenomena that can dramatically enhance light absorption in semiconductor materials, their application towards realizing dramatic increases in the efficiency of ultrathin-film photoelectrochemical (PEC) devices for water splitting is only in its infancy. In this presentation, several collaborative research efforts within the Center on Nanostructuring for Efficient Energy Conversion (CNEEC) are discussed that illustrate how these two phenomena can be tailored at the nanoscale and employed judiciously in PEC devices to enhance their performance. We show that performance enhancements can naturally result from a better match of the critical optical length-scales (absorption depth of sunlight) and electronic length-scales (charge carrier diffusion length).

4:40 PM

D-III-4: MAXIMIZING LIGHT ABSORPTION IN NANOSTRUCTURES

[LMI] Harry A. Atwater, Emily D. Kosten, Dennis M. Callahan, Kelsey Whitesell, Bryce Sadtler, Nathan S. Lewis

California Institute of Technology, Pasadena, CA 91125

We describe three approaches to maximizing light absorption in nanostructures using superlattice photonic crystals, angle restriction of radiative emission, and light-directed absorber layer growth. Broadband solar light absorption can be increased through the use of photonic crystals by generating modes in the frequency range where photovoltaic absorbers are optically thin. Appropriately designed superlattice and defect mode photonic crystals can approach the $4n^2$ light-trapping limit for < 5 μm thick Si layers, and we discuss approaches to exceeding this limit. In a conventional flat plate solar cell under direct sunlight, light is received from the solar disk, but is re-emitted isotropically. This isotropic emission corresponds to a significant entropy increase in the solar cell, with a corresponding drop in efficiency. We show that limiting the emission angle of a high-quality GaAs solar cell is a feasible route to achieving power conversion efficiencies above 38% with a single junction. The highest efficiencies are predicted for a thin, light-trapping cell with an ideal back reflector, though the scheme is robust to a non-ideal back reflector. Comparison with conventional planar cell geometries illustrates that limiting emission angle in a light trapping geometry not only allows for much thinner cells, but also for significantly higher overall efficiencies with an excellent rear reflector. Light-directed phototropic growth of semiconductors enables one to create complex, nanostructured semiconductor materials via feedback between illumination and

the morphology that develops in response to optical excitation. Ordered nanoscale lamellar patterns developed spontaneously in electrodeposited selenium–tellurium (Se–Te) alloy films grown under uniform illumination on unpatterned substrates in an isotropic electrolyte solution. These inorganic nanostructures exhibited phototropic growth in which lamellar stripes grew towards the incident light source, adopted an orientation parallel to the light polarization direction, and showed an increased growth rate with increasing light intensity.

Session IV: Friday, July 19, 2013, 8:30 – 9:30; Salon 3

8:30 AM – Graduate Student Finalist

D-IV-1: HYPERVALENT SURFACE INTERACTIONS FOR COLLOIDAL STABILITY AND DOPING OF SILICON NANOCRYSTALS

[CASP] Lance M. Wheeler[1], Nathan R. Neale[2], Ting Chen[1], Uwe R. Kortshagen[1]
[1] *University of Minnesota, 111 Church St. SE, Minneapolis, MN 55414, United States*
[2] *National Renewable Energy Lab, 15013 Denver West Parkway, Golden, Colorado 80401, United States*

Solar cells based on colloidal nanocrystals (NCs) are a prominent example of so-called third-generation of photovoltaics (PVs), which seek high efficiencies from low cost devices through exploitation of advanced physical phenomena. NCs can be inexpensively processed from solution in the same way numbers are screen-printed onto little league baseball jerseys. At the same time, they offer the unique ability to capture the excess energy of solar photons that is lost as heat in conventional PV devices by creating extra current through a process known as multiple exciton generation (MEG).

MEG is now routinely measured in NCs isolated in solution; however, multiple excitons are only useful for harnessing solar energy if they can be efficiently extracted when assembled into a PV device. There are two significant barriers to achieving this. The first is coping with the insulating ligands on the NC surfaces that provide the colloidal stability needed to deposit thin film devices. Secondly, the use of intentional impurities, or dopants, is paramount to achieving conductive films and internal electric fields needed for efficient charge carrier extraction. Recently, we demonstrated a new surface chemistry technique that confronts both of these challenges *simultaneously*.[1] Silicon NCs featuring chlorine termination exhibit a unique surface polarization that renders surface silicon atoms electron deficient, and therefore Lewis acidic and susceptible to hypervalent interactions with donor molecules. These donor molecules not only stabilize NCs into colloidal solution *without ligands*, but also produce controllable *n*-type doping in the NCs that can be retained in deposited films.

We believe this study on silicon NCs is a proof-of-concept of a more general approach to providing colloidal stability, facile thin film deposition, and doping of NCs. Thus, it may represent only the first of many efforts to explore the application of hypervalent interactions between a range of NC materials and surface dopants for improved performance in NC-based PV devices.

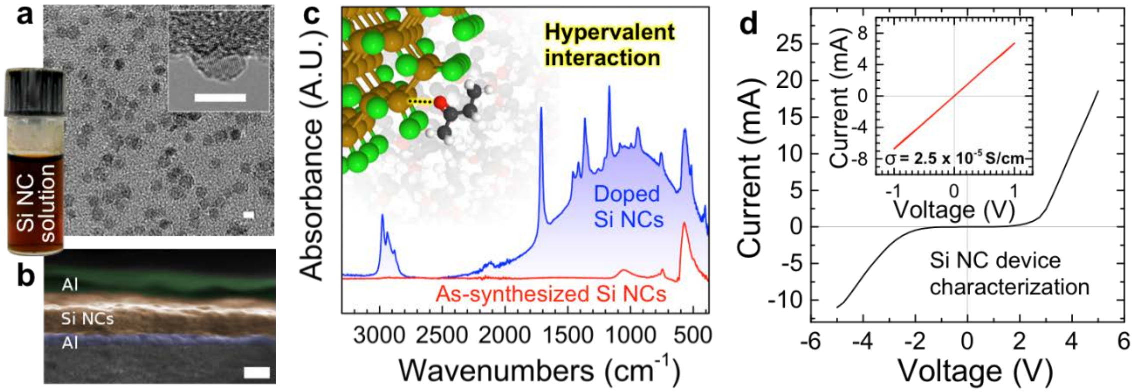


Figure 2: Cl-terminated Si NCs form a stable colloidal solution Lewis basic solvents. Si NCs are solvated without bound ligands, which can be seen the transmission electron micrograph (a) (scale is 8 nm). Films of Si NCs can be cast from the solution to fabricate optoelectronic devices (b) (scale is 2 µm). Colloidal stability is derived from hypervalent interactions at the Si NC surface. The interaction also provides doping, observed as a free carrier absorption using infrared spectroscopy (c, blue spectrum). Preliminary experiments suggest these carriers are active in optoelectronic devices (d).

References: 1. Wheeler, L. M. *et al*. *Nature Communications* (accepted).

8:50 AM

D-IV-2: SOLAR CELLS AND LEDS BASED ON NANOSTRUCTURED SEMICONDUCTORS

[CEN] P. Daniel Dapkus, Yenting Lin, Ting Wei Yeh, Chun Yung Chi, Maoqing Yao, Chongwu Zhou
University of Southern California

Nanowires and nanosheets have proven to be important materials structures to consider for future generations of high performance but low cost solar cells and light emitting diodes (LEDs). Owing to their small lateral dimensions, these nanostructures can potentially allow integration of materials with differing lattice constants without the formation of dislocations and also allow their synthesis on low cost substrates. Furthermore, the nanostructures themselves are bounded by crystalline facets that present opportunities for fabrication of three dimensional active region structures that enhance light generation in LEDs and carrier collection in solar cells. In the Center for Energy Nanoscience we have explored nanostructures in GaAs and other materials for the assembly of tandem solar cells and InGaN / GaN nanostructures for the fabrication of efficient, reduced-droop LEDs for solid state lighting. In this talk, we will present the common principles that apply to the growth of these structures by selective area growth. We will describe how the structures can enhance the performance of both types of devices and show that sufficient science is now developed that will allow their fruitful exploitation in both device types. Finally, we will describe the performance of InGaN/GaN core-shell nanowire LEDs that exhibit nearly monochromatic emission in the blue and green region of the spectrum and describe how this process may be extended to the fabrication of phosphor – free RGB white LEDs.

9:10 AM

D-IV-3: MAKING THE MOST OF A SOLAR PHOTON: *SEMICONDUCTOR NANOCRYSTALS AND SOLAR ENERGY CONVERSION*

[CASP] Lazaro A. Padilha,[1] John T. Stewart,[1] Wan Ki Bae,[1] Weon-kyu Koh,[1] Jeffrey M. Pietryga,[1] Aaron G. Midget,[2] Joseph M. Luther,[2] Matthew C. Beard,[2] Arthur J. Nozik,[2] Victor I. Klimov[1]
[1]Chemistry Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545; [2]Chemical and Material Sciences Center, National Renewable Energy Laboratory, Golden, Colorado 80401

This presentation provides an overview of research activities in the Center for Advanced Solar Photophysics (CASP) in the area of spectroscopy of semiconductor nanocrystals, with emphasis on processes relevant to solar energy conversion. One such process is carrier multiplication (CM) whereby absorption of a single photon produces multiple electron-hole pairs (excitons). Potentially, it can boost the efficiency of single-junction photovoltaics (PVs) to above 40% by increasing the photocurrent. The first spectroscopic observation of efficient CM in PbSe quantum dots (Schaller & Klimov, *Phys. Rev. Lett*. **92**, 2004) stimulated fervent activity in this area, including spectroscopic and theoretical studies of multiexciton generation and extraction, the development of practical devices exploiting CM, as well as theoretical modeling of CM-based solar cells. CASP's demonstration of *p-n* junction nanocrystal PVs with greater-than-unity external quantum efficiencies (Semonin *et al*., *Science* **334***,* 2011) establishes the relevance of this process to practical photovoltaic technologies. This presentation overviews CASP's recent progress in the understanding of CM in quantum-confined nanostructures, and our efforts on the development of materials with enhanced CM performance. Specifically, it will describe experimental results on the effect of structural parameters such as nanocrystal size, shape, and composition on multiexciton yields and discuss them within a phenomenological framework that treats CM in terms of two competing energy relaxation pathways. It will also overview CASP's efforts on structurally engineered nanocrystals with enhanced CM achieved by controlling parameters such as electron-electron Coulomb coupling and the rate of intraband energy losses.

Session V: Friday, July 19, 2013, 11:00 – 12:00; Salon 3

11:00 AM

D-V-1: RECENT PROGRESS IN QUANTUM-DOT SOLAR CELLS: *ACHIEVING QUANTUM EFFICIENCIES GREATER THAN UNITY*

[CASP] Joseph M. Luther,[1] Jianbo Gao,[1] Jason Tolentino,[2] Rachelle Ihly,[2] Octavi E. Semonin,[1] Arthur J. Nozik,[1] Matt Law,[2] Matthew C. Beard[1]

[1]Chemical and Material Sciences Center, National Renewable Energy Laboratory, Golden, Colorado 80401; [2]Department of Physics and Astronomy, University of California, Irvine, Irvine, California 92697

Exploiting the novel photophysics inherent in quantum-confined nanostructures to enhance solar energy conversion is a driving motivation of the Center for Advanced Solar Photophysics (CASP). To this end, we have studied several exploratory solar cell architectures that employ quantum dot-(QD-) layers as the active absorber as well as the electron and hole transport media. In addition to studies of transport within solar cells and field-effect transistors (FETs), new optoelectronic characterization techniques have provided important insights into charge-separation and recombination processes. These studies have led to the development of surface chemistries that allow for tuning important parameters such as inter-QD electronic coupling, carrier-cooling rates, and the concentration of free carriers within these layers, resulting in, *e.g.*, x1000 fold increase in the electron mobility in PbSe QD layers. We demonstrate that these QD layers can exploit multiple exciton generation (MEG) to produce external photocurrent quantum efficiencies greater than 100% in photovoltaic devices. We have also incorporated these layers in state-of-the-art, environmentally stable, and efficient PbS QD solar cells. This presentation discusses the design principles and methods for incorporating QDs into solar conversion architectures capable of achieving very high solar energy conversion efficiencies.

11:20 AM

D-V-2: COMBINING THEORY AND EXPERIMENT TO UNDERSTAND OPTICAL PROPERTIES AND CARRIER GENERATION IN P-TYPE OXIDES

[CID] David S. Ginley,[1] Haowei Peng,[1] Andriy Zakutayev,[1] Stephan Lany,[1] Tula R. Paudel,[1] Mayeul d'Avezac,[1] Paul F. Ndione,[1] John D. Perkins,[1] Arpun R. Nagaraja,[2] Nicola H. Perry,[2] Thomas O. Mason,[2] Vladan Stevanovic,[3] Michael F. Toney[4] and Alex Zunger[5]

[1] National Renewable Energy Laboratory, Golden, CO 80401, USA, [2] Northwestern University, Evanston, IL 60208, USA, [3]Colorado School of Mines, Golden, CO 80401, USA, [4]SLAC National Accelerator Laboratory, Menlo Park, CA 94025, USA, [5]University of Colorado Boulder, CO 80309, USA

P-type transparent conducting oxides (TCOs) are long sought-after as contacts in photovoltaics, solid state lighting and in oxide-based thin film transistors. Potentially they provide a new dimension in tunability of electronic devices. To date, no high performing (conductivity and transparency) materials exist either because nature abhors them, or we do not have the right design rules. We have used a set of basic design principles to define what would be needed to get p-type behavior, exemplified by our identification of the d^{10} CoZnNiO family of spinels. We then used defect calculations followed by experimental verification to identify where holes can be generated intrinsically, without significant hole killers to prevent p-type carriers. We also demonstrated that theory-suggested dopants can increase conductivity, by orders of magnitude, resulting in a range of inverse and normal p-type spinels in this system with an ultimate conductivity of 200 S/cm. Additionally, we examined d^5 CrMnO spinels, which show promise for conductivity and transparency.

Knowing the transition metal spinels can be good p-type materials, we began a search for new or "missing" spinels across a broad range of possible elemental compositions. "Missing," in this context, means "stable by theory but not previously made." P-type materials developed were successfully employed as hole selective layers in organic photovoltaic devices. Overall, we show how the tools employed in the inverse design of new TCOs coupled with identifying potentially new materials can be broadly employed for a wide range of functionalities.

11:40 AM

D-V-3: LUMINESCENT CONCENTRATION WITH SEMICONDUCTOR QUANTUM RODS

[LMI] A. Paul Alivisatos[1,2], Noah D. Bronstein[1], Lanfang Li[3], Yuan Yao[4], Lu Xu[4], Ralph G. Nuzzo[4]
[1]*Department of Chemistry, University of California, Berkeley, California 94720*
[2]*Materials Science Division, Lawrence Berkeley National Laboratory, Berkeley, California 94720*
[3]*Department of Materials Science and Engineering, Frederick Seitz Materials Research Laboratory, University of Illinois at Urbana-Champaign, 1304 West Green Street, Urbana, IL 61801*
[4]*Department of Chemistry, University of Illinois at Urbana-Champaign, Urbana, Illinois, 61801*

Luminescent concentration of sunlight onto high quality solar cells allows the manipulation and concentration of both direct and diffuse light for enhanced photovoltaic conversion efficiency. In addition, luminescence converts photons to spectral regions that are efficiently captured by the photovoltaic device. We utilize CdSe/CdS seeded nanorods as a tunable luminophore for luminescent concentration. These quantum rods are resistant to photobleaching, have high luminescent quantum yields, have tunable absorption and emission spectra, and have emission polarized along the nanorod axis. These nanorods are compatible with free-radical initiated polymers, facilitating ease of integration into large-area devices. Transfer-printed, ultrathin crystalline Si solar cells are embedded directly into the luminescent concentrator, allowing for mechanical flexibility. By tuning the size of the CdS rod with respect to the luminescent CdSe seed, the reabsorption of propagating photons is dramatically reduced. At long distances, this reduced reabsorption can overcome the diminished quantum yield inherent to the larger semiconductor structures, which is studied with lifetime spectroscopy. An accurate model is developed to explain the performance of the luminescent concentrator, and is then used as a design tool to determine the upper limits of concentration using luminescent concentrators based on CdSe/CdS seeded nanorods. Exploring some hypothetical light-trapping scenarios, we show how an efficient light-trapping design can allow the LSC to operate in the high-concentration regime.

E. ENERGY CONSERVATION AND CONVERSION

Session I: Thursday, July 18, 2013, 10:30 – 12:10; Virginia Suite B

10:50 AM – Graduate Student Finalist

E-I-1: GROWTH OF NOVEL SUPERCONDUCTORS BY ATOMIC LAYER BY LAYER MOLECULAR BEAM EPITAXY

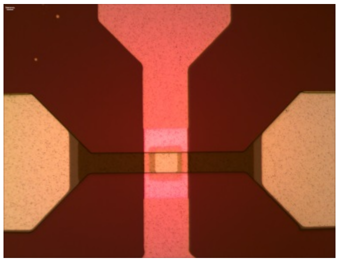
[CES] Mao Zheng[1], Can Zhang[1], Brian Mulcahy[1], Xiaoxiao Wang[1], Hefei Hu[2], Han Zhang[1], Hamood Z. Ahram[1], Ying Jia[3], Ulrich Welp[3], Alexey Koshelev[3], Jian-Min Zuo[1], Laura Greene[1], James N. Eckstein[1]

[1]Fredrick Seitz Materials Research Laboratory, University of Illinois Urbana-Champaign; [2]Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory; [3]Materials Science Division, Argonne National Laboratory

We have studied the growth of novel superconducting phases and multilayers involving them using Atomic Layer by Layer Molecular Beam Epitaxy (ALL-MBE). This growth technique is accurate enough to sequence the atomic layer content of crystalline samples so as to form new phases, heterojunctions with clean and flat interfaces as well as device structures for investigating fundamental properties of high Tc superconductors.

In one set of experiments we investigated the growth and physical properties of films and superlattices of LnT_2Ge_2, where Ln was La or Ce and T was Fe or Cu. The Ce compounds were heavy fermions and the Ce magnetism was found to be strongly coupled to the itinerant states below around 20 K. Since $CeCu_2Ge_2$ is superconducting, this may allow us to investigate spin mediated electron pairing in a system other than cuprates.

We have also studied how oxygen dopes FeTe films to make them superconducting. We found that oxygen can interact with the iron and tellurium in two different ways, illustrating how non-equilibrium growth by ALL-MBE provides another route to synthesis that is able to obtain material different from what equilibrium techniques like single crystal growth get. In particular, oxygen leading to superconductivity is interstitial and not chemically bonded to the iron atoms. Under conditions which cause oxygen to substitute for tellurium no superconductivity is found. We have also studied the way in which



Using these growth processes, we have fabricated tunnel junctions to test a prediction by Koshelev that if the order parameter symmetry of the FeTe:O is S± wave, then this should exhibit an unusual proximity effect into a thin adjacent S wave superconductor placed in intimate contact. To do this we made bilayers of FeTe:O with a thin aluminum overlayer. This is followed by a thin Al2O3 barrier layer and capped with a gold layer that acts as a tunnel junction injector. The films have been processed into mesa style devices. Such devices reveal the electronic density of states (DoS) which is proportional to the tunneling conductance. Measurements show a gap in the aluminum DoS that develops below the FeTe:O transition temperature showing that superconductivity in the FeTe:O is able to “leak into” the aluminum film. This suggests that the order parameter symmetry is not S±. However, Koshelev’s prediction of specific features in the conductance requires us to test the junctions at temperatures below the superconducting transition temperature of alumimum and preferably significantly below this. We are in the process of doing this now and will report the final results at the meeting.

11:10 AM

E-I-2: IRON-BASED SUPERCONDUCTORS – ROSETTA STONE OF ROOM TEMPERATURE SUPERCONDUCTIVITY

[CES] J. C. Séamus Davis[1,2], Freek Masse[2], Jon Rameau[1], John Tranquada[1], Peter Johnson[1], Karen Kihlstrom[3], Wai-Kwong Kwok[3], Alexei Koshelev[3], Ulrich Welp[3], George Crabtree[3], Hamood X. Arham[4], Juan Atkinson[4], Raffi Budakian[4], Laura H. Greene[4], James N, Eckstein[4], Dale J. van Harlingen[4], Philip W. Phillips[4], Anthony J. Leggett[4]

[1]Brookhaven National Laboratory, [2]Cornell University, [3]Argonne National Laboratory, [4]University of Illinois at Urbana-Champaign

As CES was being launched in 2009, iron-based high temperature superconductors were just being discovered. High temperature superconductivity portends revolutionary applications in power generation/transmission, transport, information technology, science, and medicine. The strong repulsive electron-electron interactions invoked to explain this superconductivity (SC) more usually cause commensurate magnetism. And, indeed, suppression of antiferromagnetism (AF) is the proximate cause of unconventional superconductivity in cuprates. However, intervening between the cuprate AF and SC phases, 'intertwined' electronic ordered phases of an exotic nature were also discovered. For this reason, it has been extremely difficult to distinguish the microscopic essence of the cuprate superconductivity from the often-spectacular epiphenomena of the intertwined phases. CES recognized that the novel iron-based compounds represented a golden opportunity to distill, by comparison with cuprates, the essence of the high temperature Cooper pairing mechanism. For this reason CES launched a concentrated and synergistic effort that lead to the prediction and then discovery of the 'intertwined' nematic phase of iron-based superconductors; exploration of their electronic phase diagram relating the magnetism, nematicity and superconductivity; discovery of the momentum space structure of the high temperature Cooper pairs; determination of the atomic scale effects of the dopant atoms; enhancement of the impressively high critical currents, and many other observations. The results of CES program reveal a general conceptual framework describing the relationship between antiferromagnetic electron-electron interactions, intertwined ordered phases and correlated superconductivity. This 'Rosetta Stone' allows us to distinguish the essence of correlated superconductivity from spectacular epiphenomena associated with the intertwined phases, and thereby focuses attention on the correct route towards room-temperature superconductivity.

11:30 AM

E-I-3: NANOPARTICLE ELECTRONICS WITHOUT SEMICONDUCTORS

[NERC] Bartosz A. Grzybowski
Department of Chemical and Biological Engineering, Northwestern University, Evanston, IL

The design of electronic circuits from metal nanoparticles has been a challenge because arrays of metal nanoparticles typically exhibit linear current-voltage characteristics: such characteristics are only useful for the construction of resistors. Here we report a class of ligand-stabilized metal nanoparticles that greatly expands the range of electronic properties that can be accessed. We present six electrical components that are built from metal nanoparticles: transistors, diodes, resistors, thermistors, and two types of sensors. In most cases, the nanoparticles have alkanethiols ligands that are terminated in the omega-position with N,N,N-trimethylammonium chloride. We describe how the coupling of ionic current from the charged ligand with the electronic current via electron tunneling leads to non-linear current-voltage characteristics that enable these new components. We show how these components can be combined to construct complex circuits, including logic gates, a half-adder circuit, and random access memory. At the same time, the individual components—most especially, the thermistors—provide a performance that exceeds that of state-of-the-art semiconductors. In this way, we illustrate how materials assembled from nanoparticles may emerge as an important new platform in new classes of electronic devices.

11:50 AM

E-I-4: MATERIALS DISCOVERY EFFORT IN THE CENTER FOR EMERGENT SUPERCONDUCTIVITY

[CES] Peter Abbamonte[1], James N. Eckstein[1], Laura H. Greene[1], Philip W. Phillips[1], Wei-Cheng Lee[1], Anthony J. Leggett[1], Wai-Kwong Kwok[2], Karen Kihlstrom[2], Ulrich Welp[2], Mercouri G. Kanatzidis[2], Duck Young Chung[2], Lei Fang[2], Bing Shen[2], Qiang Li[3], Ivan Božović[3], Genda Gu[3], Cedomir Petrovic[3]
[1]University of Illinois at Urbana-Champaign [2]Argonne National Laboratory [3]Brookhaven National Laboratory

The phenomenon of high temperature superconductivity has the potential to revolutionize the storage, production, and transmission of electrical power, transforming the power grid and contributing the sustainability of our energy future. One of the prime missions of the Center for Emergent Superconductivity (CES) is to discover new superconducting materials with improved properties, such as higher transition temperature, higher critical current, or lower anisotropy. In this talk I will describe the materials discovery strategy adopted by the CES, based on layering favorable combinations of ionic materials in a manner that optimizes conditions for superconductivity, and discuss the progress and milestones achieved to date. We will also discuss future plans for the Center, including the possibility of closer integration with high-performance computing methods, which will help guide future materials discovery efforts.

Session II: Thursday, July 18, 2013, 1:40 – 3:20; Virginia Suite B

1:40 PM

E-II-1: RECORD-BREAKING THERMOELECTRIC PERFORMANCE IN PBTE: *ROLE OF ALL LENGTH-SCALE HIERARCHICAL ARCHITECTURE*

[RMSSEC] Vinayak P. Dravid[1], Kanishka Biswas[1], Jiaqing He[1], Ivan D. Blum[1], David N. Seidman[1], Mercouri G. Kanatzidis[1], Chun-I Wu[2], and Timothy P. Hogan[2]
[1]*Northwestern University;* [2]*Michigan State University*

Nanostructures in bulk thermoelectrics have proven to be effective scatterers of phonons for a significant portion of the phonon spectrum, resulting in rapid improvement in the thermoelectric figure of merit, ZT, during the past few years. However, in nominally nanostructured thermoelectrics, phonons with longer mean free paths remain largely unaffected and thus contribute to the total thermal conductivity. By controlling the mesoscale architecture of nanostructured chalcogenide compounds, we have shown that long-wavelength phonons can also be scattered significantly. Thus, by considering sources of phonon scattering across all relevant length scales in a hierarchical fashion—from atomic-scale lattice disorder and nanoscale endotaxial precipitates to mesoscale grain boundaries—we achieve a significant reduction in lattice thermal conductivity and thus a large increase in the thermoelectric performance of PbTe; a figure of merit ZT of 2.2 at 900K. This all-scale hierarchical architecture is achieved by combining alloy scattering, precipitate scattering from nanostructures of endotaxially embedded SrTe, and interface scattering from small grains achieved using spark-plasma sintering (SPS). This “panascopic” approach highlights the role of multiscale hierarchical architecture in controlling phonon scattering in bulk thermoelectrics. A key feature of these materials is the close lattice match between SrTe and PbTe, allowing for the efficient transport of carriers across interfaces without degradation in mobility. The presence of these SrTe nanoprecipitates is confirmed using high resolution transmission electron microscopy and atom probe tomography.

2:00 PM – Graduate Student Finalist

E-II-2: COHERENT PHONON HEAT CONDUCTION IN SUPERLATTICES

[S3TEC] Maria N. Luckyanova[1]; Jivtesh Garg[1]; Keivan Esfarjani[1]; Adam Jandl[2]; Zhiting Tian[1]; Bo Qiu[1]; Mayank T. Bulsara[2]; Aaron J. Schmidt[3]; Austin J. Minnich[4]; Shuo Chen[5]; Mildred S. Dresselhaus[6]; Zhifeng Ren[5]; Eugene A. Fitzgerald[2]; Gang Chen[1]

[1]Department of Mechanical Engineering, MIT; [2]Department of Materials Science and Engineering, MIT; [3]Department of Mechanical Engineering, Boston University; [4]Division of Engineering and Applied Science, California Institute of Technology; [5]Department of Physics, University of Houston; [6]Department of Electrical Engineering and Computer Science, MIT

As the critical dimensions of a wide range of emerging technologies, from consumer electronics to nanoscale energy conversion systems, get ever smaller, the importance of having a fundamental understanding of the material properties gets ever larger. The behaviors of electrons and photons, electronic and electromagnetic energy carriers respectively, have been widely studied both experimentally and theoretically. By exploiting their wavelike characteristics, the transport properties of these energy carriers can now be tailored using artificial nanostructures. By comparison, a fundamental understanding of the behavior of phonons, a major thermal energy carrier, in the presence of material interfaces, boundaries, or defects has remained elusive, hampering the ability to tailor the thermal properties of materials and nanostructures. This work aims at enhancing the understanding of the fundamental properties of phonons by examining their wavelike nature, or coherence, during thermal conduction. Coherent phonons maintain wavelike characteristics and experience predictable interference effects whereas incoherent phonons are expected to lose phase information at materials boundaries and interface.

Since thermal transport involves broadband phonons, the challenge lies in discerning the coherent and incoherent contributions to heat conduction. To address this challenge, superlattices (SLs) comprised of periodic layers of GaAs and AlAs thin films on the order of 10 nm in thickness, were synthesized (Fig. 1A). In contrast with most SL-based studies of phonon behavior, the thicknesses of the individual layers were held constant while the total number of periods was varied. This approach gives unique access to the changing role of coherent phonons during heat conduction. The temperature-dependent thermal conductivities of the SLs were measured using the time-domain thermoreflectance technique and were shown to increase nearly linearly with total sample thickness (Fig. 1B), indicating the presence of coherent phonon heat conduction. The results of this experimental study, in tandem with computational results from both density functional theory (DFT, Fig. 1C) and Green's function calculations showed for the first time the important role of coherent phonons during thermal transport.

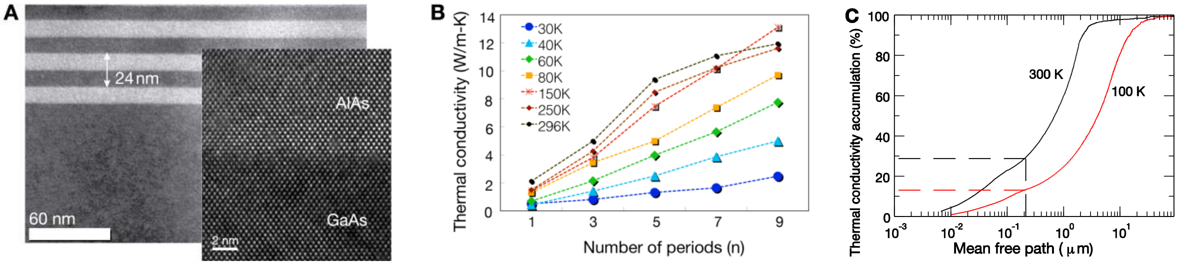


Figure 3 (A) TEM and HRTEM images of GaAs/AlAs SL; (B) Time-domain thermoreflectance measurements show increasing thermal conductivity with increasing number of periods; (C) first-principles calculations of the SL thermal conductivity accumulation functions show the importance of coherent phonons and agree well with experimental results.

M.N. Luckyanova, J. Garg, K. Esfarjani, A. Jandl, M.T. Bulsara, A.J. Schmidt, A.J. Minnich, S. Chen, M.S. Dresselhaus, Z. Ren, E.A. Fitzgerald, and G. Chen. *Science* **338**, 936-9 (2012).

2:20 PM

E-II-3: ANHARMONICITY ENGINEERING: A NEW WAY TO REDUCE THE LATTICE THERMAL CONDUCTIVITY

[RMSSEC] Joseph P. Heremans[1], Michele D. Nielsen[1], Vidvuds Ozolins[2], Yi Xia[2], Fei Zhou[2], Donald T. Morelli[3], Xu Lu[3], Ctirad Uher[4], and Hang Chi[4]
[1]Ohio State University; [2]University of California-Los Angeles; [3]Michigan State University; [4]University of Michigan

Minimizing the thermal conductivity without affecting the electronic properties is one of the main goals of research in new thermoelectric (TE) materials. Because heat is conducted mostly by phonons, impeding their transport has been achieved classically by alloying TE materials, and in the last decade by nanostructuring them or by adding atoms that locally "rattle" and scatter phonons. To these techniques, we add here a new one: engineer solids in which the phonons that carry heat have highly anharmonic properties. This promotes phonon-phonon interactions: indeed, when the bond is anharmonic, the atom displacements due to the passage of one phonon change the local bond strength and perturb the field for a second phonon. We will show how specific types of chemical bonds can be selected and designed to maximize these effects, thereby reducing the lattice thermal conductivity of the material to its minimum possible value, the amorphous limit. We will show two classes of thermoelectric solids as examples, the I-V-VI$_2$ compounds (I=group I element, etc...) in a CaF$_2$ crystal structure, and the tetrahedrite compounds. In the I-V-VI$_2$ compounds, the anharmonicity arises from the lone pair electrons on the group V element; in the tetrahedrite, it is the electrons on the Cu. In both cases, the atomic displacements that accompany the passage of a phonon distort the orbitals of these electrons (polarizes them) in strongly non-linear ways. The approach enables the design of hundreds of potential new thermoelectric compounds, several of which have already shown ZT values excess of unity.

2:40 PM

E-II-4: PROBING AND ENGINEERING PHONONS AND ELECTRONS TRANSPORT IN NANOSTRUCTURED THERMOELECTRIC MATERIALS

[S3TEC] Gang Chen[1]
1. Mechanical Engineering Department, MIT

Thermoelectric devices exploit thermal energy carried by electrical charges for the conversion between heat and electricity for cooling, heating, and power generation applications. Efficient thermoelectric energy conversion calls for materials with good electrical conductivity and large Seebeck coefficient, but low thermal conductivity. This talk will start with an introduction to the Solid-State Solar-Thermal Energy Conversion Center, and move on to discuss a few examples from the S3TEC Center research in understanding and engineering phonon and electron transport in thermoelectric materials to improve the materials' performance. On phonon transport, first-principles simulations together with neutron spectroscopy yield detailed understanding of phonon transport properties. Ballistic phonon transport is observed experimentally, and exploited to develop optical techniques for mapping phonon mean free distribution. On electrons, modulation doping approach used for 2D electron gas is extended to 3D nanostructures and new concepts in electromagnetic metamaterial are applied to electron waves to design nanostructures such that all three parameters in the thermoelectric figure-of-merit can be improved. New understandings gained from these fundamental studies enable development of high performance thermoelectric materials and devices, which will be discussed along the way.

3:00 PM

E-II-5: ENERGY DISSAPATION IN ATOMIC-SCALE DEVICES

[CSTEC] Woochul Lee[1], Kyeongtae Kim[1], Wonho Jeong[1], Pramod Reddy[1,2]
[1]*Department of Mechanical Engineering, University of Michigan, Ann Arbor, Michigan, 48109, USA*
[2]*Department of Materials Science and Engineering, University of Michigan, Ann Arbor, Michigan, 48109, USA*

Atomic and single-molecule junctions represent the ultimate limit to the miniaturization of electrical circuits. They are also ideal platforms to test quantum transport theories that are required to describe charge and energy transfer in novel functional nanodevices. Recent work has successfully probed electric and thermoelectric phenomena in atomic-scale junctions. However, energy conversion and transport in atomic-scale devices remain poorly characterized due to experimental challenges. In this talk, we describe how we have recently[1] used custom-fabricated scanning probes with integrated nanoscale thermocouples, to show that heat dissipation in the electrodes of molecular junctions, whose transmission characteristics are strongly dependent on energy, is asymmetric, *i.e.* unequal and dependent on both the bias polarity and the identity of majority charge carriers (electrons vs. holes). In contrast, we found that junctions whose transmission characteristics show weak energy dependence do not exhibit appreciable asymmetry. We will also describe how our results unambiguously relate the electronic transmission characteristics of atomic-scale junctions to their heat dissipation properties establishing a framework for understanding heat dissipation in a range of mesoscopic systems where transport is elastic.

1. W. Lee, K. Kim, W. Jeong, L. A. Zotti, F. Pauly, J. C. Cuevas, P. Reddy. Heat Dissipation in Atomic-Scale Junctions, *Nature* (DOI 10.1038/nature12183)

Session III: Thursday, July 18, 2013, 3:40 – 5:00; Virginia Suite B

3:40 PM – Postdoctoral Researcher Finalist

E-III-1: FIRST-PRINCIPLES STUDIES OF LOSS MECHANISMS IN LIGHT-EMITTING DIODES

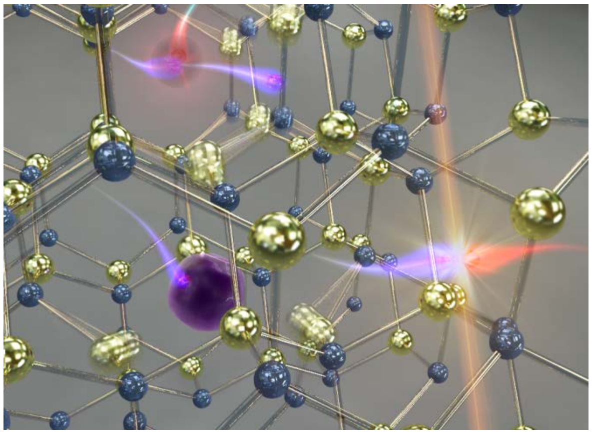
[CEEM] Daniel Steiauf[1], Qimin Yan[2], Emmanouil Kioupakis[3], and Chris G. Van de Walle[1]
[1]*Materials Department, University of California, Santa Barbara;* [2]*Molecular Foundry, Lawrence Berkeley National Laboratory;* [3]*Department of Materials Science and Engineering, University of Michigan*

Indium gallium nitride alloys are successfully being used for light emitting diodes (LEDs) in the green to ultraviolet part of the optical spectrum. These devices are the key enablers to Solid-State Lighting, which promises to significantly cut electricity consumption. Applications are still limited, however, by the declining efficiency of LEDs at high currents (“droop”), particularly at longer weavelengths.

Several mechanisms have been suggested as the cause of this efficiency loss, such as Auger recombination and free carrier absorption. Experimentally it is very difficult to discriminate between different nonradiative processes. We have therefore addressed the loss mechanisms based on state-of-the-art first-principles computational theory. We use *ab initio* wave functions and bands that are accurate throughout the entire Brillouin zone (as opposed to **k.p** band structures). Various scattering mechanisms have been taken into account, including scattering by alloying, defects, and phonons. The electron-phonon coupling is explicitly evaluated; this interaction is usually modelled by the Fröhlich expression and this is the first time that the validity of this model is verified from *ab initio* data.

For Auger recombination we find that both electron-electron-hole and hole-hole-electron processes contribute, and that indirect processes assisted by alloy scattering and by electron-phonon coupling dominate. The magnitude of the resulting Auger coefficient indicates that Auger recombination is indeed responsible for the efficiency reduction at high carrier densities.

Calculations for other III-V materials shed light on the microscopic mechanism of this process. Based on simulations of quantum-well structures we also investigate the interplay of polarization fields and Auger recombination in the efficiency droop of nitride light-emitting diodes, pointing to approaches to mitigate the effect of this intrinsic loss mechanism.



Schematic depiction of radiative and nonradiative recombination processes in a nitride crystal. In a radiative process (right), electrons and holes recombine and a photon is emitted. In a defect-assisted nonradiative process (bottom left), an electron is trapped by a defect (here a nitrogen vacancy, represented by a dark wave function). In Auger recombination (top left), an electron and hole recombine but the energy is transferred to a third carrier which is excited to a higher-energy state.

4:00 PM

E-III-2: NANOWIRES FOR SOLID-STATE LIGHTING

[SSLS] [1]George T. Wang
[1]*Sandia National Laboratories, Albuquerque, NM 87185*

Nanowires based on the III nitride (AlGaInN) materials system have attracted attention as potential nanoscale building blocks in LEDs, lasers, sensors, photovoltaics, and high speed electronics. Compared to conventional LEDs based on planar architectures, future LEDs based on III-nitride nanowires have several potential advantages which could enable cheaper and more efficient lighting. However, before their promise can be fully realized, several challenges must be addressed in the areas of controlled nanowire synthesis, understanding and controlling the nanowire properties, and nanowire device integration. I will describe a recent "top-down" approach for fabricating ordered arrays of high quality GaN-based nanowires with controllable height, pitch and diameter. Using this top-down approach, both axial and radial nanowire light emitting heterostructures can be realized. The fabrication, structure, optical properties, lasing characteristics, and performance of top-down-fabricated nanowires and nanowire LEDs and lasers will be discussed.

Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

4:20 PM

E-III-3: DIRECT MEASUREMENT OF AUGER ELECTRONS EMITTED FROM A SEMICONDUCTOR LIGHT-EMITTING DIODE UNDER ELECTRICAL INJECTION: IDENTIFICATION OF THE DOMINANT MECHANISM FOR EFFICIENCY DROOP

[CEEM] Justin Iveland[1], L Peretti[2], Martinelli[2], James S. Speck[1] and Claude Weisbuch[1,2]
[1]Mater. Dept., Univ. of California, Santa Barbara, Santa Barbara, CA, USA; [2]Lab. de Phys. de la Mater. Condensee, Ecole Polytech., Palaiseau, France.

We report on the unambiguous detection of Auger electrons by electron emission spectroscopy from a cesiated InGaN/GaN light-emitting diode under electrical injection. Electron emission spectra were measured as a function of the current injected in the device. The appearance of high energy electron peaks simultaneously with an observed drop in electroluminescence efficiency shows that hot carriers are being generated in the active region (InGaN quantum wells) by an Auger process. A linear correlation was measured between the high energy emitted electron current and the droop current - the missing component of the injected current for light emission. We conclude that the droop phenomenon in GaN light-emitting diodes originates from the excitation of Auger processes.

4:40 PM

E-III-4: OPTICAL AND ELECTRICAL CHARACTERIZATION OF DEFECTS IN NANOSCALE INGAN/GAN HETEROSTRUCTURES

[SSLS] [1]Andrew M. Armstrong, [1]Mary H. Crawford, [1]Daniel D. Koleske, [1]Stephen R Lee
[1]Sandia National Laboratories, Albuquerque, NM 87185

Commercialization of GaN-based light emitting diodes (LEDs) has enabled widespread adoption of energy-efficient solid-state lighting. Despite this success, crystal defects continue to have a strong and often undesired impact on the opto-electronic properties of InGaN/GaN LEDs. The physical origin of these defects and their optical and electrical properties are not well understood due to the unmet challenges of 1) quantitatively studying defect physics in (In)GaN semiconductors with large band gap energy (0.9 - 3.4 eV) that are capable of emitting visible light, and 2) non-destructively resolving the spatial distribution of atomic defects among nanoscopic multi-quantum well (MQWs) heterostructures that generate light within LEDs. This talk will discuss new developments in the technique of deep level optical spectroscopy (DLOS) to quantitatively study deep level defect states in the MQWs of InGaN/GaN LEDs with nanoscale depth resolution. Using DLOS, defect incorporation was found to evolve drastically over the first 200 Å of MQW growth, and a strong interaction among point defects and extended defects was observed. The microscopic origin of observed defect states and their influence on the electrical and optical properties of GaN-based LEDs will be discussed.

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F. MATERIALS AND CHEMISTRY FOR NUCLEAR ENERGY APPLICATIONS

Session I: Thursday, July 18, 2013, 10:30 – 12:10; Salon 3

10:50 AM – Postdoctoral Researcher Finalist

F-I-1: MICROSTRUCTURAL INVESTIGATIONS OF KR AND XE IRRADIATED UO_2

[CMSNF] Lingfeng He[1], Mahima Gupta[1], Billy Valderrama[2]. Hunter B. Henderson[2], Abdel-Rahman Hassan[3], Janne Pakarinen[1], Jian Gan[4], Marquis A. Kirk[5], Michele V. Manuel[2]. Anter A. El-Azab[3], Todd R. Allen[1,3]
[1]University of Wisconsin at Madison, [2]University of Florida, [3]Purdue University, [4]Idaho National Laboratory, [5]Argonne National Laboratory

Revealing the microstructural damage of nuclear fuels under irradiation is of significance in understanding and modeling the thermal transport in nuclear fuels. In this study, both single-crystal and polycrystalline UO_2 were irradiated with in situ Kr and Xe ions at room temperature and high temperatures. The ion dose dependence of defect microstructure (dislocation loops, dislocations and gas bubbles) was investigated by an in situ transmission electron microscopy (TEM). A dislocation loop denuded zone near the surface and grain boundary indicates they are good sinks for irradiation-induced defects. Interstitial-type dislocation loops with a Burgers vector along <110> were observed in the irradiated UO_2. Further, stoichiometry and gas distribution in the irradiated UO_2 were characterized by atom probe tomography (APT) and electron energy loss spectroscopy (EELS). The stoichiometry of UO_2 is stable during irradiation and the gas distribution shows a similar profile with SRIM calculation but the measured gas content is much lower than the calculated one.

11:10 AM

F-I-2: CREATING RADIATION-RESISTANT MATERIALS BY TAILORING INTERFACES

[CMIME] Michael J. Demkowicz
Massachusetts Institute of Technology.

Irradiation of structural materials creates defects that are deleterious to critical properties such as strength and ductility. Interfaces and grain boundaries may absorb these defects, healing radiation damage. However, not all interfaces and grain boundaries are equally effective sinks for radiation-induced defects. By combining modeling and experiments, we have developed a figure of merit for the defect sink efficiency of different interfaces and grain boundaries. Using this insight, we have created bulk nanocomposite materials that are strong, stable, and radiation resistant.

11:30 AM

F-I-3: FIRST PRINCIPLES AND MODEL HAMILTONIANS WORKING IN CONCERT TO UNDERSTAND DEFECTS IN IRON AND IRON BASED ALLOYS

[CDP] Don M. Nicholson,[1] Malcolm G. Stocks,[1] Dilina Perera,[2] David P. Landau,[2] Markus Eisenbach,[1] Junqi Yin,[1] Gregory Brown,[3] Kh. Odbadrakh,[1] Yang Wang,[4] Roger Stoller,[1] German Samolyuk[1]
[1]Oak Ridge National Laboratory; [2]Center for Simulational Physics, The University of Georgia; [3]Florida State University, [4]Carnegie Mellon University, Pittsburgh Supercomputing Center

We present results of large-scale O(N) ab initio studies of extended defects, including dislocation cores and dislocation loops, to study structure, magnetism and energetics of these defects in iron and iron-based alloys. These calculations have been utilized to develop combined spin/molecular

dynamics Hamiltonians to examine defect dynamics of these materials. Under extreme conditions, energy and stress in a lattice may be dissipated through the formation and motion of defects. Defects can also cause stress in the lattice, and change the local response of the material. The large distances and times over which defect processes play out has motivated the use of large-scale molecular dynamics and kinetic Monte Carlo. Models large enough to incorporate defect phenomena range from a few thousand to a few million. Using order-N density functional codes we can evaluate energies, energy gradients and the underlying electronic and magnetic structure of configurations drawn straight from MD. Dynamics is controlled by gradients of the energy with respect to system degrees of freedom. Accurate treatment of defects in Fe alloys requires inclusion of spin degrees of freedom. We discuss the construction and use of first principles based model Hamiltonians for MD that includes spin dynamics (MD-SD) in the evolution of large defect models. We illustrate how first principles electronic/magnetic structure calculations on large configurations drawn from MD-SD give a rich description of defect events.

11:50 AM

F-I-4: DEFECT DISORDER AND ELECTROCHEMICAL EFFECTS OF VOIDS IN UO_2

[CMSNF] Abdel-Rahman Hassan[1], Janne Pakarinen[2], Michele V. Manuel[3], Todd R. Allen[4] and Anter A. El-Azab[1]
[1]Purdue University, [2]University of Wisconsin at Madison, [3]University of Florida, [4]Idaho National Laboratory

A defect disorder model of UO_2 founded on density functional theory results of defect energetics has been extended to investigate local off-stoichiometry near UO_2 surfaces. While bulk UO_2 crystals contain defects and electronic charge carrier densities that solely depend on the oxygen partial pressure and temperature, surfaces were found to significantly modify the defect equilibrium states. Analysis of local defect densities near flat surfaces in UO_2 showed that significant defect segregation occurs and that, under fixed thermo-chemical environment, local stoichiometry can change from hyper to hypo as a function of distance from the surface. A generalization of the theory to void surfaces has led to the discovery that voids in UO_2 must contain oxygen gas. This important finding implies that, as a major component of UO_2, oxygen may have a bigger role to play in the irradiation response of the material than previously believed. It was also found that voids are surrounded by significant defect segregation regions at void sizes in the range few tens to few hundred nanometers. This discovery also implies that the average O:U ratio of irradiated UO_2 crystals containing ensembles of voids will be different from the unirradiated material under the same thermo-chemical conditions. The discovered electrochemical aspect of voids in UO_2 gave us new insight into how to construct microstructure evolution models. A number of chemical characterization experiments are now being designed to validate this prediction.

Session II: Thursday, July 18, 2013, 1:40 – 3:20; Salon 3

1:40 PM

F-II-1: PROPERTIES OF NANOSCALE URANIUM CAGE CLUSTERS IN AQUEOUS SOLUTION

[MSA] Peter C. Burns[1]
1- University of Notre Dame

A family of about 80 nanoscale uranyl peroxide cage clusters has been found to self-assemble in aqueous solution under ambient conditions. Selected clusters have been purified by crystallization and dissolved in aqueous solution to probe their properties in solution. Upon dissolution in relatively dilute solutions, the negatively charged clusters are dispersed dominantly as isolated units. U60, which contains 60 uranyl peroxide polyhedra arranged in a fullerene topology, persists in water upon dissolution for months, with an approximate charge of -18. Addition of cations to solution changes the mass of the clusters, as shown by ESI-MS, reducing their negative charge and leading to aggregation into blackberry-like objects with diameters of 10s of nanometers. Cluster U24Py12, which contains pyrophosphate units, also readily dissolves and is stable in water, as shown by NMR spectroscopy. Its charge can be reduced by protonation of non-bridging O atoms, triggering aggregation into blackberry-like objects. NMR spectra have demonstrated that U24Py12 remains intact in aqueous solution upon heating to 65°C, although an interchange between its solid-state oblong structure and a more symmetric configuration occurs with increasing temperature, without breakdown of the cluster. The oblong configuration, which has a lower volume than the symmetric form, is favored by increasing pressure. These clusters provide useful insights into the properties of nanoscale objects in solution, and have a variety of potential applications in an advanced nuclear energy system.

2:00 PM

F-II-2: CARBON NANOMATERIALS FROM HIGH PRESSURE REACTIONS OF BENZENE

[EFree] Thomas C. Fitzgibbons[1], Malcolm Guthrie[2], Enshi Xu[3], Stephen Davidowski[4], Jeffery Yarger[4], Roald Hoffmann[5], Vincent Crespi[3], John V. Badding[1]
[1]Department of Chemistry, Pennsylvania State University, University Park, PA; [2]Geophysical Laboratory, Carnegie Institution of Washington, Washington DCl [3]Department of Physics, Pennsylvania State University, University Park, PA; [4]Department of Chemistry and Biochemistry, Arizona State University, Tempe AZ; [5]Department of Chemistry and Chemical Biology, Cornell University, Ithaca NY

The ability of carbon to bond in different ways allows for a range of optical, electrical, and physical materials properties unmatched by any other element. High pressure could provide a route for synthesizing extended carbon solids with deliberately tailored structures and properties. We discuss the polymerization of benzene via a kinetically controlled reaction mediated by high pressure at room temperature. The reaction product is a colorless, solid material with predominantly (85%) sp^3 bonding. Through a broad use of resources within the EFree Center (high energy x-ray and neutron diffraction, SSNMR, TEM and theory) we gained great insight into the nature of this material. The diffraction shows well-defined short range order strongly reminiscent of adamantane. And, strikingly, it also reveals long range order out to several nanometers. Our brightfield TEM investigations are consistent with this and reveal both the presence of beading at or near the periodicity of the experimental diffraction and extended, linear structures out to ~10nm. Finally, this suggests that structures chemically defined on at least this length scale are being synthesized rather than merely amorphous materials. There appear to be striking parallels between these observations and several previously predicted sp^3 hybridized nanotubes.

2:20 PM – Graduate Student Finalist

F-II-3: REACTION DYNAMICS OF A NANOMETER-SIZED URANYL CLUSTER IN SOLUTION

[MSA] Rene L. Johnson;[1] C. André Ohlin;[2] Kristi L. Pellegrini;[3] Peter. C. Burns;[3,4] William H. Casey[1,5]

1.Department of Chemistry, University of California - Davis, Davis, CA (USA); 2. School of Chemistry, Monash University, Clayton, Victoria (Australia); 3. Department of Civil and Environmental Engineering and Earth Sciences, University of Notre Dame, South Bend, IN (USA); 4. Department of Chemistry and Biochemistry, University of Notre Dame, South Bend, IN (USA); 5. Department of Geology, University of California – Davis, Davis, CA (USA)

A large and previously unsuspected class of uranyl-peroxide clusters was discovered less than a decade ago as nanometer-size ions that form spontaneously in aqueous solutions. Little is known about the chemistry of these ions in spite of their obvious importance as soluble forms of actinide elements which are potentially present in the environment. Here we show reversible structural changes in an example uranyl(VI) cluster of this class that is ~2 nm in diameter. It contains 24 uranyl moieties, and 12 pyrophosphate units that are detectable via ^{31}P NMR and has a nominal stoichiometry of $[(UO_2)_{24}(O_2)_{24}(HP_2O_7)_6(H_2P_2O_7)_6]^{30-}$. NMR spectroscopy shows that the ion has two distinct forms, aspherical and spherical, that interconvert (Figure 1. Left) on the millisecond to second time scale depending upon temperature and the size of the counterions. For a solution with only Na^+ counterions we estimated $k_{298} = 9.7\pm0.6\ s^{-1}$, as compared to $k_{298} = 0.40\pm0.02\ s^{-1}$ estimated for a solution with Na^+ and tetramethyl ammonium counterions. This dynamic interconversion (Figure 1. Right) may relate to the onset of dissociation of the cluster into smaller fragments. High-pressure (up to 300 MPs) experiments yielded an activation volume of $\Delta V^{\ddagger} = +11.6\pm0.5\ cm^3\ mol^{-1}$, showing that the difference in volume between the isomers is about the volume of a water molecule. Extrapolated broadly, these results support a model where nanometer-size features at the oxide-solution interface have sets of accessible low-energy metastable states that control isotope exchanges and dissociation.

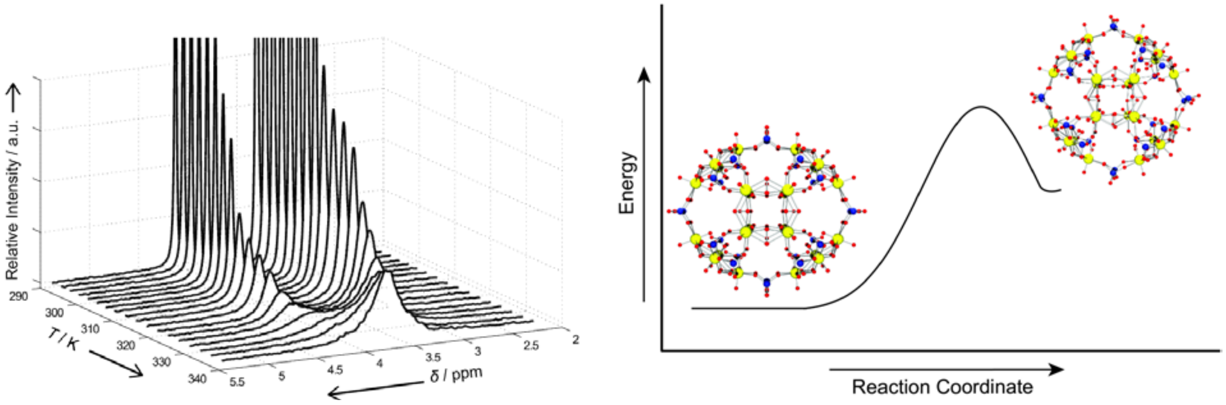


Figure 1. **Left:** Stacked ^{31}P solution-NMR plot of the uranyl-peroxo-pyrophosphate cluster as a function of temperature. This plot shows the interconversion of the aspherical form of the cluster to the spherical form. **Right:** A proposed reaction coordinate for the conformational change from the stable aspherical molecule to the metastable spherical molecule.

* R. L. Johnson, C. A. Ohlin, K. Pellegrini, P. C. Burns, W. H. Casey, *Angew. Chem. Int. Ed.* **2013**, In Print. DOI: 10.1002/anie.201301973

2:40 PM

F-II-4: CRITERIA FOR INTERFACIAL STABILITY IN BULK NANOCOMPOSITES SUBJECTED TO EXTREME MECHANICAL STRAINS

[CMIME] Irene J. Beyerlein[1], Nathan A. Mara[1], John S. Carpenter[1], Shijian Zheng[1], Jonathan LeDonne[2], Anthony D. Rollett[2], Thomas Nizolek[3], Tresa Pollock[3], Jason R. Mayeur[1], Keonwook Kang[1], Jian Wang[1]
[1]Los Alamos National Laboratory; [2]Carnegie Mellon University, [3]University of California, Santa Barbara

We utilize Accumulative Roll-Bonding (ARB) to process bulk nanolamellar composites from 2 mm thick high-purity polycrystalline sheet down to layer thicknesses of 10 nm. This processing technique has the advantage of producing bulk quantities of nanocomposite material, and also exposes the interface and bulk constituents to large strains (1000's of percent). Recently, we applied this process to a composite consisting of two dissimilar metals with the aim of exploring stability of bimetal interfaces in mechanical extremes. Atomic to meso-scale characterization of the bimetal interfaces revealed a remarkable ordering in interface character and atomic structure that prevailed over the material. Specifically after extreme mechanical straining, when the spacing between the neighboring bimetal interfaces reduced below 100 nm, the initially random distribution of interfacial character transformed into one that consisted of highly oriented single crystals and interfaces containing minimal defects. Using molecular dynamics and crystal plasticity theory and simulation, we identify two criteria for mechanical stability of interfaces: 1.) The crystallographic orientation of each layer must provide for symmetric slip in each phase and 2.) the formation energy of the interface must correspond to a local energy minimum. We show that only a few interfaces meet such stringent criteria, which explains the intense preference towards a singular form observed after extreme strains. These findings provide a direct connection between the evolution of stable interface structures and the mechanical processing pathway. This further implies that the properties of interfaces can be controlled at the atomic level via design of severe plastic deformation methods.

3:00 PM

F-II-5: ENERGETICS OF COMPLEX ACTINIDE MATERIALS – CALORIMETRIC AND COMPUTATIONAL STUDIES

[MSA] Alexandra Navrotsky[1]
1 - University of California, Davis

The thermodynamic stability of complex actinide materials ranging from reactor fuels to waste forms is a critical factor in determining their synthesis, use, and long term behavior. At the same time, knowledge of energetic and entropic parameters sheds light on fundamental physics and chemistry, including structure, defect chemistry, order-disorder, magnetic and electronic properties, and oxidation states. Experimental calorimetric determinations of enthalpies of formation and DFT calculations of energetic parameters go hand-in-hand. Here I report studies of two classes of materials- uranium and thorium oxides doped with rare earths and cerium, thorium, and uranium based garnets. The charge-balanced ionic substitutions of different sized cations and vacancies lead to complex defect formation and clustering and influence the oxidation states of variable valence cations. Determination of heats of formation by high temperature oxide melt solution calorimetry is coupled with DFT calculations of mixing energies, cluster formation and charge transfer to provide a comprehensive picture of energetics with potential predictive capability.

Session IV: Friday, July 19, 2013, 8:30 – 9:30; Virginia Suite B

8:30 AM

F-IV-1: INVESTIGATIONS OF ANHARMONIC PHONON PROPERTIES AND THERMAL TRANSPORT OF UO_2 BY INELASTIC NEUTRON SCATTERING AND FIRST-PRINCIPLES SIMULATIONS

[CMSNF] Judy W.L. Pang[1], Aleksandr Chernatynskiy[2], Bennett C. Larson[1], Simon R. Phillpot[2], William J.L. Buyers[3], Mark D. Lumsden[1], Douglas L. Abernathy[1]
[1]Oak Ridge National Laboratory, [2]University of Florida, [3]Chalk River Laboratories,

We have used inelastic neutron scattering to probe anharmonicity and the microscopic phonon physics of thermal transport in UO_2, the most widely used nuclear fuel. In stark contrast to existing simulations, high-resolution phonon lifetime measurements in UO_2 have shown that highly-anharmonic pure oxygen phonons and low-velocity uranium modes are strong transporters of heat despite their short lifetimes and low velocities, respectively. We have further performed the first ab initio simulations of phonon lifetimes for UO_2 in which the strong heat transport by the low-velocity uranium and pure oxygen phonon modes is predicted correctly. Observations of a significant impact of phonon dispersion on first principles phonon lifetime simulations will be discussed through direct comparisons of measurements of the phonon density of states for UO_2 with anharmonic lifetime broadened ab initio density of states simulations. Phonon density of states investigations of the relative effects of anharmonicity and fission product impurities (5% ceria doping) will be discussed showing that ceria preferentially impacts zone boundary phonons with pure uranium and pure oxygen vibrations – the two strongest heat carrying phonon branches in UO_2. The comprehensive phonon measurements provide a new level of insight into anharmonicity and thermal transport in UO_2 and they further provide stringent benchmarks for ab initio modeling of the electronic structure for UO_2 that will impact simulations of all physical properties including thermal transport.

8:50 AM

F-IV-2: CASCADE-INDUCED DEFECT FORMATION AND EVOLUTION IN IRON: A COMPARISON OF COMPUTATIONAL AND EXPERIMENTAL RESULTS

[CDP] H. Xu,[1] R. E. Stoller,[1] Yu. N. Osetskiy,[1] B. C. Larson,[1] G. M. Stocks,[1] V. McCreary,[2] I. M. Robertson[2,3]
[1]Oak Ridge National Laboratory, Oak Ridge, TN; [2]University of Illinois, Champaign-Urbana, IL; [3]University of Wisconsin, Madison, WI

Atomistic and *ab initio* approaches have been developed to enable direct comparison between their predictions and relevant experimental results. The timescale for radiation-induced defect formation in atomic displacement cascades is ~10 picoseconds, followed by short-term evolution (~10^{-3} to 10^{3} sec). The shorter timescale is amenable to atomistic simulations, but a challenge for experimental methods. New atomistic approaches, particularly the CDP-developed self-evolving atomistic Kinetic Monte Carlo (SEAKMC) method, enable simulation of the cascade debris evolution for times long enough (>milliseconds) to enable direct comparisons. Importantly, it is found that there are strong qualitative correlations between short-time molecular dynamics simulations (MD) in Fe and Fe-Cr and the results of our own ion irradiation experiments and a larger body of neutron irradiation data. The computational methods and the results obtained will be described, and comparisons will be shown between these simulations and CDP-conducted *ex situ* x-ray diffuse scattering measurements and *in situ* transmission electron microscopy (TEM) observations. Predictions of the lower limit for vacancy loop collapse will be correlated with x-ray diffuse scattering, and the nature of small dislocation loops predicted by SEAKMC and MD will be compared with TEM examination of ion-irradiated Fe and Fe-Cr. These examples demonstrate the synergy between the simulations and

experiments, with atomistic insights garnered from simulations explaining experimental observations and experiments testing predictions from simulations. For example, segregation of Cr to loops hinders loop mobility which biases loop character and predicts a shift to small loop sizes; this effect and prediction are supported experimentally.

9:10 AM

F-IV-3: HIGH PRESSURE NEUTRON DIFFRACTION WITH DIAMONDS

[EFree] Malcolm Guthrie[1], Reinhard Boehler[1], Kuo Li[1], Jamie. J. Molaison[2], António M. dos Santos[2], Christopher A. Tulk[2], Guoyin Shen[3], Stanislav Sinogeikin[3]

[1]Geophysical Laboratory, Carnegie Institution of Washington, Washington DC; [2]Neutron Sciences Directorate, Oak Ridge National Laboratory, Oak Ridge, TN; [3]High Pressure Collaborative Access Team, Carnegie Institution of Washington, Argonne IL

Neutron diffraction conveys a wealth of advantages compared to other structural probes. Key among these are its sensitivity to light atom locations (H^2,Be,B^{11},C), its ability to measure long range magnetic order and its unmatched utility in measurement of non-crystalline structure. These capabilities hint at the broad importance of this technique across the scientific thrusts of the EFree Center. However, critical limitations in maximum achievable pressures (typically < 25 GPa) have acted as a severe limit on its applicability. Driven by these needs, we established a neutron group within the Center with the goal of doubling accessible pressures to enable EFree science. The success of this project has stemmed from a "Center modality" allowing the melding of expertise in high-pressure and neutron-diffraction techniques through strong relationships with key DOE facilities.

We have focused on the SNAP beamline at the Spallation Neutron Source (ORNL), one of the most powerful neutron sources in the world. To achieve sufficient signals, we developed a new design of diamond-anvil cell with ~100-fold increase in volume. Implementation of the cell was accelerated by drawing on EFree's synchrotron expertise where we identified substantial technical overlap. We have greatly exceeded our original goals: measuring neutron diffraction at over 94 GPa and there is now great promise for a substantially expanded role for neutron diffraction. Here, we will present some details of the method and describe a recent study of the structure of heavy water ice under unprecedented pressures.

G. CARBON CAPTURE AND SEQUESTRATION

Session II: Thursday, July 18, 2013, 1:40 – 3:20; Virginia Suite A

1:40 PM

G-II-1: EMERGENT BEHAVIOR DURING CO_2 TRANSPORT WITHIN FAULTS – OBSERVATIONS BASED ON THE CRYSTAL GEYSER ANALOG

[CFSES] Peter Eichhubl[1], Jon Major[1], Matthew Balhoff[1], Honkyu Yoon[2], Sean McKenna[2], Thomas Dewers[2], Young Kim[1], Harpreet Singh[1], and Sanjay Srinivasan[1]

[1]University of Texas Austin, [2]Sandia National Laboratories

Faults, which can extend from storage reservoir depths to shallow groundwater aquifers, play a crucial role in geologic carbon storage security. We gathered samples from the natural analog at

Crystal Geyser, Utah and the observed CO_2 seeps along the Grand Wash fault. We also developed multi-scale modeling capabilities to examine two scenarios for CO_2 migration and seepage along the Grand Wash fault. A small-scale modeling framework enabled us to attribute the difference in surface expression of CO_2 leakage to a physical cause.

A key observation at the Crystal Geyser site is the lateral migration of CO_2 seep sites over time, which we have confirmed by isotope studies. By incorporating a pore-scale model for calcite precipitation, our multiscale model predicts permeability reduction at the continuum scale. In addition, a pore-scale model coupled with experimental results in a microfluidic pore network provides fundamental mechanistic explanations of how calcite precipitation alters flow paths by pore plugging. This behavior combined with percolation theory calculations at the macroscopic scale shows that permeability alterations cause re-routing of local flows. These in turn result in lateral migration of surface CO_2 seeps at rates comparable to those established by isotope dating.

Measurements on samples of CO_2-altered and unaltered sandstone from the Crystal Geyser site revealed that the peak strength of sandstone is reduced by 40% with alteration. This suggests, consistent with our sampling transects across the CO_2 alteration zones, that leakage could persist in the vicinity of an existing pathway as that pathway becomes cemented with calcite.

This work is supported as part of the Center for Frontiers of Subsurface Energy Security, 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-SC0001114. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

2:00 PM

G-II-2: SYNCHROTRON OBSERVATIONS OF 3D SCCO_2 DISTRIBUTION IN RESERVOIR MATERIALS: IMPLICATIONS FOR MODELING & SITE CHARACTERIZATION

[NCGC] Jonathan B. Ajo-Franklin[1], Marco Voltolini[1], Steven R. Pride[1], Tae-Hyuk Kwon[2]

[1] Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA; *[2] Korea Advanced Institute of Science and Technology, Republic of Korea*

Pore morphology, topology, and surface properties directly control scCO_2 distribution within porous materials. This distribution of scCO_2 controls a variety of processes including CO_2 dissolution rate, capillary trapping, and residual brine fraction. Few direct measurements of the pore-scale distribution of scCO_2 in geological samples have been made, leaving models describing multi-phase fluid dynamics, reactive transport, and geophysical properties reliant on analog systems or theoretical models describing phase configurations. In zones where capillary flow is dominant, capillary fingering should lead to a scCO_2 distribution determined by the distribution of pore entry pressures and pore topology during drainage. We have developed a system for making synchrotron micro-tomography measurements of pore-scale scCO_2 distribution in reservoir materials at in situ P/T conditions, allowing exploration of fluid distribution in scenarios where CO_2 and brine have field appropriate properties. In this presentation we will show results from scCO_2 invasion experiments conducted on sandstones from a variety of GCS sites & analogs. Segmentation and network analysis of the pore space reveals brine localization in small pores with high entry pressures as would be expected in capillary fingering. Development of a flow modeling system based on the MIS algorithm and invasion-percolation (IP) theory allowed a spatial comparison of the scCO_2 distribution to that predicted; results suggest that IP-based approaches can predict pore scale CO_2 distribution across

large model domains. Calculations of this class should allow determination of a variety of sub-grid hydrologic parameters currently unconstrained at many GCS sites and improve the reliability of field scale predictions of $scCO_2$ fate.

2:20 PM

G-II-3: GEOMECHANICS OF GEOLOGIC CARBON STORAGE: HAZARDS, LONG-TERM SEALING, AND STORAGE SECURITY

[CFSES] Thomas Dewers[1], Alex Rinehart[1], Jon Major[2], Peter Eichhubl[2], Pania Newell[1], Mario Martinez[1], Joseph Bishop[1], Steven Bryant[2]
[1]Sandia National Laboratories, [2]University of Texas Austin

Injection of waste fluids including CO_2 into the subsurface modifies the local state of stress in saline formations and in overlying caprock. Reservoir and caprock mechanical integrity both pre- and post-injection require an assessment of geologic heterogeneity and the attendant ranges in geomechanical response. Using examples of the Mt. Simon Sandstone in the Illinois Basin, and the Mancos Shale from the San Juan Basin, we discuss how variability in reservoir and caprock architecture and mechanical properties present challenges for predictive models and hazard mitigation associated with pore pressure increases. In particular, mudstone heterogeneity at all length scales presents difficulties for monitoring and prediction. Risk assessment approaches have focused on the injection interval and associated pressure-up as representing the main CCUS risk. We examine the possibility that long term time-dependent coupled processes may lead to emergent caprock leakage.

This work is supported as part of the Center for Frontiers of Subsurface Energy Security, 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-SC0001114. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

2:40 PM – Graduate Student Finalist

G-II-4: CONTROLS ON MINERALIZATION IN VOLCANOGENIC RESERVOIR ROCKS

[CFSES] Shuo Zhang[1,2], Donald J. DePaolo[2], Tianfu Xu[2], Marco Voltolini[2]
[1]*University of California, Berkeley, CA 94720, USA;* [2]*Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA*

We proposed to use volcanogenic sandstones for CO_2 sequestration. Such sandstones with a relatively high percentage of volcanic rock fragments (VRF) could be a promising target for CO_2 sequestration in that they have a sufficient percentage of reactive minerals to allow substantial mineralization of injected $scCO_2$, which provides the most secure form of CO2 storage, but can also be porous and permeable enough to allow injection at acceptable rates. The limitation in using volcanogenic sandstones as CO_2 reservoir rocks is that porosity and permeability tend to decrease with increase of volcanic rock fragments (VRF) and with the length and complexity of the diagenetic history. Decreased porosity limits the rate at which CO_2 can be injected. We evaluated these tradeoffs to assess the feasibility of using volcanogenic sandstone to achieve highly secure CO_2 storage. Using relationships between VRF percent, porosity and permeability from available geological data, the reactive transport code TOUGHREACT was used to estimate the rate and extent of CO_2 mineralization over 1000 years, and the trade-off between higher reactivity and lower porosity and permeability. For the parameter set that we believe is defensible, the optimal VRF percent for the largest amount of mineralized CO_2 is around 10-20%. The results show that as much as 80% CO_2 mineralization could occur in 1000 years and still allow sufficient injectivity so that ca. 1 megaton of CO_2 can be injected per year per well. The key to estimating how much CO_2 can be injected and mineralized is the relationship between permeability (or injectivity) and reactive mineral content. The overall relationships can be reduced to a simple equation that relates the fraction of injected CO_2 that becomes mineralized in 1000 years to the volume fraction of reactive minerals. We have sampled examples of volcanogenic sandstones from Miocene Etchegoin Formation, central California to examine these relationships. Characterizations of these samples by SEM, XRF and XRD show that they are very rich in reactive minerals with around 32% plagioclase, 10% clinopyroxene, 2% diopside, and 1% ilmenite. Porosities range from 10% to 20%, and permeabilities range from 10 mD to 1000 mD. Batch experiments are also in progress to obtain realistic reactivity estimates.

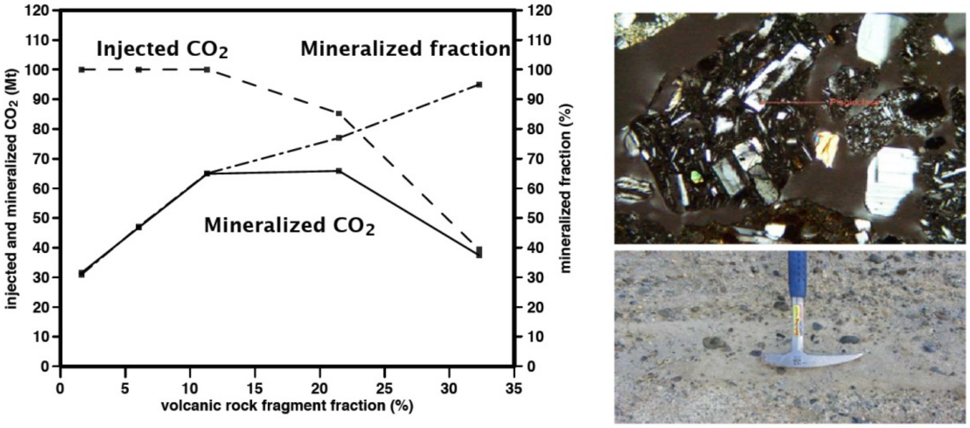


Figure 1. (Left) Amount of injected CO_2, mineralized CO_2 and mineralized fraction for different volcanic rock fragment (VRF) fractions, showing the largest amount of mineralized CO_2 at around VRF =10%-20%. (Right) Photomicrograph and outcrop photo showing volcanic mineralogy and abundant pore space from Miocene Etchegoin Formation, central California

3:00 PM – Graduate Student Finalist

G-II-5: SOLID, POROUS MATERIAL FOR IMPROVED EFFICIENCY OF GASOLINE PRODUCTION AND LOW-COST AND NON-TOXIC ENHANCEMENT OF GASOLINE QUALITY

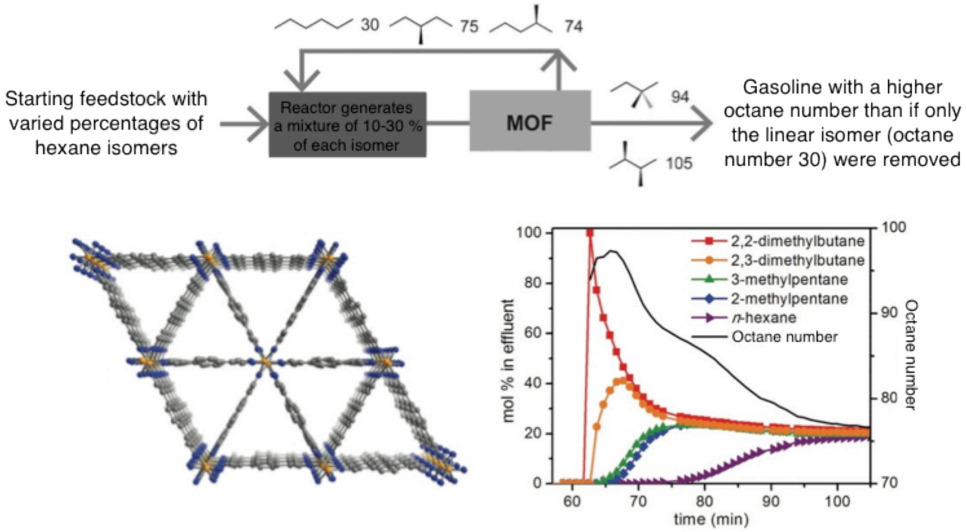
[CGS] Zoey R. Herm,[1] Brian M. Wiers,[1] Jarad A. Mason,[1] Jasper M. van Baten,[2] Norberto Masciocchi,[3] Rajamani Krishna,[2] Jeffrey R. Long[1]

[1]Department of Chemistry, University of California, Berkeley, CA 94720, USA. [2]Van't Hoff Institute for Molecular Sciences, University of Amsterdam, Science Park 904, 1098 XH Amsterdam, Netherlands..
[3]Dipartimento di Scienza e Alta Tecnologia, Università dell'Insubria, via Valleggio 11, I-22100 Como, Italy.

The discovery presented here could render the refining of petroleum more efficient and, as a result, save substantial energy worldwide. Further, if fewer low octane number hydrocarbons were added to gasoline, fewer toxic additives would be required to boost quality – benefiting both human health and the environment.

Saturated hydrocarbons such as pentane (C_5H_{12}), hexane (C_6H_{14}), and heptane (C_7H_{16}) each have multiple isomers in which the same number of carbons can be connected linearly or with branch points. These isomers are components of gasoline and have drastically varying value in the petroleum industry due to their wide-ranging octane numbers. Currently, some of the low-quality isomers end up in gasoline because they cannot be removed efficiently, and high-octane additives which require energy to generate and also are often toxic are added to the gasoline to compensate.

Through collaboration between theoretical modeling and the development of new experimental techniques (bottom right below), the solid iron based material $Fe_2(BDP)_3$ reported here (bottom left below) was pinpointed and shown to efficiently separate the most valuable isomers because of the rare triangular shape of its pores.



Top: Schematic of the proposed hexane isomer separation. The numbers next to the hexane isomers are octane numbers. *Bottom Right:* The crystal structure of $Fe_2(BDP)_3$ showing Fe (orange), N(blue), and C(gray) atoms, viewing along the *c*-axis. *Bottom Left:* Results of a breakthrough experiment in which a mixture of hexane isomers were moved through a bed of $Fe_2(BDP)_3$. The more valuable dimethylbutane isomers elute first and are therefore possible to separate.

Herm, Z. R.; Wiers, B, M.; Mason, J. A.; van Baten, J. M.; Hudson, M. R.; Zajdel, P.; Brown, C. M.; Masciocchi, N.; Krishna, R.; Long, J. R. *Science* **2013**, *340*, 960-964.

Session V: Friday, July 19, 2013, 11:00 – 12:00; Delaware Suite B

11:00 AM

G-V-1: DRAWING CORRELATIONS BETWEEN STRUCTURE AND GAS-ADSORPTION/SEPARATION PROPERTIES OF METAL-ORGANIC FRAMEWORKS

[CGS] Wendy L. Queen[1], Craig M. Brown[2], Eric D. Bloch[3], Jeffrey R. Long[3]

[1]The Molecular Foundry, Lawrence Berkeley National Laboratory, Berkeley CA; [2]Center for Neutron Research, National Institute of Standards and Technology, Gaithersburg, MD; [3]Department of Chemistry, University of California, Berkeley, CA

Metal organic frameworks (MOFs) are crystalline materials that contain metal-ions or metal-ion clusters as nodes and organic ligands as linkers to form 1-, 2-, and 3-D structures. In addition to their convenient modular synthesis and chemical tunability, this class of materials has been under intense investigation for gas storage and separation applications due to the discovery of many 3-D frameworks with high internal surface areas. Through careful selection of the ligand and metal, which control pore size/shape and MOF-adsorbate interactions, their uptake properties, such as gas selectivity, can be tuned. We have shown that an effective strategy to increase the binding energy of guest species is through the generation of MOFs that, upon solvent removal, contain high concentrations of coordinatively unsaturated metal centers (UMCs) on the framework surface. Due to their highly reactive, electron deficient nature, UMCs can drastically enhance gas uptake / selectivity, increase adsorbate surface packing density, and in some instances allow charge transfer between the framework and bound guest species. In order to obtain a better understanding of how structure dictates function during adsorption/ desorption processes we have performed detailed neutron and X-ray diffraction experiments on several porous frameworks with UMCs. These experiments have allowed us to probe structural changes in the framework as well as the exact positions, occupancy, and site affinity of several small molecules such as CO_2.

11:20 AM

G-V-2: UPSCALING CARBONATE MINERAL GROWTH RATES FROM THE NANO- TO PORE- SCALES

[NCGC] Andrew G. Stack[1], Carl I. Steefel[2], Glenn A. Waychunas[2], Alejandro Fernandez-Martinez[3], Gernot Rother[1], Lawrence M. Anovitz[1], Jacquelyn N. Bracco[4]

[1]Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA; *[2]Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA*; *[3]Université Joseph-Fourier Grenoble I & CNRS, Grenoble Cedex 9, France*; *[4]Wright State University, Dayton, OH 45435, USA*

The ability to quantitatively predict and control the rate and locales of carbonate mineral precipitation in porous media is an important factor necessary to evaluate and constrain the long-term success of geologic carbon sequestration. Efficient carbonate mineral growth will ensure that available aquifer pore space in an aquifer is filled by a high storage security solid phase and seals leaks in cap-rocks. Precipitation processes are ultimately driven by atomic-scale reactions on surfaces, but it is impractical to evaluate these directly at the reservoir scale: methods to upscale atomic- or nano-scale rates must therefore be used. We will focus on our recent work to develop expressions describing the precipitation of carbonate minerals valid at the nanoscale, but macroscopically applicable, and the effects of pores. Calcite ($CaCO_3$) precipitation has been used as a generalized carbonate mineral due to its fast reaction rate at room temperature. Initially, nanoscale measurements of the intrinsic reaction rate of the mineral's surface sites and their density will be discussed, as well as theory to upscale these observations to the macroscale. The rates obtained from this "process-based" approach are quantitatively consistent with many

macroscopic measurements made under a range of solution conditions. At the pore scale, we have examined precipitation onto synthetic and natural samples using X-ray and neutron scattering. We find that the surface chemistry between the precipitating mineral and the host substrate affect the size of pores into which precipitation preferentially occurs, but that rates nominally consistent with reactive transport models can be made in porous media.

11:40 AM

G-V-3: COMPUTATIONAL APPROACHES IN GAS SEPARATION

[CGS] Allison L. Dzubak,[1] Laura Gagliardi, [1] Maciej Haranczyk,[4] Jihan Kim,[3] Kuyho Lee,[3] Li-Chiang Lin, [2] Richard L. Martin,[4] Jeffrey B. Neaton,[3] Johanna Obst, [2] Nora Planas,[1] Berend Smit,[2]

[1]Department of Chemistry, University of Minnesota, MN; [2]Department of Chemical and Biomolecular Engineering, University of California, Berkeley, CA; [3]Materials Science Division, Lawrence Berkeley National Laboratory, Berkeley, CA; [4]Computational Research Division, Lawrence Berkeley National Laboratory, Berkeley, CA

In this presentation we describe how computational techniques can be used to screen materials for carbon capture. Our starting point is the question how to define the optimal material. We introduce the concept of parasitic energy as a metric to compare different materials; the best material is the material that minimizes the loss of efficiency of a power plant. To compute this parasitic energy one need information on the mixture isotherms of the various components of flue gasses. We show how quantum chemical calculations can be used to predict the adsorption energies. In addition, we show how these calculations can be used to develop a force field that allows us to predict the adsorption properties. We will apply these methods for materials for which experimental data is lacking, and for materials that have not yet been synthesized.

H. CATALYSIS

Session I: Thursday, July 18, 2013, 10:30 – 12:10; Virginia Suite A

10:50 AM

H-I-1: ALD OVERCOATS: A NEW TOOL FOR HIGH PERFORMANCE CATALYST DESIGN

[IACT] Junling Lu[1], Christian Canlas[2], Natalie Ray[2], Brandon O'Neil[3], David H. K. Jackson[3], Anthony J. Crisci[3], Carrie A. Farberow[3], Fengyuan Shi[3], Paul J. Dietrich[4], Christopher L. Marshall[1], Jeffrey T. Miller[1], Sungsik Lee[1], Jeffrey W. Elam[1], Randall E. Winans[1], Justin M. Notestein[2], Paul M. Voyles[3], Manos Mavrikakis[3], Thomas F. Kuech[3], James A. Dumesic[3], Jeffrey Greeley[4], Fabio H. Ribeiro[4], Peter C. Stair[1,3]
[1]Argonne National Lab; [2]Northwestern University; [3]University of Wisconsin; [4]Purdue University

The atom-efficient conversion of chemical energy feedstocks into desirable fuels and chemicals is an important objective for the design of new catalytic materials. The ability of atomic layer deposition (ALD) to form conformal coatings whose thickness and composition can be controlled with atomic precision makes possible new designs for heterogeneous catalysts that possess exceptionally long-lasting and selective performance. A particularly effective design positions the active catalytic site, either a late transition metal or an early transition metal oxide, at the bottom of a very short (1-5 nm) pore. This motif serves to stabilize the catalytic material against leaching or sintering that degrades performance while simultaneously controlling access by reagents to the catalyst. Synthesis of this structure has been accomplished by either 1) overcoating the catalytic material with a controlled thickness of ALD alumina, followed by high temperature annealing to open pores through the overcoat or 2) depositing ALD alumina around a molecular template chemisorbed on the catalyst surface, followed by removal of the template to generate a channel to the catalyst. For supported noble metal nanoparticle catalysts the ALD overcoats impart selectivity and stability by anchoring and blocking under-coordinated atoms located at edges and corners while leaving facets open on the nanoparticle surface. Size-selective catalysis has been demonstrated using calixarenes and adamantane carboxylic acids as molecular templates.

11:10 AM

H-I-2: A STEP TOWARDS SYNTHESIS AND IN SITU CHARACTERIZATION OF CATALYSTS WITH ATOMIC-PRECISION

[CALCD] Katla Sai Krishna,[1,4] Chelliah V. Navin,[1] Sanchita Biswas,[1] Yuehao Li,[2] Krishnaswamy Nandakumar,[2] Jeffery T. Miller,[3] James Spivey,[2, 4] Jing Liu,[1] Yaroslov B. Losovyj,[1] Ulrike Diebold,[5] Challa S. S. R. Kumar,[1, 4]
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One of the main challenges for developing effective catalysts from first principles is lack of tools for synthesizing and characterizing catalysts with atomic-precision, in real time and under practical experimental conditions. To address this challenge, we have utilized computational fluid dynamic simulations to design various millifluidic chips for synthesis and in situ characterization of catalysts in a continuous flow device. In these chips, solutions containing the soluble catalyst precursors are mixed in a flow channel of millimeter dimensions, and clusters of the metals nucleate and grow, and

can be deposited on the channel walls. We show that by probing the reaction using synchrotron radiation-based X-ray absorption spectroscopy, these simple devices can be used for in-situ time-resolved characterization of gold cluster formation at the scale of atoms, with a time resolution in micro seconds. X-ray tomography experiments revealed that width and thickness of the gold coating formed varied with deposition time. These gold depositions were found to be catalytically active for conversion of 4-nitrophenol into 4-aminophenol, providing an example of potential opportunities for flow catalysis and for time resolved analysis of catalytic reactions.

11:30 AM

H-I-3: RATIONAL DESIGN OF MOLECULAR ELECTROCATALYSTS FOR OXIDATION AND PRODUCTION OF H_2 USING FIRST ROW TRANSITION METALS

[CME] Michael P. Stewart, Wesley A. Hoffert, Stefan Wiese, R. Morris Bullock, Monte L. Helm
Center for Molecular Electrocatalysis, Physical Sciences Division, Pacific Northwest National Laboratory, P.O. Box 999, K2-57, Richland, Washington 99352

Recent advances in bio-inspired catalysts obtained in the Center for Molecular Electrocatalysis at Pacific Northwest National Laboratory demonstrated the electrocatalytic oxidation and production of H_2 using inexpensive, abundant metals such as Ni, Mn and Fe. A key feature in our studies is the incorporation of a pendant amine as a proton relay into the ligand, generally at a distance that will preclude formation of a M-N bond. In these catalysts the transformation between H_2 and protons proceeds via an interplay between proton and electron transfer steps and involves the interaction of a H_2 molecule with both a metal center and pendant amine bases. The use of careful energy matching of intermediates along catalytic cycles, key to designing catalysts with enhanced activity, will be discussed in this presentation. The synthesis, characterization and electrochemical analysis of new Ni and Fe H_2 oxidation catalysts will be discussed. Additionally, we will discuss recent advances in the synthesis and study of water-soluble Ni electrocatalysts for H_2 production from H_3O^+.

11:50 AM – Postdoctoral Researcher Finalist

H-I-4: ADSORBATE INDUCED ADATOM MOBILITY IN A MODEL CATALYST: PD/FE$_3$O$_4$

[CALCD] Parkinson G.S.
Vienna University of Technology, Vienna, Austria

Industrial catalysts often comprise metal nanoparticles residing on a metal-oxide support. As part of the center for atomic level catalyst design, we are searching for model systems that will allow us to disentangle the fundamental processes underlying heterogeneous catalysis, and with which to test the limits of current theoretical modeling. Recently, we discovered that the Fe_3O_4(001) surface[1] stabilizes single metal adatoms of catalytically active metals to high temperatures; Au atoms, for example, remain isolated up to 400 °C[2]. This remarkable property facilitates very interesting, previously impossible, experiments. For example, one can test the hypothesis of "single-atom catalysis" to unambiguously show whether single atoms can really catalyze chemical reactions. If single atoms are catalytically active, the amount of precious metal required, and with it much of the cost of a catalyst, could be slashed.

In this presentation, we use the Fe_3O_4(001) adatom template to investigate how gas molecules affect the stability of a model Pd/Fe_3O_4 catalyst[3]. Under ultrahigh vacuum conditions, atomically resolved scanning tunneling microscopy (STM) movies show that single Pd atoms are completely stationary over many hours. In the presence of CO, however, highly mobile Pd-carbonyl species form, and mass transport is initiated at the surface. When a critical number of Pd-carbonyls meet, clusters nucleate. The cluster nuclei are themselves mobile, diffusing across the surface, collecting nearby adatoms until a stable size is reached. Tracking the evolution of the system atom-by-atom allows all the details of the sintering process to be discerned. Complementary DFT calculations show that CO lifts the Pd atoms from the surface, vastly reducing the barrier for diffusion One particularly interesting finding is that reaction with surface hydroxyl groups stabilizes Pd atoms against carbonyl formation, preventing the sintering mechanism. These results shed new light on the sintering process, and hint that pretreatment with relevant molecules could be a viable strategy for extending catalyst lifetimes.

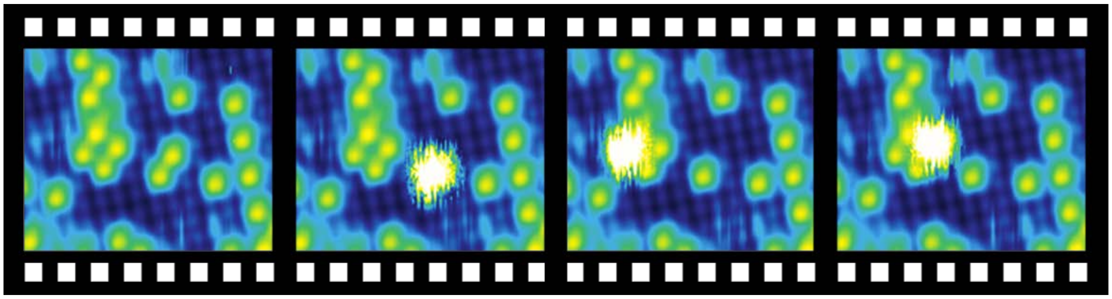


Figure 1: Selected frames from an STM movie showing the formation and subsequent mobility of a Pd-carbonyl in the Pd/Fe_3O_4(001) model catalyst

1. G. S. Parkinson, T. A. Manz, Z. Novotny, P. T. Sprunger, R. L. Kurtz, M. Schmid, D. S. Sholl, and U. Diebold, Phys. Rev. B 85, 195450 (2012).
2. Z. Novotny, G. Argentero, Z. Wang, M. Schmid, U. Diebold, G.S. Parkinson, Phys. Rev. Lett., 108, 216103 (2012)
3. G. S. Parkinson Z. Novotny, G. Argentero, M. Schmid, J. Pavelec, R. Kosak, P. Blaha, U. Diebold, Nature Materials, in press (2013).

Session III: Thursday, July 18, 2013, 3:40 – 5:00; Virginia Suite A

3:40 PM

H-III-1: DEVELOPMENT OF WELL DEFINED SINGLE-SITE CATALYSTS SUPPORTED ON MESOPOROUS SILICA NANOPARTICLES: APPLICATION TOWARD HYDROCARBON FUNCTIONALIZATION

[CCHF] T. Brent Gunnoe[1], Brian G. Trewyn[2], Andrei N. Vedernikov[3], Tristan S. Gray[1], Jeremy R. Andreatta[1], Theodore D. Matson[1], Pranaw Kunal[2], Daoyong Wang[3]
[1]Department of Chemistry, University of Virginia; [2]Department of Chemistry and Geochemistry, Colorado School of Mines; [3]Department of Chemistry and Biochemistry, University of Maryland

The catalytic functionalization of hydrocarbons is central to the petrochemical industry including the production of higher value compounds and fuel processing; however, many current processes operate under high temperature and pressure, are energy intensive and often exhibit poor selectivity. It is challenging to systematically alter heterogeneous catalysts to optimize reaction selectivity. In contrast, the development of molecular catalysts offers opportunities to enhance selectivity for hydrocarbon functionalization, but many molecular catalysts suffer from rapid deactivation. Molecular Pt complexes have been demonstrated to functionalize alkanes, and our groups have developed new Pt complexes that mediate olefin hydroarylation and olefin oxidation. Mesoporous silica nanoparticles (MSNs) are attractive for catalysis because of the ability to control pore size and vary surface functionality. The covalent attachment of a variety of molecular Pt complexes to MSNs will be discussed, including characterization data. Also, it has been demonstrated that these new materials exhibit improvements over the corresponding molecular catalysts, including increased catalyst stability and longevity as well as access to new aerobic oxidation transformations.

4:00 PM

H-III-2: PRODUCT SELECTIVITY IN THE ELECTROCHEMICAL REDUCTION OF CO_2 AT CU ELECTRODES

[CALCD] John Flake[1], Evan Andrews[1], Maoming Ren[1], Ziyu Zhang[2], Phillip Sprunger[2], Richard Kurtz[2], Aravind Asthagiri[3], Wenjia Luo[3], Xiaowa Nie[3], and Michael Janik[4]

[1]Department of Chemical Engineering, Louisiana State University, Baton Rouge, LA 70803; [2]Department of Physics, Louisiana State University, Baton Rouge, 70803; [3]Department of Chemical Engineering, The Ohio State University, Columbus, OH 432104; [4]Department of Chemical Engineering, Pennsylvania State University, University Park, PA 16802

The ability to store electrical energy in chemical bonds provides an attractive alternative to batteries. Liquid fuels generated from basic feedstocks such as CO_2 and water can be easily stored and used in a variety of energy generating systems such as engines and fuel cells. Historically, there have been relatively few examples of electrocatalysts capable of reducing CO_2 beyond CO to form higher value fuels such as methane or methanol. Further, research in this area has largely been limited to trial-and-error experimental work with little understanding of fundamental mechanisms that control rate limiting steps and selectivity. In this talk, we examine the roles of water and kinetics in determining the selectivity of products generated from the electrochemical reduction of CO_2.

Results from DFT calculations including activation barriers show the CO reduction step is the key selectivity determining step for CO_2 at Cu(111) electrodes. The dominant path proceeds via reduction of CO to COH, which leads to CH_x species, and produces mostly methane and some ethylene. If the CO is reduced to a CHO intermediate instead of COH, methanol is the preferred product over methane. The proposed pathways are consistent with the experimental data including in-situ FTIR analysis showing C-H, CHO, CH_2O, CH_3O intermediates under reduction conditions. These results suggest that future design of heterogeneous catalysts for CO_2 reduction should focus on the relative energetics of COH versus CHO to selectively produce liquid fuels such as methanol.

4:20 PM

H-III-3: HYDROCARBON OXYGENATION AND HALOGENATION WITH MANGANESE CATALYSTS

[CCHF] Wei Liu[1], Xiongyi Huang[2], Mu-Jeng Cheng[1], Robert J. Nielsen[1], William A. Goddard III[1], John T. Groves[2]

[1]Materials and Process Simulation Center, California Institute of Technology; [2]Department of Chemistry, Princeton University

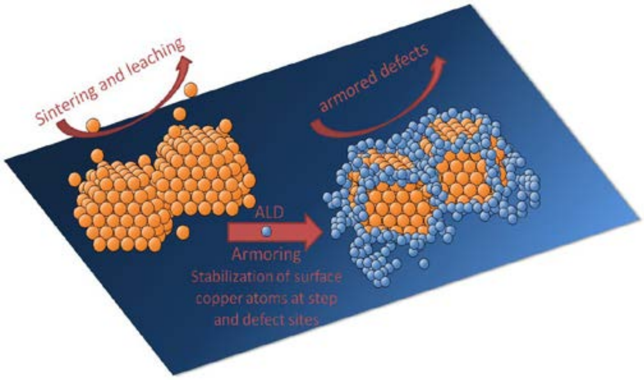
Despite the growing importance of halogenated organic compounds, including alkyl fluorides, there are few direct protocols for the selective halogenation of aliphatic C-H bonds. Manganese porphyrin and manganese salen complexes have long been known to catalyze oxygen transfer reactions. We have recently discovered that these manganese complexes also catalyze C-H halogenation under mild conditions. Significantly, alkyl C-H fluorination reactions were also found to be selective and efficient using conveniently handled fluoride salts as the only fluorine source. Simple alkanes, terpenoids, and more complex molecules were selectively fluorinated at otherwise inaccessible sites in 50 to 60% yield. Decalin was fluorinated preferentially at the methylene sets over the usually more reactive tertiary C-H bonds. The talk will focus on the combined use of experiment and DFT theory to discover these reactions and to real their interesting and novel mechanisms.

4:40 PM – Graduate Student Finalist

H-III-4: STABILIZATION BY ATOMIC LAYER DEPOSITION OF COPPER CATALYSTS FOR LIQUID PHASE REACTIONS

[IACT] Brandon J. O'Neill[1], David H. K. Jackson[2], Anthony J. Crisci[1,3], Carrie A. Farberow[1], Fengyuan Shi[2], Junling Lu[4], Paul J. Dietrich[5], Xiangkui Gu[5],Christopher L. Marshall[6], Peter C. Stair[6,7], Jeffrey W. Elam[8], Jeffrey T. Miller[6], Fabio H. Ribeiro[5], Paul M. Voyles[2], Jeffrey Greeley[5], Manos Mavrikakis[1], Susannah L. Scott[3,9], Thomas F. Kuech[1,2], and James A. Dumesic[1]

[1]Department of Chemical and Biological Engineering, University of Wisconsin, Madison, WI 53705, USA; [2]Materials Science Program, University of Wisconsin, Madison, WI 53705, USA; [3]Department of Chemistry and Biochemistry, University of California, Santa Barbara, California 93106, USA; [4]Department of Chemical Physics, University of Science and Technology of China, Hefei 230026, China; [5]Department of Chemical Engineering, Purdue University, West Lafayette, IN47907, USA; [6]Chemical Science and Engineering, Argonne National Laboratory, Argonne, IL 60439, USA; [7]Department of Chemistry and the Center for Catalysis and Surface Science, Northwestern University, Evanston, IL 60208, USA; [8]Energy Systems Division, Argonne National Laboratory, Argonne, IL 60439, USA; [9]Department of Chemical Engineering, University of California, Santa Barbara, California 93106, USA.



Precious metal catalysts are used extensively in the petrochemical industry and are anticipated to have a significant role in future biorefineries. While it would be desirable to replace precious metal catalysts (e.g., platinum) with base metals that are more abundant (e.g., copper), these base metal catalysts are susceptible to sintering and leaching under liquid-phase reaction conditions. Atomic layer deposition (ALD) of an alumina coating can be employed to stabilize a base-metal catalyst (e.g., copper) for liquid-phase catalytic reactions (e.g., hydrogenation of biomass-derived furfural in alcohol or water solvents), thereby eliminating the deactivation of conventional catalysts by sintering and leaching into the reaction medium. This method of catalyst stabilization reduces the need to employ precious metals (e.g., platinum) in liquid-phase catalytic processing. The alumina overcoat initially covers the active catalyst surface completely. We show using solid state nuclear magnetic resonance, powder X-ray diffraction, and electron microscopy that high temperature treatment (973 K) opens porosity in the overcoat by forming crystallites of γ-Al_2O_3. Infrared spectroscopic measurements, density functional theory, and scanning tunneling microscopy studies of trimethylaluminum ALD on Cu(111) show that the remarkable stability imparted to copper nanoparticles arises from selective armoring of highly under-coordinated copper atoms on the nanoparticle surface by the overcoating alumina.

The ability to stabilize base metals could have important applications beyond catalysis such as in electronics and especially in batteries. This project is an example of how IACT's collaborative structure brings together advanced synthesis, experimentation, theory, and characterization to advance fundamental scientific understanding and provide breakthrough solutions to real world problems.

IA. PREDICTIVE THEORY AND MODELING

Session IV: Friday, July 19, 2013, 8:30 – 9:30; Virginia Suite A

8:30 AM

Ia-IV-1: PREDICTING THE PERFORMANCE OF ALTERNATIVE FUELS

[CEFRC] William H. Green,[1] Stephen J. Klippenstein,[2] Ronald K. Hanson,[3] Chih-Jen Sung,[4] Donald G. Truhlar,[5] Fokion N. Egolfopoulos,[6] Chung K. Law,[7] Nils Hansen[8]

[1]Massachusetts Institute of Technology, [2]Argonne National Laboratory, [3]Stanford University, [4]University of Connecticut, [5]University of Minnesota, [6]University of Southern California, [7]Princeton University, [8]Sandia National Laboratories

A large number of potential alternative fuels have been proposed, and most discussions have focused on the challenges associated with producing each proposed fuel. However, an equally important question is 'how will the proposed fuel perform in engines?'. The Combustion EFRC has been focusing on developing efficient ways to answer that question. Here we report a combined theoretical and experimental study of the combustion of several proposed biofuels, including several isomers of butanol. Butanol is particularly interesting because it is near commercialization and because its isomers have very different chemistry and combustion performance. We find that certain fuel properties can be measured and/or predicted very accurately, while other fuel performance properties are much more challenging. In several cases the computer models and experiments significantly disagree; we have tracked down the origins of many of these discrepancies: some are due to experimental issues, some are due to errors in calculations and databases, and some have led us to discover important unexpected new types of chemical reactions. The current status and prospects for predicting fuel performance will be summarized.

8:50 AM

Ia-IV-2: MECHANISTIC ANALYSIS AND DESIGN OF HETEROGENEOUS CATALYSTS FOR BIOMASS CONVERSION

[IACT] Bin Liu[1], Jessica Scaranto[2], Suyash Singh[2], Rajeev Assary[1], Lei Cheng[1], Xiangkui Gu[3], Paul J. Dietrich[3] Junling Lu[1], Yu Lei[1], Brandon O'Neil[2], Carrie A. Farberow[2], Christopher L. Marshall[1], Jeffrey W. Elam[1], Linda Broadbelt[4], James A. Dumesic[2], Peter C. Stair[1,4], Jeffrey T. Miller1, Fabio H. Ribeiro[3], Larry Curtiss[1], Manos Mavrikakis[2], Jeffrey Greeley[3]

[1]Argonne National Lab; [2]University of Wisconsin; [3]Purdue University; [4]Northwestern University

The production of fuels from biomass-related feedstocks is a critical challenge motivating the study and design of new catalysts. First principles computational techniques, in close synergy with experimentally-based studies of catalyst synthesis, characterization, and testing, are well positioned to contribute to these efforts. Within IACT, approaches have been pioneered to apply first principles methods to biomass-relevant reactions ranging from aqueous phase reforming to the conversion of fructose to HMF. Methods under development and applied within IACT include 1) an approach to rapidly estimate the thermodynamics and kinetics of complex biomass reaction networks on metal catalyst surfaces, 2) prediction of volcano plots and novel catalyst structures for hydrogen production reactions, and 3) analysis of acid-catalyzed reaction networks in bulk, liquid-phase solutions. Related strategies have also been successfully employed to understand atomic layer deposition of alumina layers on late transition metal substrates and their stabilizing effect. Taken together, these computational efforts contribute to all aspects of IACT's work by both providing

molecular-level interpretations of our state-of-the-art experiments and producing testable predictions for improved catalysts.

9:10 AM

Ia-IV-3: HIGH-FIDELITY SIMULATIONS OF TURBULENCE-CHEMISTRY INTERACTIONS TOWARDS PREDICTIVE MODELS FOR ENERGY CONVERSION DEVICES WITH ALTERNATIVE FUELS

[CEFRC] Jacqueline H. Chen,[1] Stephen B. Pope,[2] Chung K. Law,[3] Rolf D. Reitz[4]
[1]Sandia National Laboratories, [2]Cornell University, [3]Princeton University [4]University of Wisconsin-Madison

Petascale computing has made it possible to glean fundamental physical insight into 'turbulence-chemistry' interactions in simple laboratory-scale turbulent flames using high-fidelity numerical approaches: direct numerical simulations (DNS) [i,ii] and large-eddy simulation with the probability density function approach (LES/PDF) [iii]. A principal objective of the Combustion Energy Frontier Research Center is to develop validated predictive models of combustion from the quantum chemistry to the turbulent flame scales characteristic of future energy conversion devices using alternative fuels. At the largest scale in the Center's multi-scale approach, LES/PDF and DNS in concert with coordinated experiments have focused on canonical configurations intended to illuminate key 'turbulence-chemistry' interactions featuring mixed-modes of combustion far from chemical equilibrium: lifted turbulent jet flame stabilization in autoignitive co-flows; transient ignition and weak flame propagation into stratified mixtures; ignition timing and pressure rise rate in homogeneous and spark-assisted compression ignition, and flashback in turbulent flame propagation in channels. These configurations were chosen because they isolate many of the underlying processes in low-temperature, high pressure engines and hydrogen-enriched combustion for carbon capture and storage that are poorly understood and for which current models are not applicable.

[i] Chen, J.H., Choudhary, A., de Supinski, B., DeVries, M., Hawkes, E.R., Klasky, S., Liao, W.K., Ma, K.L., Mellor-Crummey, J., Podhorski, N., Sankaran, R., Shende, S., Yoo, C.S., (2009), *Computational Science and Discovery* 2.
[ii] Chen J.H., (2011), *Proc. Combust. Inst*. 33, 99-123.
[iii] Yang, Y., Wang, H., Pope, S. B., Chen, J. H., (2013), *Proc. Combust. Inst.* 34, 1241–1249.

Session V: Friday, July 19, 2013, 11:00 – 12:00; Virginia Suite A

11:00 AM

Ia-V-1: EMERGENT PHENOMENA IN DRIVEN SYSTEMS OF ACTIVE COLLOIDS

[NERC] N. Nguyen[1], M. Spellings[2], D. Klotsa[2], M. Engel[2], B. Grzybowski[3], S.C. Glotzer[2,4]
[1]Mechanical Engineering, University of Michigan, Ann Arbor, MI; [2]Chemical Engineering, University of Michigan, Ann Arbor, MI; [3]Department of Chemical and Biological Engineering, Northwestern University, Evanston, IL; [4]Materials Science and Engineering, University of Michigan, Ann Arbor, MI

Active matter is an emerging branch of non-equilibrium soft matter that encompasses novel, dissipative structures formed from collections of particles driven via externally applied local forces. Examples include self-propelled particles and switchable colloids. Such systems can exhibit nontrivial, emergent behavior fundamentally different from behavior seen in traditional thermodynamic equilibrium, and for which there is no established theoretical framework and no general predictive capability. As such, active matter lies at the forefront of basic energy science. In this talk we describe new simulation studies of active colloidal matter in which externally applied forces drive the formation of unexpected structures, producing emergent, effective, interparticle interactions arising solely from the driven, active aspects of the system. We show that in some cases these emergent forces can be harnessed to perform meaningful work.

11:20 AM

Ia-V-2: ELECTRONIC STRUCTURE IN THE CETM-EFRC: TOWARDS A FUNDAMENTAL UNDERSTANDING OF ELECTROCATALYTIC (DE-)HYDROGENATION

[CETM] Ingolf Warnke[1], Steven Konezny[1], C. Moyses Araujo[1], Daniel L. Kellenberger[2], Mark Doherty[3], Davide Simone[3], Matthew Rainka[3], Peter Bonitatibus Jr. [3], John Kerr[4], John Arnold[2], Kristen Brownell[5], Antonio de Crici[5], Kate Waldie[5], Oana R. Luca[1], Robert H. Crabtree[1], Grigorii Soloveichik[3], Victor S. Batista[1]
[1]Yale University,[2]UC Berkeley, [3]GE Global Research, , [4]Lawrence Berkeley National Laboratory, [5]Stanford University

The energy frontier research center for electrocatalysis, transport phenomena, and materials (CETM) aims to develop fundamental understanding on catalytic electrodehydrogenation /electrohydrogenation of an organic carrier as 'virtual hydrogen storage'. We apply and develop electronic structure modeling methods in close collaboration with our experimental partners. Cross validating computational and experimental results enables characterization and design of (de-)hydrogenation catalysts and organic 'virtual hydrogen' carriers.

The selection of organic fuels is guided by density functional theory (DFT) calculations of the free energy changes associated with their dehydrogenation reaction energy profiles. In an extensive benchmark study, we have developed a protocol to reduce systematic uncertainties in DFT redox potentials. For several promising (de-)hydrogenation (electro-)catalysts, such as [Ir(trop$_2$DACH)], we provide insights into the nature of catalytic mechanisms. We focus on the role of transition metal hydrides in the C-H activation reactions and mechanisms associated with non-innocent ligand systems. Comparison to experiment is provided by means of electrochemical data, characterization of key-intermediates, and equilibrium constants. We currently investigate hydricities and proticities of metal hydride intermediates, and the influence of the ligands on structure/function relations. These properties are key for hydrogenation reactions and allow experimental characterization of transient intermediates. We use our insight to understand trends observed in a series of homolog

bipyridine derivatives as ligands for Rh-complexes, used for electrocatalytic oxidation of hydrogen carriers.

11:40 AM

Ia-V-3: FIRST-PRINCIPLES DESIGN OF ELECTROCATALYSTS FOR ENERGY STORAGE AND PRODUCTION: H_2 OXIDATION AND H_2 PRODUCTION

[CME] Ming-Hsun Ho, Shentan Chen, Roger Rousseau, Michel Dupuis, Daniel L. DuBois, R. Morris Bullock and Simone Raugei

Center for Molecular Electrocatalysis, Physical Sciences Division, Pacific Northwest National Laboratory, P.O. Box 999, K1-83, Richland, Washington 99352

Our research has demonstrated the possibility of cleaving H_2 or generating H_2, with turnover frequencies comparable or superior to those of hydrogenase enzymes, using complexes of inexpensive, abundant metals containing pendant amines in the metal coordination sphere. Using large-scale *ab initio* molecular dynamics, advanced statistical mechanics tools for free energy calculations and microkinetic modeling, we carried out an exhaustive characterization of molecular catalysts based on nickel. Our studies revealed that the metal center and the pendant amine act as a frustrated Lewis acid/base pairs, making the H_2 bond cleavage or formation a facile process. To maximize catalytic rates, it is of critical importance to precisely control the delivery of protons to the pendant amines and to match the energetics of various species involved in the catalysis. Toward the rational design of catalysts with optimal rates and overpotentials, we will discuss the development of linear free energy relationships, based on extensive *ab initio* thermodynamic and kinetic data, to be employed in a theoretically driven refinement of catalysts.

IB. PREDICTIVE THEORY AND MODELING

Session IV: Friday, July 19, 2013, 8:30 – 9:30; Virginia Suite B

8:30 AM – Postdoctoral Researcher Finalist

Ib-IV-1: NEW TERNARY MATERIALS DISCOVERED BY INVERSE DESIGN

[CID] Romain Gautier,[1] Xiuwen Zhang,[2] Andriy Zakutayev,[2] Arpun R. Nagaraja,[1] Feng Yang,[1] Liping Yu,[3] Stephan Lany,[2] David S. Ginley,[2] Thomas O. Mason,[1] Kenneth R. Poeppelmeier,[1] Alex Zunger[3]
[1]Northwestern University, Evanston, IL 60208, USA; [2]National Renewable Energy Laboratory, Golden, CO 80401, USA; [3]University of Colorado, Boulder, CO 80309, USA

The experimental realization of new inorganic compounds is limited by the large number of possible combinations of elements and the difficulties to identify and structurally characterize the new materials. In this context, the Inverse Design approach greatly accelerated the discovery of missing ABX ternary materials that satisfy the 18-electron valence rule by predicting their stability and crystal structures [1]. Synthesis of the predicted "missing" compounds by arc melting and vacuum annealing of stoichiometric ABX mixtures of pure elements resulted in the identification of TaCoSn [2], TaIrGe, ScRhTe, ZrRhBi, HfIrSb, VIrSi, VRhSi and HfRhP, all eight adopt the crystal structure predicted. Interesting optical and electronic properties were targeted such as for TaIrGe which is a transparent hole conductor.

Experimental realization of these materials demonstrates that theoretical prediction is key to identifying stable missing materials and in providing accurate information about the symmetry of these crystal structures. This latter information is critically important to accelerate the characterization of any newly made phase.

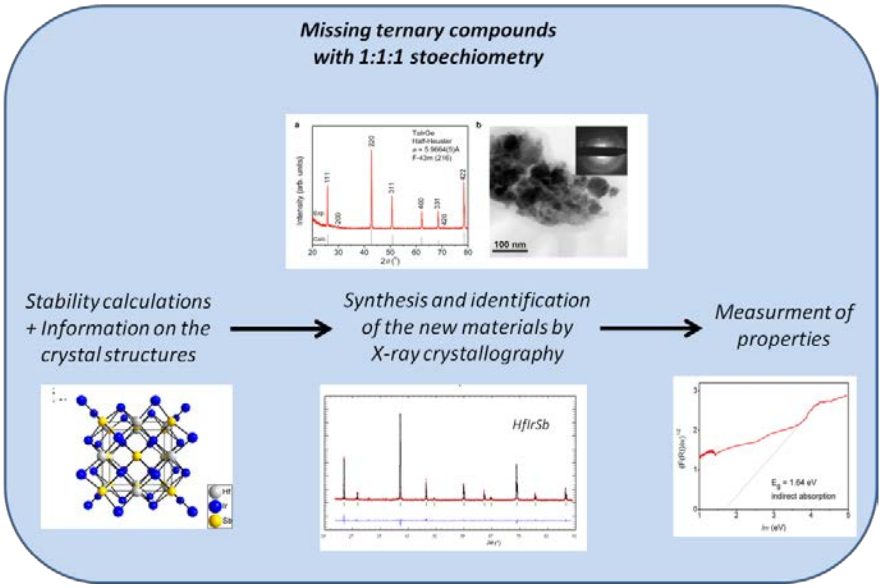


Figure 1. The discovery of missing ABX materials by Inverse Design.

References:
[1] X. Zhang, L.P. Yu, A. Zakutayev and A. Zunger, **Adv. Funct. Mater.** 22, 1425–1435 (2012).
[2] A. Zakutayev, X. Zhang, A.R. Nagaraja, L.P. Yu, S. Lany, T.O. Mason, D.S. Ginley, and A. Zunger, *Accepted*, ***J. Am. Chem. Soc.*** (2013).

8:50 AM – Graduate Student Finalist

Ib-IV-2: PREVENTING HELIUM-INDUCED DAMAGE THROUGH INTERFACE ENGINEERING

[CMIME] Abishek Kashinath[1], Michael J. Demkowicz[1]

[1] *Department of Materials Science and Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA.*

He implanted into metals precipitates into nanoscale bubbles that may later grow into voids, degrading the properties of engineering alloys in nuclear energy applications. However, using multiscale modeling, we find that at fcc-bcc interfaces, He is initially trapped in the form of stable, sub-nanometer platelet-shaped clusters, not bubbles[1]. This behavior occurs due to the spatial heterogeneity of the interface energy (Figure 1): He wets high energy, "heliophilic" regions while avoiding low energy, "heliophobic" ones. This insight allows us to predict the maximum He concentration that can be stored without forming bubbles at any interface in terms of its location-dependent energy distribution. We confirmed our modeling predictions with neutron reflectometry measurements, which showed that interfacial He bubbles form only above a critical He concentration and provided evidence for the presence of stable He platelets below the critical He concentration. Our work paves the way for the design of composite structural materials with increased resistance to He-induced degradation by tailoring the types of interfaces they contain. Such materials are indispensible for advanced fission and future fusion reactors.

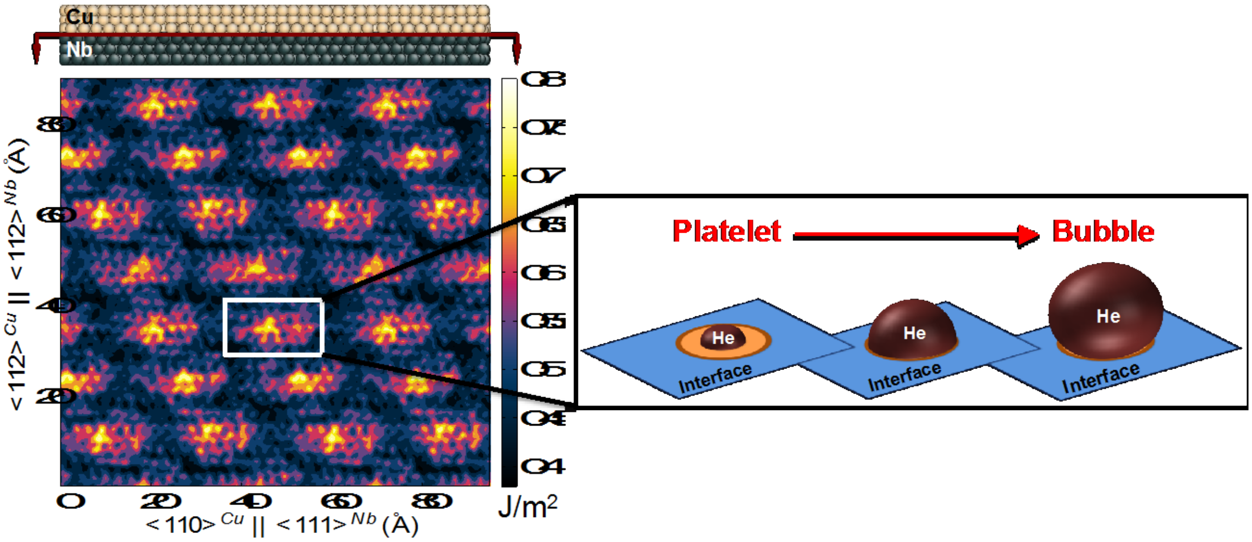


Figure 1. (left) Location dependence of Cu-Nb interface energy looking normal to the interface plane. Patches of highest energy are "heliophilic." (right) Schematic showing the growth of a He platelet and its eventual transformation into a bubble upon exhausting the "heliophillic" interface patch.

References:

1. A. Kashinath, A. Misra, and M.J. Demkowicz, Physical Review Letters **110**, 086101 (2013).

9:10 AM

Ib-IV-3: PREDICTIVE THEORY AND MODELING OF NEW MATERIALS AND NEW FUNCTIONALITIES VIA INVERSE DESIGN

[CID] Alex Zunger,[1] University of Colorado, Boulder Colorado 80309 and CID Collaborators [1,2,3,4,5,6]
[1]University of Colorado Boulder, CO 80309, USA, [2]National Renewable Energy Laboratory, Golden, Colorado 80401, USA, [3]Northwestern University, Evanston, IL 60208, USA, [4] Oregon State University, Corvallis OR 97331, USA, and [5]SLAC National Accelerator Laboratory, Menlo Park, CA 94025, USA, [6]Colorado School of Mines, Golden, CO 80401, USA.

We address, via integration of predictive theory and experiment, three of the currently leading obstacles to discovery of technologically important functional materials.

Obstacle 1 is that, whereas artificial materials can be made in the laboratory via layer-by-layer (superlattice) growth, we don't know *a priori* which of the countless number of possible layer sequences and ensuing mesoscopic structures has the material functionality we need. We address this bottleneck by genetic algorithm search of the configuration with given calculated electronic property ("Modality 1 Inverse Design"). This is illustrated for identifying the layer sequence of InAs/GaSb with target IR absorption and the Si-Ge structure with direct, allowed band gap.

Obstacle 2 is that we do not know even the basic materials properties of thousands of materials with known crystal structures documented in the inorganic literature, making it difficult to select suitable candidates for material-specific technologies. We address this bottleneck by theoretically developing computable metrics associated with particular target functionalities and screening computationally numerous materials, identifying a small number of "best of class" subjected to iterative experiment-theory scrutiny ("Modality 2 Inverse Design"). This is illustrated for newly discovered super strong PV absorbers and novel transparent conductors.

Obstacle 3 is that there are thousands of compounds that are missing altogether from current material compilations. We address this bottleneck by using functionality-directed first-principles thermodynamics to identify stable "missing compounds" ("Modality 3 Inverse Design"). This is illustrated for laboratory realization of our predicted, but previously unreported ABX compounds, including TaCoSn, and the new transparent hole conductor TaIrGe.

Session V: Friday, July 19, 2013, 11:00 – 12:00; Virginia Suite B

11:00 AM

Ib-V-1: NANOPHOTONICS FOR ENERGY-CONVERSION APPLICATIONS

[S3TEC] Marin Soljacic[1]
1. Physics Department, MIT

By nano-structuring materials at length scales smaller than the wavelength of light, one can create effective materials, exhibiting optical properties unparalleled in any naturally occurring materials. The power of this approach is illustrated via a number of important examples. Firstly, it is shown that the control over the density of photonic states via such effective materials provides an optimal way to control the far field emission of radiation. Angularly selective absorbers, or transmitters could be enabled; these could enhance performance of solar absorbers. Moreover, this approach can be used to control black body emission, which can now be tailored almost at-will. It is also shown that such materials offer unprecedented opportunities for tailoring the near-field. In the photonic near-field, thermal transfer can be orders of magnitude stronger at a given temperature than the black-body thermal transfer. And since over 90% of all primary energy sources are converted into electrical and mechanical energy via thermal processes, exciting energy-related applications could be enabled.

11:20 AM

Ib-V-2: DESIGN AND DISCOVERY OF NOVEL ELECTRODE MATERIALS FOR SOLID OXIDE FUEL CELLS

[HeteroFoaM] Andreas Heyden[1]
[1]*University of South Carolina*

As a result of the recent shale gas development there are abundant supplies of natural gas in the U.S. Considering that it is furthermore likely that the role of natural gas will continue to increase when greenhouse gas emissions are constrained, there is a critical need for a highly efficient and environmentally friendly natural gas-to-electrical energy conversion technology. Solid oxide fuel cell (SOFC) technology offers great promise for such an efficient and cost-effective conversion; however, state-of-the-art SOFC nickel cermet anodes suffer from coking and sulfur poisoning upon direct oxidation of hydrocarbon fuels. Hence, identifying alternative anode materials has become an important objective in the development of SOFC technology. Among the novel anode catalysts, perovskite based materials are of interest since they can accommodate various dopants and incorporate cations with multiple oxidation states which often improves the electrocatalytic activity and provides a mechanism for mixed electronic and ionic conductivity. Nevertheless, perovskite based anode materials generally display low electrochemical performance even for hydrogen fuels. To better understand the reasons for the low performance and to identify design criteria for the rational discovery of improved electrode materials for SOFCs, we investigated the electrocatalytic performance of $Sr_2Fe_{1.5}Mo_{0.5}O_{6-\delta}$ (SFM). Specifically, we first introduced a novel computational approach for modeling fuel cell performance from first principles and then studied the SFM (001) surface to identify the active surface composition, reaction mechanism, and rate controlling step for the electrochemical hydrogen oxidation. Finally, we propose strategies for the design of improved oxide based anode materials for SOFCs.

11:40 AM

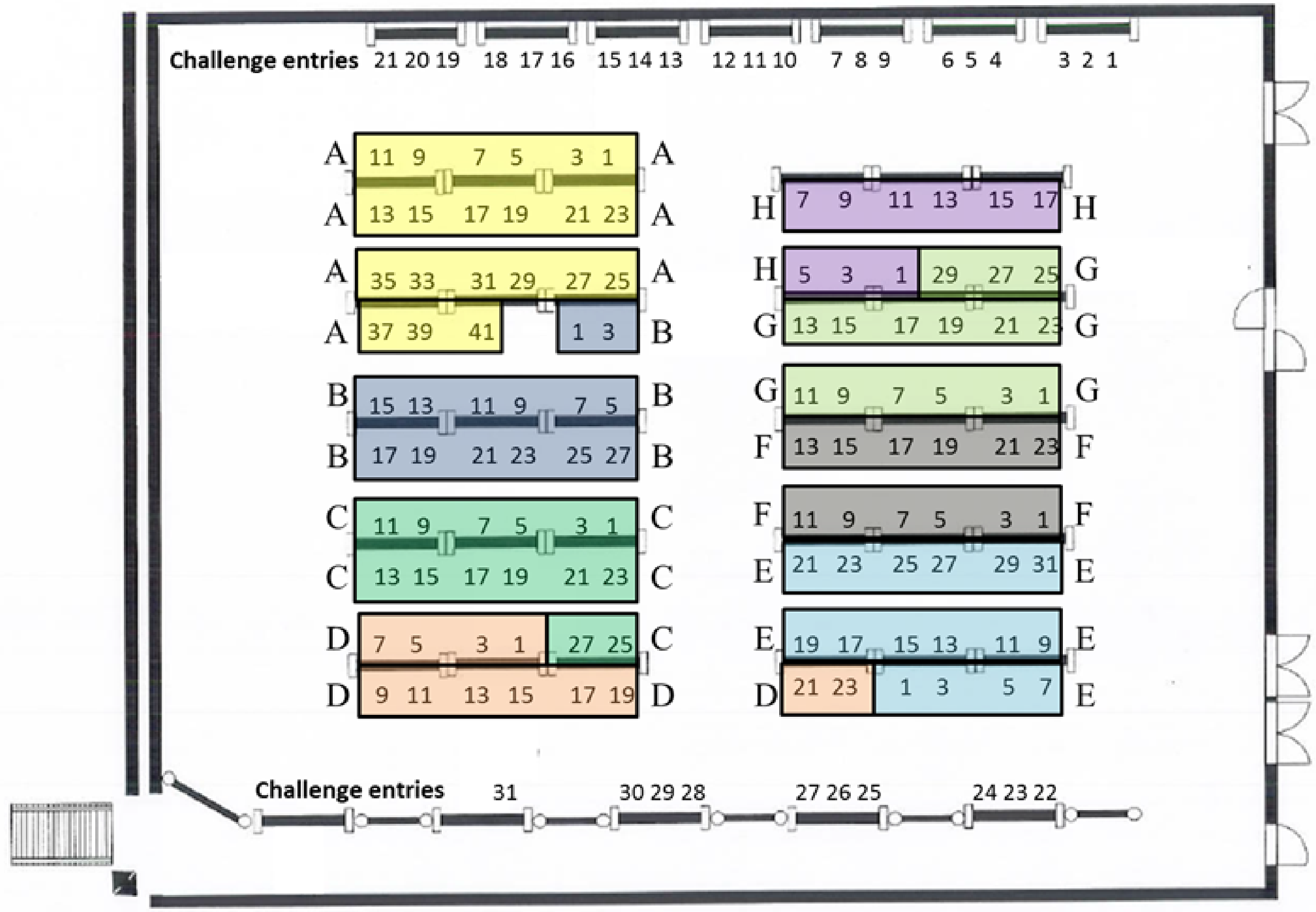
Ib-V-3: EXPERIMENTALLY GUIDED MODEL DEVELOPMENT AND PREDICTIVE THEORY IN THE FIRST CENTER

[FIRST] Paul R.C. Kent

Center for Nanophase Materials Science and Computer Science and Mathematics Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831

A central focus of the Fluid, Interface Reactions, Structure and Transport (FIRST) EFRC is the development of models and predictive theory strongly guided by experiments. We exploit the overlap of length and time scales sampled by different theoretical and experimental probes to enable a critical and informative comparison of results, and, in favorable cases, to develop a robust link between the experimental observations and underlying microscopic or atomistic processes. I will give examples of this approach including (i) water-graphene interactions, studied using classical and ab initio molecular dynamics contrasted with X-ray reflectivity data, (ii) the development and validation of molecular dynamics and classical density functional based models of the pore-size dependence of supercapacitance, (iii) ab initio molecular dynamics simulations of incipient solid electrolyte interphase formation at lithium ion battery anodes, and (iv) the related development of benchmarked reactive force fields (ReaxFF) to greatly extend the length and timescales accessible in simulations of lithium ion electrolyte and electrode systems, enabling a meaningful comparison with experiment.

Poster Session I – Thursday, July 18, 2013 – Marriot Salon 3
All Odd Numbered Posters



A. Solar Fuels and Biomass	D. Inorganic Photovoltaics	G. Carbon Capture and Sequestration
B. Energy Storage	E. Energy Conservation and Conversion	H. Catalysis
C. Organic Photovoltaics	F. Materials and Chemistry for Nuclear Energy Applications	I. Predictive Theory and Modeling

A. SOLAR FUELS AND BIOMASS

P-A-1: NANOSTRUCTURED METAL OXIDE BASED MATERIALS FOR APPLICATION IN DYE-SENSITIZED PHOTOELECTROSYNTHESIS CELLS

[UNC] James F. Cahoon[1], Byron H. Farnum[1], Leila Alibabaei[1], Wenjing Song[1], Robert J. Brown[1], Hanlin Luo[1], Cory J. Flynn[1], Dennis A. Ashford[1], Michael R. Norris[1], Paul G. Hoertz[2], Javier J. Concepcion[1], M. Kyle Brennaman[1], Thomas J. Meyer[1]

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P-A-3: A MUTATION IN INOSITOL POLYPHOSPHATE BIOSYNTHETIC PATHWAY LINKS TOR KINASE SIGNALING TO LIPID ACCUMULATION IN THE GREEN ALGA *CHLAMYDOMONAS REINHARDTII*

[CABS] Inmaculada Couso-Lianez[1], Spencer Diamond[2], Garret Anderson[3], James Umen[1]

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P-A-5: PHOTOINDUCED CHARGE TRANSFER DYNAMICS AT THE CHROMOPHORE AND ASSEMBLY-SEMICONDUCTOR INTERFACE

[UNC] Erik M. Grumstrup[1], Stephanie E. Bettis[1], Dennis L. Ashford[1], Derek M. Ryan[1], Michael R. Norris[1], Paul G. Giokas[1], Li Wang[1], Zhen Fang[1], Kenneth Hanson[1], Steven A. Miller[1], Robert J. Brown[1], Wenjing Song[1], Robin R. Knauf[1], Leila Alibabaei[1], Javier J. Concepcion[1], M. Kyle Brennaman[1], Jillian L. Dempsey[1], Andrew M. Moran[1], Marcey L. Waters[1], John M. Papanikolas[1], Thomas J. Meyer[1]

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P-A-7: IMPROVING OUR UNDERSTANDING AND CONTROL OF PHOTO- AND ELECTRO- CATALYSIS IN COMPLEX OXIDES—A THIN FILM APPROACH

[emc^2] Joel Brock[1]; Charles M. Brooks[2] (Darrell); Xin Huang[1]; Hanjong Paik[2]; Manuel Plaza[2]; Joaquín Rodríguez-López[3]; Héctor Abruña[3]; Tomás Arias[4]; Craig Fennie[1]; Darrell Schlom[2]

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P-A-9: PRODUCTION OF MONO- AND SESQUITERPENES IN SEEDS OF *CAMELINA SATIVA*

[CABS] Jörg M. Augustin[1], Yasuhiro Higashi[1], Xiaohong Feng[1], Toni M. Kutchan[1]

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P-A-11: CODOPING TIO_2 NANOWIRES WITH (W, C) FOR ENHANCING PHOTOELECTROCHEMICAL PERFORMANCE

[CNEEC] In Sun Cho[1], Chi Hwan Lee[1], Yunzhe Feng[1], Manca Logar[1], Pratap M. Rao[1], Lili Cai[1], Dong Rip Kim[1], Robert Sinclair[2] and Xiaolin Zheng[1]

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P-A-13: INTEGRATION OF MULTIPLE CHROMOPHORES WITH NATIVE PHOTOSYNTHETIC ANTENNAS TO ENHANCE SOLAR ENERGY CAPTURE AND DELIVERY

[PARC] Michelle A. Harris[1], Pamela S. Parkes-Loach[2], Joseph W. Springer[1], Jianbing Jiang[3], Elizabeth C. Martin[4], Pu Qian[4], Jieying Jiao[5], Dariusz M. Niedzwiedzki[1], Christine Kirmaier[1], John D. Olsen[4], David F. Bocian[5], Dewey Holten[1], C. Neil Hunter[4], Jonathan S. Lindsey[3], Paul A. Loach[2]

[1]Washington University in St. Louis, St. Louis, MO, [2]Northwestern University, Evanston, IL, [3]North Carolina State University, Raleigh, NC, [4]University of Sheffield, Sheffield, United Kingdom, [5]University of California- Riverside, Riverside, CA

P-A-15: BIOMIMETIC CHALCOGELS FOR SOLAR FUEL CATALYSIS

[ANSER] Abhishek Banerjee[1], Yurina Shim[1], Benjamin D. Yuhas[1], Amanda L. Smeigh[1], Alexios P. Douvalis[1], Eric A. Margulies[1], Michael R. Wasielewski[1], Mercouri G. Kanatzidis[1]

[1]Northwestern University

P-A-17: DE NOVO DESIGN OF ARTIFICIAL HYDROGENASES

[BISFuel] Anindya Roy[1], Michel Vaughn[1], Chris Madden[1], and Giovanna Ghirlanda[1]

[1]Department of Chemistry and Biochemistry, Center for Bio-Inspired Solar Fuel Production, Arizona State University, Tempe, Arizona 85287

P-A-19: TAILORING BIOMASS FOR ITS USE IN CATALYTIC AND HYDROPYROLYTIC CONVERSION PATHWAYS

[C3Bio] Maureen C. McCann[1], Nickolas A. Anderson[2], Hui Wei[3], Haibing Yang[4], Mauricio Antunes[1], Joseph Cox[4], Peter Ciesielski[3], Jeong Im Kim[2], Nate Mosier[5], Barron Hewetson[5], Mahdi Abu-Omar[6], Bryon Donohoe[3]; Clint Chapple[2], Michael E. Himmel[3], Angus Murphy[4], Wendy Peer[4], and Melvin P. Tucker[3]

Departments of [1]Biological Science, [2]Biochemistry, [4] Horticulture & Landscape Architecture, [5]Agricultural & Biological Engineering, and [6]Chemistry, Purdue University, West Lafayette, IN, [3]National Renewable Energy Laboratory, Golden, CO

P-A-21: ROLE OF SILANOL GROUPS IN SN-BETA ZEOLITE FOR GLUCOSE ISOMERIZATION AND EPIMERIZATION REACTIONS

[CCEI] Neeraj Rai[1], Stavros Caratzoulas[1], Dionisios G. Vlachos[1]

[1]University of Delaware

P-A-23: DEVELOPMENT OF NONPRECIOUS METAL CATALYSTS FOR THE OXYGEN EVOLUTION REACTION GUIDED BY *AB INITIO* THEORY AND PEC EFFICIENCY MODELING

[CNEEC] Linsey C. Seitz,[1] Zhebo Chen,[1] Arnold J. Forman,[1] Blaise A. Pinaud,[1] Jesse D. Benck,[1] Dennis Nordlund,[2] and Thomas F. Jaramillo[1]

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P-A-25: CATALYST DEVELOPMENT: WATER OXIDATION AND CO_2 REDUCTION

[UNC] Alexander J. M. Miller[1], Aaron K. Vannucci[1], Zuofeng Chen[1], Javier J. Concepcion[1], Robert A. Binstead[1], Chuncheng Chen[1], Peng Kang[1], David R. Weinberg[1], Daniel P. Harrison[1], M. Kyle Brennaman[1], Michael R. Norris[1], Paul G. Hoertz[2], Leila Alibabaei[1], Kenneth Hanson[1], Alessa A. Gambardella[1], Katherine E. Michaux[1], Cynthia K. Schauer[1], Maurice S. Brookhart[1], Royce W. Murray[1], Thomas J. Meyer[1]

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P-A-27: STUDY OF CELLULOSE STRUCTURES AND DEPOSITION PATTERNS IN INTACT PLANT CELL WALLS USING CELLULOSE-SPECIFIC VIBRATION SPECTROSCOPY

[CLSF] Christopher M. Lee[1], Kabindra Kafle[1], Yongbum Park[2], Candace Haigler[3], Daniel J. Cosgrove[2], and Seong H. Kim[1]

[1]Department of Chemical Engineering and [2]Department of Biology, Pennsylvania State University; [3]Department of Plant Biology, North Carolina State University

P-A-29: ADSORPTION OF THE COMPOUNDS ENCOUNTERED IN MONOSACCHARIDE DEHYDRATION IN ZEOLITES

[CCEI] Marta León[1], T. Dallas Swift[1], Vladimiros Nikolakis[1], Dionisios G. Vlachos[1]

[1]University of Delaware

P-A-31: BIO-INSPIRED PHOTOELECTROCHEMICAL TANDEM CELLS

[BISFuel] Dalvin D. Méndez-Hernández[1], Marely Tejeda-Ferrari[1], Jackson D. Megiatto, Jr.[1], Benjamin D. Sherman[1], Robert Godin[1], Maxime Fournier[1], Thomas Mallouk[2], Thomas A. Moore[1], Devens Gust[1], Vladimiro Mujica[1] and Ana L. Moore[1]

*[1]Department of Chemistry and Biochemistry, Center for Bio-Inspired Solar Fuel Production, Arizona State University, Tempe, Arizona 85287; [2]*Pennsylvania State University, University Park, PA 16801

P-A-33: MECHANISTIC UNDERSTANDING OF THE FAST PYROLYSIS OF OLIGOSACCHARIDES AND CELLULOSE

[C3Bio] John C. Degenstein[1], Matthew R. Hurt[2], Vinod K. Venkatakrishnan[1], Mckay W. Easton[1], Guannan Li[2], Huaming Sheng[2], Linan Yang[2], John J. Nash[2], Rakesh Agrawal[1], W. Nicholas Delgass[1], Fabio H. Ribeiro[1], Hilkka I. Kenttamaa[2]

[1]School of Chemical Engineering and [2]Department of Chemistry, Purdue University, West Lafayette, IN

P-A-35: MULTIPLE ROLES OF ZEOLITES IN FRUCTOSE DEHYDRATION

[CCEI] Jacob S. Kruger[1], Marta León[1], Vladimiros Nikolakis[1], Dionisios G. Vlachos[1]

[1]University of Delaware

P-A-37: TOWARD PHOTODRIVEN WATER OXIDATION BY A MOLECULAR IRIDIUM-BASED CATALYST

[ANSER] Julianne M. Thomsen[1], Rebecca J. Lindquist[2], Leah E. Shoer[2], Eric A. Margulies[2], Michael R. Wasielewski[2], Robert H. Crabtree[1], Gary W. Brudvig[1]

[1]Yale University, [2]Northwestern University

P-A-39: INTERCHROMOPHORE INTERACTIONS IN ARTIFICIAL PHOTOSYNTHETIC ANTENNAS

[BISFuel] Yuichi Terazono[1]; Gerdenis Kodis[1]; Ana L. Moore[1]; Thomas A. Moore[1]; Devens Gust[1]

[1]Department of Chemistry and Biochemistry, Center for Bio-Inspired Solar Fuel Production, Arizona State University, Tempe, Arizona 85287

P-A-41: QUANTUM AND CLASSICAL MECHANICAL MODELING OF CELLULOSE INTERACTIONS IN PLANT CELL WALLS

[CLSF] James D. Kubicki[1], Heath D. Watts[1], Zhen Zhao[1], Daniel J. Cosgrove[2], Linghao Zhong[3]

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B. ENERGY STORAGE

P-B-1: EVALUATION OF LIQUID ORGANIC FUELS IN FLOW/FUEL CELLS

[CETM] John Kerr[1], Elise Deunf[1], Leah Rubin[2], Kyle Clark[1], Eric Stenehjem[3], Chris Chidsey[3], Lakshmi Krishnan[4], Gary Yeager[4], Sydney Laramie[4], Grigorii L. Soloveichik[4]

[1]Lawrence Berkeley National Laboratory, [2]UC Berkeley, [3]Stanford University, [4]GE Global Research

P-B-3: DEVELOPMENT OF NOVEL MEMS-LEVEL ENABLING APPROACHES FOR NANOSCALE ENERGY STORAGE

[NEES] Ekaterina Pomerantseva[1,2], Markus Gnerlich[1,2], Hyun Jung[1,2], Xinyi Chen[3], Konstantinos Gerasopoulos[1,2,3], Gary Rubloff[2,3], and Reza Ghodssi[1,2,3]

[1]MEMS Sensors and Actuators Laboratory, Department of Electrical and Computer Engineering, [2]Institute for Systems Research, [3]Department of Materials Science and Engineering, University of Maryland College Park, MD 20742

P-B-5: ELECTROCATALYTIC OXIDATION OF FORMATE WITH RH(III) ELECTROCATALYSTS AND RELATED REACTIVITY FOR PEM FUEL CELL APPLICATIONS

[CETM] Daniel L. Kellenberger[1], Ingolf Warnke[2], Elise Deunf[3], Victor S. Batista[2], John Arnold[1], John Kerr[3]

[1]UC Berkeley, [2]Yale University, [3]Lawrence Berkeley National Laboratory

P-B-7: IN-SITU ELECTRICAL CHARACTERIZATION OF MNO_2 NANOWIRE CATHODES

[NEES] Mya Le Thai[1], Wenbo Yan[1], Brad Corso[2], Rajan Dutta[2], Philip Collins[2], Reginald Penner[1]

[1]Dept of Chemistry, University of California, Irvine, 92697, [2]Dept of Physics & Astronomy, University of California, Irvine, 92697

P-B-9: NEUTRON PROBES OF INTERFACIAL FLUID DYNAMICS

[FIRST] J.L. Banuelos[1], Alexander I. Kolesnikov[1], D.M. Anjos[1], G.M. Brown[1], Y. Cai[2], S.M. Chathoth[1], P.T. Cummings[1,3], G. Feng[3], Y. Gogotsi[4], E. Mamontov[1], M. Neurock[5], S.H. Overbury[1], D.J. Wesolowski[1], Z. Wu[1]

[1]Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA, [2]University of Virginia, Charlottesville, VA 22904, USA, [3]Vanderbilt University, Nashville, TN 37235, USA, [4]Drexel University, Philadelphia, PA 19104, USA, [5]University of Virginia, Charlottesville, VA 22904

P-B-11: FACTORS CONTROLLING THE NATURE OF THE SOLID ELECTROLYTE INTERPHASE AT LI-ION BATTERY ANODES

[CEES] Hadi Tavassol[1], Maria Chan[2], Andrew Gewirth[1]

[1]University of Illinois at Urbana-Champaign, [2] Argonne National Laboratory

P-B-13: SOLID-STATE NMR AND X-RAY SCATTERING CHARACTERIZATION OF NAFION-BASED FUEL CELL MEMBRANES: STRUCTURE AND DYNAMICS

[CETM] Matthew Dodd[1], Kyle Clark[2], Jeff Reimer[1], John Kerr[2]

[1]UC Berkeley, [2]Lawrence Berkeley National Laboratory

P-B-15: IN SITU TEM STUDY ON SODIATION/DESODIATION OF EXPANDED GRAPHITE

[NEES] Yang Wen[1], Kai He[2], John Cumings[2], Chunsheng Wang[1]

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P-B-17: UNRAVELING THE MYSTERIES BEHIND HYSTERESIS IN INTERCALATION AND CONVERSION REACTIONS

[NECCES] Hui-Chia Yu[1], Donghee Chang[1], Aziz Abdellahi[2], Katsuyo Thornton[1], Gerbrand Ceder[2], Anton Van der Ven[1]

[1]University of Michigan, [2]MIT

P-B-19: NEW CONCEPTS AND ADVANCES IN LI-O_2 ELECTROCHEMISTRY

[CEES] Maria Chan[1], Michael Thackeray[1], Andrew Gewirth[2]

[1]Argonne National Laboratory, [2]University of Illinois at Urbana-Champaign

P-B-21: NANOSCALE STRUCTURE OF ELECTROLYTES AT CHARGED AND UNCHARGED SURFACES

[FIRST] Ahmet Uysal[1], Hua Zhou[2], Guang Feng[3], Michael Rouha[3], Hugh Docherty[3], Paul Fenter[1], Peter Cummings[3], Pasquale Fulvio[4], Sheng Dai[4], John McDonough[5], Volker Presser[6], Yury Gogotsi[5]

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P-B-23: OBSERVATION OF ELECTROCHEMICAL PHASE TRANSFORMATIONS AT SINGLE PARTICLE LEVEL

[NECCES] Ulrike Boesenberg[1], Young-Sang Yu[1], Jaroslaw Syzdek[1], Robert Kostecki[1], Jordi Cabana[1], Dhamodaran Santhanagopalan[2], Y. Shirley Meng[2], Danna Qian[2], Fiona Strobridge[3], Clare P. Grey[3]

[1]Lawrence Berkeley National Laboratory, [2]U. California at San Diego, [3]Cambridge University

P-B-25: AUTONOMOUS PROTECTION, REPAIR, AND SHUTDOWN OF LITHIUM-ION BATTERIES

[CEES] Marta Baginska[1] and Jeffrey Moore[1]

[1]University of Illinois at Urbana-Champaign

P-B-27: UNDERSTANDING SNCO-CARBON NANOCOMPOSITES AS ANODE FOR LI-ION BATTERIES

[NECCES] Hyeyoung Jung,[1] Ruigang Zhang,[2] Natasha A. Chernova,[2] Dongli Zeng,[3] Sung-Wook Kim,[3] Feng Wang,[3] Kyung-Wan Nam,[3] Qi Wang,[2] Ruibo Zhang,[2] Fred Omenya,[2] Zhixin Dong,[2] Olaf Borkiewicz,[4] Karena W. Chapman,[4] Peter J. Chupas,[4] Yushan Zhang,[5] Jaroslaw Syzdek,[5] Xiao-Qing Yang,[3] Lin-Shu Du,[1] Jason Graetz,[3] M. Stanley Whittingham,[1,2] and Clare P. Grey[1,6]

[1]Stony Brook University, [2]Binghamton University, [3]Brookhaven National Laboratory, [4]Argonne National Laboratory, [5]Lawrence Berkeley National Laboratory, [6]University of Cambridge

C. ORGANIC PHOTOVOLTAICS

P-C-1: EFFECT OF NANOCRYSTAL SURFACE MODIFICATION ON THE PERFORMANCE OF HYBRID POLYMER:NANOCRYSTAL SOLAR CELLS

[CEN] Matthew J. Greaney[1], Elsa Couderc[1], Lijun Li[2], Joe C. Campbell[2], Stephen E. Bradforth[1], Richard L. Brutchey[1]

[1]University of Southern California and [2]University of Virginia

P-C-3: VISUALIZATION OF EXCITON DIFFUSION IN SPACE, TIME, AND ENERGY

[CE] Gleb M. Akselrod[1], Parag Deotare[1], Nicholas Thompson[1], Jiye Lee[1], Marc A. Baldo[1], Vinod Menon[2], Vladimir Bulovic[1]

[1]Center for Excitonics, Massachusetts Institute of Technology, Cambridge, MA, [2]Dept of Physics, Queens College of CUNY, NY

P-C-5: HIGH PERFORMANCE SOLUTION-PROCESSED SMALL MOLECULE SOLAR CELLS

[CEEM] Thuc-Quyen Nguyen

Chemistry Dept., University of California, Santa Barbara

P-C-7: ELECTRONIC STRUCTURE OF ORGANIC/METAL-OXIDE SEMICONDUCTOR INTERFACES AS DETERMINED BY INTRINSIC DEFECTS

[CISSEM] David A. Racke,[1] Leah L. Kelly,[1] Laura K. Schirra,[1] K. Xerxes Steirer,[1] Delvin Tadytin,[1] Philip Schulz,[2] Hong Li,[3] Paul Winget,[3] Veaceslav Coropceanu,[3] David Beljonne,[3] Jaewon Shim,[3] Hyungchul Kim,[3] Ajaya K. Sigdel,[4] Matthew Gliboff,[5] Dennis Nordlund,[6] David S. Ginger,[5] Joseph J. Berry,[4] Samuel Graham,[3] Bernard Kippelen,[3] Jean-Luc Brédas,[3] Antoine Kahn,[2] Neal R. Armstrong,[1] Oliver L.A. Monti[1]

[1]The University of Arizona, [2]Princeton University, [3]Georgia Institute of Technology, [4]National Renewable Energy Laboratory, [5]University of Washington, [6]SLAC National Accelerator Laboratory

P-C-9: PROBING ELECTRONIC STRUCTURE AND CHARGE TRANSFER BY NON-CONTACT AFM AND KELVIN PROBE FORCE MICROSCOPY

[CST] Raluca I. Gearba,[1] Peter A. Veneman,[1,2] Kory M. Mueller,[1,2] Calvin Chan,[3] Bradley J. Holliday,[1,2] Keith J. Stevenson[1,2]

[1]Center for Nano- and Molecular Science, The University of Texas at Austin, [2]Department of Chemistry, The University of Texas at Austin, [3]Sandia National Laboratories

P-C-11: MOLECULAR DESIGN, SUPERCRITICAL CO_2 PROCESSING, AND MORPHOLOGICAL OPTIMIZATION OF CONJUGATED POLYMERS FOR ORGANIC PHOTOVOLTAICS

[CSTEC] Jojo Amonoo[1], Bong-Gi Kim[2], Bing Huang[3], Hengxi Yang[4], Xiao Ma[3], Hossein Hashemi[3], Xi Chen[3], John Kieffer[1], Jinsang Kim[2,3,5], and Peter F. Green[1,2,3,5]

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P-C-13: TOPOLOGICALLY PROTECTED ONE-WAY EXCITON CHANNELS IN TWO-DIMENSIONAL PORPHYRIN ARRAYS

[CE] Joel Yuen

Center for Excitonics, Massachusetts Institute of Technology, Cambridge, MA

P-C-15: AN INTEGRATED VIEW OF CRITICAL CHARGE HARVESTING INTERFACES IN THIN-FILM PHOTOVOLTAICS

[CISSEM] Neal R. Armstrong,[1] Jeanne E. Pemberton,[1] Jean-Luc Brédas,[2] Antoine Kahn,[3] David S. Ginger,[4] S. Scott Saavedra,[1] Oliver L.A. Monti,[1] Seth R. Marder,[2] Dominic V. McGrath,[1] Dennis Nordlund,[5] Joseph J. Berry,[6] Dana C. Olson,[6] David S. Ginley,[6] Bernard Kippelen,[2] Erin L. Ratcliff,[1] Samuel Graham[2]

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P-C-17: USING SCANNING PHOTOCURRENT MICROSCOPY TO STUDY RECOMBINATION IN LANGEVIN AND NON-LANGEVIN POLYMERS

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P-C-19: CONTROLLING THE MORPHOLOGY OF ORGANIC PHOTOVOLTAICS USING SEQUENTIAL PROCESSING OF NOVEL POLYMERS AND FULLERENE DERIVATIVES

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P-C-21: COOPERATIVE COMPUTATIONAL AND EXPERIMENTAL APPROACH TO CONJUGATED PENDANTS IN DONOR-ACCEPTOR POLYMERS

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P-C-23: EXCITONS IN SUPRAMOLECULAR LIGHT-HARVESTING ANTENNAE

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P-C-25: EVAPORATION INDUCED SELF-ASSEMBLY AND CHARACTERIZATION OF NANOPARTICULATE FILMS: A NEW ROUTE TO BULK HETEROJUNCTIONS

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P-C-27: NEW GENERATION OF LIGHT-HARVESTING CONSTRUCTS WITH NATURALLY OCCURRING PROTEINS AND SYNTHETIC PIGMENTS

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D. INORGANIC PHOTOVOLTAICS

P-D-1: DESIGN OF HIGHLY-EFFICIENT, NANOSTRUCTURED SOLAR CELLS AND LEDs IN THIN FILM SEMICONDUCTORS

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P-D-3: DETAILED CHARACTERIZATION OF ATOMIC AND ELECTRONIC STRUCTURE: INTEGRATING THEORY AND EXPERIMENT

[CID] Michael F. Toney,[1] Yezhou Shi,[1] Linda Lim,[1] Kevin H. Stone,[1] Paul F. Ndione,[2] Andriy Zakutayev,[2] Phillip A. Parilla,[2] John D. Perkins,[2] David S. Ginley,[2] Nicola Perry,[3] Arpun R. Nagaraja,[3] Thomas O. Mason[3]
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P-D-5: TAILORING COMPOUND SEMICONDUCTOR NANOSTRUCTURES FOR NEXT GENERATION PHOTOVOLTAICS

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P-D-7: MODELING AND CHARACTERIZATION OF SOLAR THERMOPHOTOVOLTAIC DEVICES WITH HIGH-TEMPERATURE PHOTONIC CRYSTAL EMITTERS

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P-D-9: P-GRAINS AND GRAIN BOUNDARIES IN HIGHLY-CRYSTALLINE, MONOLAYER MOLYBDENUM DISULFIDE

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P-D-11: THIN-FILM, MICRO-SOLAR CELLS THROUGH TRANSFER PRINTING FOR LIGHT MANAGEMENT

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P-D-13: BASIC STUDIES AND OPTIMIZATION OF CHARGE TRANSPORT IN HIGH-PERFORMANCE COLLOIDAL QUANTUM DOT FILMS

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P-D-15: LOCAL ATOMIC AND ELECTRONIC STRUCTURES OF CHEMICALLY DOPED MONOLAYER GRAPHENE

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P-D-17: BONDING AND OPTICAL COUPLING IN ADVANCED MULTIJUNCTION SOLAR CELLS

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P-D-19: MECHANISMS OF ENHANCED OPTICAL ABSORPTION FOR ULTRATHIN SILICON SOLAR MICRO-CELLS WITH AN INTEGRATED NANOSTRUCTURED BACKSIDE REFLECTOR

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P-D-21: ADVANCED CHEMICAL APPROACHES TO SOLAR-RELEVANT NANOMATERIALS WITH ENHANCED FUNCTIONALITY

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P-D-23: TUNABLE PHOTOVOLTAIC RESPONSE IN ATOMICALLY THIN HETEROSTRUCTURES

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E. ENERGY CONSERVATION AND CONVERSION

P-E-1: ENGINEERING LIGHT HARVESTING MAQUETTES BOTH IN VITRO AND IN VIVO

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P-E-3: SOLAR THERMOELECTRIC ENERGY CONVERSION USING NANOSTRUCTURED THERMOELECTRIC MATERIALS

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P-E-5: UNRAVELING CHEMISTRY-TRANSPORT COUPLING in Flames

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P-E-7: CRITICAL CURRENTS: BREAKING THE GLASS CEILING IN HIGH-TEMPERATURE SUPERCONDUCTING CUPRATE 2G COATED CONDUCTORS

[CES] Ulrich Welp[1], Ying Jia[1], Maxime Leroux[1], Wai-Kwong Kwok[1], Alexei E. Koshelev[1], Vitalii Vlasko-Vlasov[1], J. G. Wen[1], Dean Miller[1], George Crabtree[1], Jian-Min (Jim) Zuo[2], Qiang Li[3], Marty Rupich[4], Steve Fleshler[4], Alex Malozemoff[4], Venkat Selvamanckam[5], Asghar Kayani[6], Oscar Ayala-Valenzuela[7], Leonardo Civale[7]

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P-E-9: PHOSPHONIUM--FUNCTIONALIZED POLYETHYLENE: A NEW CLASS OF BASE-STABLE ALKALINE ANION EXCHANGE MEMBRANES

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P-E-11: THERMOELECTRIC PROPERTIES OF AND THE ROLE OF ANHARMONICITY IN I-V-VI2 COMPOUNDS

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P-E-13: LASER BASED THERMAL TRANSPORT AND PICOSECOND ACOUSTIC STUDIES OF PHONON MEAN FREE PATH

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P-E-15: QUANTUM-DOT-BASED SOLID-STATE LIGHTING WITH ELECTRIC-FIELD-TUNABLE CHROMATICITY

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P-E-17: ENHANCEMENT OF THERMOELECTRIC PROPERTIES IN ELECTRICALLY GATED SILICON NANOWIRES

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P-E-19: SUPERCONDUCTING MATERIALS: ACCOMPLISHMENTS AND FUTURE DIRECTIONS

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P-E-21: TOWARDS RATIONAL DESIGN OF HETEROFOAM SURFACES AND INTERFACES: IN-SITU CHARACTERIZATION AND MULTISCALE SIMULATION

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P-E-23: HIGH PERFORMANCE THERMOELECTRICITY IN COMPOUNDS BASED ON NATURAL MINERAL TETRAHEDRITE

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P-E-25: THERMAL QUENCHING MECHANISMS IN II-VI SEMICONDUCTOR NANOCRYSTALS

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P-E-27: FUNDAMENTAL CONCEPTS OF ELECTRON MATTER IN FE-BASED HIGH-TEMPERATURE SUPERCONDUCTORS

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P-E-29: HETEROFOAM: A NEW DESIGN CONCEPT FOR HETEROGENEOUS FUNCTIONAL MATERIALS

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P-E-31: DIODE LASERS FOR SOLID-STATE LIGHTING

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F. MATERIALS AND CHEMISTRY FOR NUCLEAR ENERGY APPLICATIONS

P-F-1: STRUCTURE AND CHEMISTRY OF METAL/OXIDE INTERFACES

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P-F-3: UNDERSTANDING PHONON-MAGNON INTERACTIONS IN BCC IRON: A COMBINED MOLECULAR AND SPIN DYNAMICS STUDY

[CDP] Dilina Perera[1], David P. Landau[2], Don M. Nicholson[1], Malcolm G. Stocks[1], Markus Eisenbach[1], Junqi Yin[1], Gregory Brown[3]
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P-F-5: IRRADIATED INTERFACES: OVERCOMING THE MD TIMESCALE PROBLEM

[CMIME] Enrique Martinez-Seaz[1], Alfredo Caro[1]
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P-F-7: INVESTIGATION OF THE ATOMIC-LEVEL CHEMISTRY AND MICROSTRUCTURE OF NUCLEAR FUEL

[CMSNF] Michele V. Manuel[1], Billy Valderrama[1], Hunter B. Henderson[1], Lingfeng He[2], Janne Pakarinen[2], Clarissa Yablinsky[2], Todd R. Allen[2]
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P-F-9: HIGH RESOLUTION STUDIES OF DISLOCATION CORE STRUCTURES IN FE AND FE-CR ALLOYS

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P-F-11: MEASUREMENT OF THERMAL CONDUCTIVITY REDUCTION IN ION IRRADIATED CERIA AND URANIA

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P-F-13: ANOMALOUS ISOSTERIC ENTHALPY OF ADSORPTION IN HIGH PRESSURE EXPERIMENTS

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P-F-15: AQUEOUS SOLUTION CHEMISTRY OF ACTINYL COMPLEXES

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P-F-17: PRESSURE EFFECTS ON STRONGLY CORRELATED MATERIALS: THE EXAMPLES OF $LaMnO_3$ AND VO_2

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P-F-19: URANYL-PEROXIDE NANOCAPSULES IN AQUEOUS SOLUTION: A COMPUTATIONAL STUDY
[MSA] Bess Vlaisavljevich[1], Pere Miro[2], Chris Cramer[1], Peter C. Burns[3], Ginger E. Sigmon[3], Riccardo Spezia, Laura Gagliardi[1]
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P-F-21: QUANTITATIVE IN SITU TEM MEASUREMENTS OF INDIVIDUAL DEFECT INTERACTIONS
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P-F-23: COMPLEX SOLID STATE ACTINYL STRUCTURES
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G. CARBON CAPTURE AND SEQUESTRATION

P-G-1: GEOLOGICAL CARBON STORAGE: A CO_2 INJECTION TEST AT CRANFIELD - ESTIMATING GEOLOGICAL FEATURES AND MODEL PREDICTION UNCERTAINTY
[CFSES] Hongkyu Yoon[1], Reza Tavakoli[2], Mojdeh Delshad[2], Bill W. Arnold[1], Mary F. Wheeler[2], and Seyyed A. Hosseini[2]
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P-G-3: METAL-ORGANIC FRAMEWORKS FOR ENERGY-RELATED GAS SEPARATIONS INCLUDING PRE-, POST-, AND OXYFUEL-COMBUSTION CARBON DIOXIDE CAPTURE
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P-G-5: INTERFACIAL AND WETTING PROPERTIES OF MINERAL-WATER-BRINE SYSTEMS FROM MOLECULAR DYNAMICS (MD) SIMULATIONS
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P-G-7: EXPERIMENTAL AND MOLECULAR DYNAMICS SIMULATION STUDY OF CARBON DIOXIDE AND BRINE CONTACT ANGLES ON MINERAL SURFACES IN DEEP SALINE RESERVOIRS

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P-G-9: GENERAL MODEL FOR GROWTH KINETICS, IMPURITY ELEMENT- AND ISOTOPIC COMPOSITION OF CALCITE

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P-G-11: FUNCTIONALIZED POLYMER MEMBRANES FOR HIGH PERFORMANCE SEPARATION OF CO_2 AND CH_4

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P-G-13: UPSCALING DISSOLUTION RATES USING DIRECT NUMERICAL SIMULATION OF PORE SCALE REACTIVE TRANSPORT IN A CRUSHED CALCITE CAPILLARY EXPERIMENT

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P-G-15: COMPUTATIONAL CARBON CAPTURE

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P-G-17: THE EFFECT OF NANOPARTICLES ON CO_2 TRAPPING IN SANDSTONE

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P-G-19: OPTICALLY RESPONSIVE METAL-ORGANIC POLYHEDRA FOR CONTROLLED CAPTURE AND RELEASE OF GUEST MOLECULES

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P-G-21: ANATOMY OF PORE NETWORKS IN CAPROCK RELEVANT TO GEOLOGIC CO_2 SEQUESTRATION

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P-G-23: IMPACTS OF CO_2 SEQUESTRATION ON DEEP SUBSURFACE MICROBIAL POPULATIONS: INSIGHTS INTO AN UNEXPLORED EXTREME ENVIRONMENT

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P-G-25: CALCIUM CARBONATE POLYMORPHS ON MICA AND QUARTZ SUBSTRATES AND THEIR INTERFACIAL ENERGIES: CRUCIAL INFORMATION FOR PREDICTING PERMEABILITY CHANGES DURING GEOLOGIC CO_2 SEQUESTRATION

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P-G-27: CHARACTERIZATION OF GAS INTERACTIONS IN METAL-ORGANIC FRAMEWORKS

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P-G-29: PARAMETRIC COUPLED FLOW AND GEOMECHANICAL ANALYSIS OF SURFACE UPLIFT AT IN SALAH

[CFSES] Pania Newell[1], Mario J. Martinez[1], Joseph E. Bishop[1], and Steven L. Bryant[2]

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H. CATALYSIS

P-H-1: COMPUTATIONAL STUDIES OF CO OXIDATION ON TITANIA SUPPORTED GOLD NANOPARTICLES

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P-H-3: C-H BOND HYDROXYLATION WITH METAL OXO CATALYSTS

[CCHF] Aaron K. Vannucci[1], Meng Zhou[2], Ulrich Hintermair[2], David Balcells[3], Brian G. Hashiguchi[4], Alexander R. Parent[2], Sara M. Hashmi[5], Menachem Elimelech[5], Roy A. Periana[4], Dan H. Ess[6], Gary W. Brudvig[2], Thomas J. Meyer[1], Robert H. Crabtree[2]

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P-H-5: REDUCTION OF DINITROGEN TO AMMONIA WITH GROUP 6 COMPLEXES SUPPORTED BY DIPHOSPHINE LIGANDS CONTAINING PROTON RELAYS

[CME] Michael T. Mock[1], Charles J. Weiss[1], Zachariah M. Heiden[1], Liezel A. Labios[1], Jonathan D. Egbert[1], Molly O'Hagan[1], Shentan Chen[1], Roger Rousseau[1], R. Morris Bullock[1]

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P-H-7: EVALUATING MOLECULAR CATALYSTS FOR HYDROCARBON OXIDATION IN SUB-SCALE FUEL CELLS

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P-H-9: ULTRAFAST CHEMICAL DYNAMICS ON CATALYTIC NANOMATERIALS MEASURED BY PUMP-PROBE VIBRATIONAL SUM-FREQUENCY GENERATION SPECTROSCOPY

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P-H-11: MANAGING PROTONS FOR CATALYTIC OXYGEN REDUCTION

[CME] Colin W. Anson,[2] Johanna M. Blacquiere,[1] James B. Gerkin,[2] Michael L. Pegis,[1] Carlos Rodriguez,[1] Xiujian Wang,[1] Yu-Heng Wang,[2] Derek J. Wasylenko,[1] James M. Mayer,[1]* Shannon S. Stahl*[2]

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P-H-13: SURFACE SCIENCE STUDIES OF ALUMINA OVERLAYERS ON PD(111), PT(111) AND CU(111) SURFACES PREPARED BY ATOMIC LAYER DEPOSITION

[IACT] Amir Gharachorlou[1], Mike Detwiler[1], Dmitry Zemlyanov[2], Yu Lei[3], Junling Lu[3], Jeffrey W. Elam[3], W. Nicholas Delgass[1], Fabio H. Ribeiro[1]

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P-H-15: HOMOGENEOUS RHODIUM CATALYSTS FOR SELECTIVE HYDROCARBON OXIDATION

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P-H-17: EXPLORING NANOCLUSTERS SELF-ASSEMBLED ON TEMPLATE SURFACES FOR MODEL CATALYSIS STUDIES

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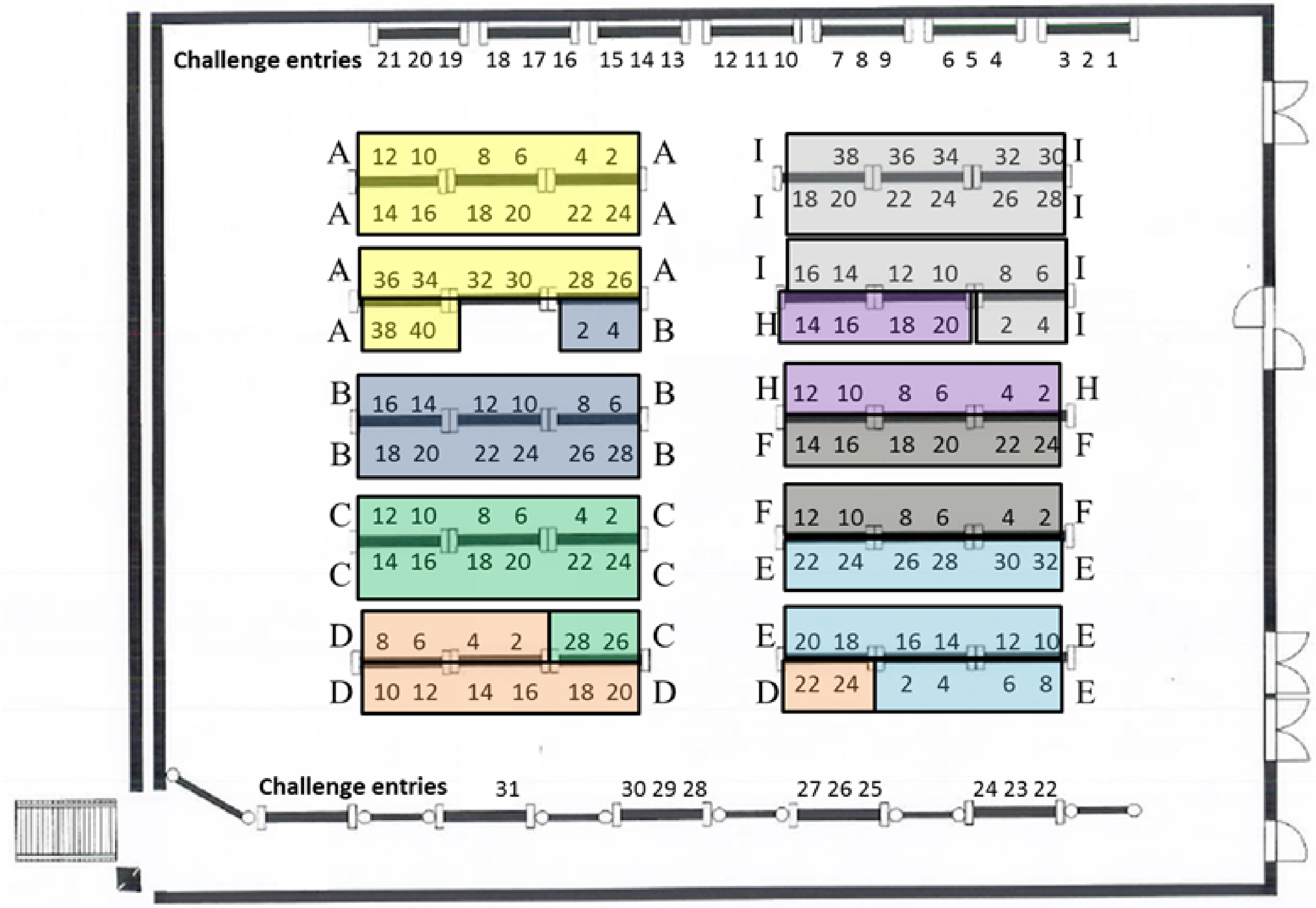
Poster Session II – Friday, July 19, 2013 – Marriot Salon 3
All Even Numbered Posters



A. Solar Fuels and Biomass	**D. Inorganic Photovoltaics**	**G. Carbon Capture and Sequestration**
B. Energy Storage	**E. Energy Conservation and Conversion**	**H. Catalysis**
C. Organic Photovoltaics	**F. Materials and Chemistry for Nuclear Energy Applications**	**I. Predictive Theory and Modeling**

A. SOLAR FUELS AND BIOMASS

P-A-2: THE DISCOVERY OF BACTERIOCHLOROPHYLL *F*: IMPLICATIONS FOR GREEN BACTERIA AND BIOHYBRID SOLAR DEVICES

[PARC] Gregory S. Orf[1,2], Dariusz Niedzwiedzki[2], Marcus Tank[3], Kajetan Vogl[3], Donald A. Bryant[3,4], and Robert E. Blankenship[1,2]

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P-A-4: LIGHT HARVESTING POLYMERS FOR ENERGY CONVERSION AND SOLAR FUELS

[UNC] Kirk S. Schanze[1], Gyu Leem[1], Toan Pho[2], Zhuo Chen[1], Junlin Jiang[1], Erik M. Grumstrup[3], Zachary A. Morseth[3], Li Wang[3], Zhen Fang[3], Shahar Keinan[3], John M. Papanikolas[3], John R. Reynolds[2]

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P-A-6: UNDERSTANDING SHORT- AND MEDIUM-CHAIN FATTY ACID BIOSYNTHESIS AND METABOLISM FOR ENHANCED BIOFUELS IN CAMELINA

[CABS] Hae Jin Kim[1], Jillian Collins-Silva[1], Umidjon Iskandarov[1] and Edgar Cahoon[1]

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P-A-8: NANOSCALE MATERIALS DEPOSITION FOR LIGHT ABSORPTION AND CATALYTIC ACTIVITY: TOWARD SOLAR FUELS

[CNEEC] C. Hägglund[1], K. L. Pickrahn[1], G. Zeltzer[1], R. Ruiz[1], I. Thomann[2,3], H. B. R. Lee[1], Y. Gorlin[1], S. W. Park[1], A. Garg[1], V. Vishwanathan[1], J. K. Norskov[1,4], T. F. Jaramillo[1], M. L. Brongersma[2], and S. F. Bent[1]

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P-A-10: LEARNING FROM PHOTOSYNTHESIS: HOW TO HARVEST LIGHT ENERGY FOR SOLAR FUEL PRODUCTION

[PARC] A.T. Gardiner[1], A.W. Roszak[1], A.-M. Carey[1], K. A. Hacking[1], S. Henry[1], K. Ashraf[1], H. Yan[2], R.J. Cogdell

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P-A-12: TRANSCRIPTIONAL REGULATORY NETWORKS DURING OIL ACCUMULATION IN *CHLAMYDOMONAS REINHARDTII*

[CABS] Mahmoud Gargouri[1], Jeong-Jin Park[1], Hongxia Wang[2], Omar Holguin[4], Rahul Deshpande[3], Yair Shachar-Hill[3], Leslie M. Hicks[2] and David R. Gang[1]

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P-A-14: III-V THIN FILMS AND NANOWIRES AS LIGHT ABSORBERS FOR PHOTOELECTROCHEMICAL ENERGY CONVERSION

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P-A-16: UNDERSTANDING HEMATITE: SOLAR-DRIVEN WATER OXIDATION WITH EARTH-ABUNDANT ELEMENTS

[ANSER] Shannon C. Riha[1], Joy M. Racowski[1], Michael D. Vermeer[2], Benjamin M. Klahr[3], Eric C. Tyo[1], Sonke Seifert[1], Michael P. Lanci[1], Jeffrey A. Klug[1], Joseph A. Libera[1], M. J. Katz[2], Nak Cheon Jeong[2], Steven T. Christensen[1], Stefan Vajda[1], Omar K. Farha[2], Thomas W. Hamann[3], Jeffrey W. Elam[1], Adam S. Hock[1], Michael J. Pellin[1,2], Joseph T. Hupp[1,2], Alex B. F. Martinson[1]

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P-A-18: DEVELOPING A BIO-INSPIRED METAL-BINDING PEPTIDE THAT FUNCTIONS AS A WATER OXIDATION CATALYST

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P-A-20: STREAMING BIOMASS INTO HIGH VALUE CHEMICALS AND FUEL

[C3Bio] Trenton H. Parsell[1], Tiffany M. Jarrel[1], Ian Klein[1], John Degenstein[2], Jeongim Kim[3], Sara L. Yohe[2], Vinod K. Venkatakrishnan[2], Harshavardhan Choudhari[2], Dhairya Mehta[2], Barron Hewetson[4], Ximing Zhang[4], Eurick S. Kim[1], Christine Bohn[1], Basudeb Saha[1], Yuan Jiang[1], Clint Chapple[3], Rick Meilan[5], Hilkka Kenttamaa[1], Nathan S. Mosier[4], Mahdi Abu-Omar[1], Rakesh Agrawal[2], W. Nicholas Delgass[2], Fabio H. Ribeiro[2]

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P-A-22: LIQUID PHASE CATALYTIC TRANSFER HYDROGENATION OF FURFURAL OVER RU/C CATALYST

[CCEI] Paraskevi Panagiotopoulou[1], Dionisios G. Vlachos[1]

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P-A-24: ANALYSIS OF PLANT CELL WALL ARCHITECTURE BY ATOMIC FORCE MICROSCOPY

[CLSF] Tian Zhang[1], Bernard Tittmann[2], Daniel J. Cosgrove[1,3]

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P-A-26: CHROMOPHORE-CATALYST ASSEMBLIES: FROM SYNTHESIS TO SPECTROSCOPY

[UNC] Dennis. L. Ashford[1], Stephanie E. Bettis[1], Zhen Fang[1], Christopher R. K. Glasson[1], Kenneth Hanson[1], Hanlin Luo[1], Animesh Nayak[1], Michael R. Norris[1], Derek. M. Ryan[1], Wenjing Song[1], Leila Alibabaei[1], M. Kyle Brennaman[1], Javier J. Concepcion[1], Thomas J. Meyer[1], John M. Papanikolas[1], J. L. Templeton[1], Marcy L. Waters[1]

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P-A-28: THE CELLULOSE SYNTHASE COMPLEX: SOMETHING OLD, SOMETHING NEW

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P-A-30: PNA-POLYPEPTIDE ASSEMBLY IN A 3D DNA NANOCAGE FOR BUILDING AN ARTIFICIAL OXYGEN EVOLVING COMPLEX

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P-A-32: SECOND GENERATION CATALYTIC PROCESSES FOR THE CONVERSION OF BIOREFINERY LIGNIN TO CHEMICALS AND FUELS

[C3Bio] Joseph J. Bozell[1], Berenger Biannic[1], Diana Cedeno[1], Alison Buchan[2], Ashley M. Frank[2], James J. Daleiden[2] Tiffany M. Jarrel[3], Hilkka I. Kenttamaa[3]

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P-A-34: SOLVATION AND HYDROGEN BONDING EFFECTS ON THE REACTIVITY OF BIOMASS DERIVATIVES

[CCEI] Tyler Josephson[1], George Tsilomelekis[1], Christina Bagia[1], Stavros Caratzoulas[1], Vladimiros Nikolakis[1], Dionisios G. Vlachos[1]

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P-A-36: IMAGING AND MODELING TO QUANTIFY PLANT CELL WALL DECONSTRUCTION

[C3Bio] Peter N. Ciesielski[1], Bryon S. Donohoe[1], Hui Wei[1], Melvin P. Tucker[1], James F. Mathews[1], Michael F. Crowley[1], Michael E. Himmel[1], Lee Makowski[2] , Nathan S. Mosier[3], Clint C.S. Chapple[4]

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P-A-38: ELECTROCATALYSIS OF TOTAL WATER SPLITTING ON PEROVSKITE OXIDES AND OXYNITRIDES

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P-A-40: FUNCTIONAL, STRUCTURAL, AND METABOLIC ANALYSIS OF PECTINS IN PLANT CELL WALLS

[CLSF] Charles T. Anderson[1,2], Chaowen Xiao[1], Melissa J. Ishler[1], Daniel D. McClosky[2]
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B. ENERGY STORAGE

P-B-2: UNDERSTANDING FUEL-MEMBRANE INTERACTIONS AND SELECTIVITY IN AN ORGANIC LIQUID FUEL CELL

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P-B-4: REVEALING THE WORKING AND DEGRADATION MECHANISMS IN LITHIUM-ION BATTERIES VIA IN-SITU TRANSMISSION ELECTRON MICROSCOPY

[NEES] Yang Liu[1], Kevin R. Zavadil[1], Katherine L. Jungjohann[1], Ju Li[2], Ting Zhu[3], S. Tom Picraux[4], John P. Sullivan[5], Chunsheng Wang[6], and Gary W. Rubloff[7]
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P-B-6: AN OLD DOG LEARNS NEW TRICKS: REDOX-ACTIVATION OF ELECTROCATALYSTS FOR THE PRODUCTION AND RELEASE OF HYDROGEN EQUIVALENTS

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[1]Yale University, [2]GE Global Research, [3]Stanford University, [4]Lawrence Berkeley National Laboratory, [5]UC Berkeley

P-B-8: ELECTROCHEMICAL ION TRANSPORT IN METAL OXIDE NANOSTRUCTURES

[NEES] Eleanor Gillette[1], Trevor Gamble[2], Jonathon Duay[1], Jaehee Song[1], Zuzanna Siwy[2], Reg Penner[3], Phil Collins[2], Sang Bok Lee[1]
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P-B-10: DIRECTED INTERCALATION BEHAVIOR IN MULTILAYER SILICON ELECTRODES FOR LI BATTERIES

[CEES] Paul Fenter[1], Andrew Gewirth[2]
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P-B-12: LITHIUM INSERTION IN NANOSTRUCTURED TIO_2(B) ARCHITECTURES

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P-B-14: OPERANDO IMAGING OF ENERGY MATERIALS IN AN ELECTROCHEMICAL CELL BY ELECTRON MICROSCOPY AND SPECTROSCOPY

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P-B-16: STRAIN-BASED IN-SITU STUDY OF CATION AND ANION INSERTION INTO POROUS CARBON ELECTRODES

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P-B-18: CHARACTERIZING THE EFFECTS OF SURFACE MODIFICATION ON LI-ION BATTERY ELECTRODES VIA X-RAY AND SCANNING PROBE TECHNIQUES

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P-B-20: UNDERSTANDING THE MECHANICAL AND SURFACE PHENOMENA OF LITHIATION IN SILICON NEGATIVE ELECTRODES

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P-B-22: THE LI/S INITIATIVE - AN INTEGRATED APPROACH TO ADVANCE HIGH CAPACITY SULFUR-CATHODE BASED BATTERIES

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P-B-24: FROM ATOMS TO ELECTRODES: ADVANCING SYNCHROTRON CHARACTERIZATION TOOLS FOR CHEMICAL ENERGY STORAGE

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P-B-26: HIGH-RATE ELECTROCHEMICAL ENERGY STORAGE WITH Nb_2O_5

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P-B-28: COMPREHENSIVE INSIGHT INTO FEOF; A MODEL OF MIXED ANION CONVERSION MATERIAL FOR SECONDARY BATTERIES

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C. ORGANIC PHOTOVOLTAICS

P-C-2: CONCERTED PROCESSES IN ORGANIC PHOTOVOLTAICS: THE RELATED CHALLENGES OF GENERATING AND COLLECTING CHARGE IN A DISORDER ENVIRONMENT

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P-C-4: ELECTRONIC STRUCTURE AT THE INTERFACE OF CONDUCTING METAL OXIDES AND ORGANIC SEMICONDUCTORS

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P-C-6: EXCITON DISSOCIATION DYNAMICS AT ORGANIC DONOR/ACCEPTOR INTERFACES

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P-C-8: THEORY OF SINGLET FISSION AND THE ROLE OF CHARGE-TRANSFER STATES

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P-C-10: Link Between Open Circuit Voltage and the Donor-Acceptor Interface Structure and Composition in Molecular Organic Solar Cells

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P-C-12: Understanding and Predicting the Singlet Fission Rate: A Combined Theoretical and Experimental Effort

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P-C-14: Structure Dependent Charge Transport Through Surfactant-Stabilized Polymer Nanoparticle Assemblies

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P-C-16: Design Guidelines for Contacts: Identifying Mechanisms at Organic/Oxide Interfaces that Control Energy Transfer

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P-C-18: Self-Assembling Polymer/Fullerene Systems for Organic Photovoltaics

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P-C-20: Morphology Characterization of Low Band Gap Polymer Based Organic Photovoltaics

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P-C-22: KEY INTERFACES FOR THE REALIZATION OF ALL-PLASTIC SOLAR CELLS AND TANDEM SOLAR CELLS: POLYMER SURFACE MODIFICATION AND ELECTRODES

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P-C-24: SOME ASSEMBLY REQUIRED: SPECTROSCOPY REVEALS THE EFFECTS OF AGGREGATION IN CONJUGATED ORGANICS, FROM SINGLE MOLECULE TO DEVICE

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P-C-26: NON-BASIC SMALL MOLECULE SEMICONDUCTOR WITH WORLD-RECORD ORGANIC PHOTOVOLTAIC EFFICIENCY

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P-C-28: MULTICHROMOPHORIC POLYMERS FOR BROADBAND LIGHT ABSORPTION IN ORGANIC PHOTOVOLTAICS

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D. INORGANIC PHOTOVOLTAICS

P-D-2: NANOSCALE ATOMS IN SOLID-STATE CHEMISTRY

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P-D-4: INVERSE DESIGN OF TERNARY ABX INORGANIC MATERIALS

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P-D-6: NEW PHOTOELECTRODE ARCHITECTURES FOR LIGHT-TO-ELECTRICAL AND LIGHT-TO-CHEMICAL ENERGY CONVERSION

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P-D-8: CHARGE GENERATION, TRANSPORT, AND COLLECTION IN QUANTUM-DOT SOLAR CELLS

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P-D-10: INVERSE DESIGN OF NOVEL HIGH ABSORPTION MATERIALS

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P-D-12: THE NEW OPTO-ELECTRONIC PHYSICS THAT BROKE THE EFFICIENCY RECORD IN SOLAR CELLS

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P-D-14: SEEING THE INVISIBLE: UNRAVELING THE EXCITON LIFECYCLE IN INFRARED NANOCRYSTALS

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P-D-16: PHOTON MANAGEMENT TECHNIQUES FOR PHOTOVOLTAICS

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P-D-18: COMPREHENSIVE THEORY OF OPTICAL PROPERTIES, CARRIER MULTIPLICATION, AUGER PROCESSES, AND CHARGE TRANSPORT IN QUANTUM-DOT

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P-D-20: NANOWIRE AND NANOSHEET SOLAR CELLS

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P-D-22: DESIGN METHODS FOR COMPLEX, MESOSTRUCTURED LIGHT ABSORBERS

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P-D-24: NOVEL SPECTROSCOPIC INSIGHTS INTO CARRIER MULTIPLICATION IN SEMICONDUCTOR NANOCRYSTALS: EFFECTS OF SIZE, SHAPE, COMPOSITION, AND INTERNAL STRUCTURE

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E. ENERGY CONSERVATION AND CONVERSION

P-E-2: PHONON SCATTERING MECHANISMS IN ROCK-SALT TELLURIDE THERMOELECTRICS STUDIED BY INELASTIC NEUTRON SCATTERING

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P-E-4: EXPERIMENTAL INSIGHTS INTO CHEMICAL KINETICS OF BIOFUEL COMBUSTION

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[1]Princeton University, [2]Sandia National Laboratories, [3]Stanford University, [4]University of Connecticut

P-E-6: III-V THERMOELECTRIC MATERIAL GROWN BY MBE WITH PRECISE AND INDEPENDENT CONTROL OF NANOSTRUCTURE AND DOPING

[CEEM] Peter G. Burke[1], Hong Lu[1], Phillip Zhuo[1], Arthur C. Gossard[1], John E. Bowers[1]
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P-E-8: PNICOGEN RINGS OF SKUTTERUDITES CONFIGURED FOR LOW THERMAL CONDUCTIVITY

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P-E-10: MULTI-SCALE MEMBRANE DESIGN

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P-E-12: MULTI-COLOR PHOTONIC CRYSTAL NANOWIRE LASER PIXELS

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P-E-14: DEVELOPMENT OF PREDICTIVE COMBUSTION KINETICS FOR MODEL BIODIESEL FUELS

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P-E-16: HUGE CRITICAL CURRENTS AND TAILORED ANISOTROPY IN FE-BASED HIGH-TEMPERATURE SUPERCONDUCTORS

[CES] Wai-Kwong Kwok[1], Lei Fang[1], Ying Jia[1], Karen Kihlstrom[1], Bing Shen[1], Yonglei Wang[1], Ulrich Welp[1], Alexei E. Koshelev[1], George Crabtree[1], Jian-Min (Jim) Zuo[2], Russell W. Giannetta[2], Qiang Li[3], Ruslan Prozorov[4], Paul Canfield[4], Asghar Kayani[5], Januz Karpinski[6], Hai-Hu Wen[7]

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P-E-18: PHONON-DRAG THERMOPOWER IN THIN FILMS GOVERNED BY THE CHOICE OF SUBSTRATE

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P-E-20: NON-EQUILIBRIUM EFFECTS IN THE DESIGN, SYNTHESIS, CHARACTERIZATION AND USE OF HETEROGENEOUS FUNCTIONAL MATERIALS (HETEROFOAMS) IN ELECTROCHEMICAL DEVICES

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P-E-22: HIGH THERMOELECTRIC PERFORMANCE VIA SYNERGISTIC APPROACHES IN THE PBSE SYSTEM

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P-E-24: 3-D MAPPING OF QUANTUM WELLS IN A GAN/INGAN CORE-SHELL NANOWIRE LIGHT EMITTING DIODE
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P-E-26: FUNDAMENTAL CONCEPTS OF ELECTRON MATTER IN CUPRATE HIGH-TEMPERATURE SUPERCONDUCTING
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P-E-28: PROCESSING AND OPTIMIZATION OF THE THERMOELECTRIC PROPERTIES OF EARTH-ABUNDANT MG-SI-SN ALLOYS
[RMSSEC] Timothy P. Hogan[1], Peng Gao[1], Isil Berkun[1], Eldon D. Case[1], Patricia Bordon Sarac[1], and Robert W. Schmidt[1]
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P-E-30: INNOVATIVE DESIGN OF HETEROFOAM ELECTRODES FOR SOLID OXIDE FUEL CELLS
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P-E-32: THE EFFECTS OF SODIUM ON THE PHASE STABILITY OF THE LEAD CHALCOGENIDES
[RMSSEC] Jeffrey W. Doak[1], Christopher Wolverton[1], Vinayak P. Dravid[1], Mercouri G. Kanatzidis[1], Jiaqing He[1], Lidong Zhao[1], and Yeseul Lee[2]
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F. MATERIALS AND CHEMISTRY FOR NUCLEAR ENERGY APPLICATIONS

P-F-2: MECHANICAL RESPONSE OF INTERFACES CONTAINING NANO-SCALE HELIUM BUBBLES
[CMIME] Nan Li[1], Amit Misra[1], Abishek Kashinath[2], Michael J. Demkowicz[2]
[1]Los Alamos National Laboratory; *[2]Massachusetts Institute of Technology*

P-F-4: MULTISCALE MODELING OF DEFECT PRODUCTION AND DEFECT CLUSTERING IN UO_2
[CMSNF] Xian-Ming Bai[1], Jiangou Yu[1], Anter A. El-Azab[2], Todd R. Allen[1.3]
[1]*Idaho National Laboratory*, [2]Purdue University, [3]University of Wisconsin at Madison

P-F-6: PREDICTING DYNAMIC FAILURE IN POLYCRYSTALLINE METALS
[CMIME] Saryu J. Fensin[1], Steve M. Valone[1], Ellen K. Cerreta[1] and George T. Gray III[1]
[1]Los Alamos National Laboratory

P-F-8: LOCAL STRUCTURE EVOLUTION IN ION IRRADIATED UO_2
[CMSNF] Mahima Gupta[1], Steve Conradson[2], Janne Pakarinen[1], Jeff Terry[3], Todd R. Allen[1,4]
[1]University of Wisconsin at Madison, [2]Los Alamos National Laboratory, [3]Illinois Institute of Technology, [4]Idaho National Laboratory

P-F-10: TEMPERATURE DEPENDENCE OF LOOP FORMATION IN FE AND FE-BASED ALLOYS
[CDP] Virginia McCreary[1], Bai Cui[1], Ian Robertson[1,2], Roger Stoller[3], Ben Larson[3,] Easo George[3]
[1]*University of Illinois;* [2]*University of Wisconsin;* [3]*Oak Ridge National Laboratory*

P-F-12: POLARON-ION CORRELATIONS IN $LiFePO_4$ STUDIED BY NUCLEAR RESONANT SCATTERING
[EFree] Sally June Tracy[1], Lisa M. Mauger[1] and Brent T. Fultz[1]
[1]*California Institute of Technology, Pasadena CA*

P-F-14: FILTRATION METHODS FOR THE AQUEOUS SEPARATION OF URANYL PEROXOCLUSTERS FROM SIMULATED USED NUCLEAR FUEL
[MSA] E. Miller Wylie[1], Kathryn M. Peruski[1], W.A. Phillip[1], Peter C. Burns[1]
[1]*University of Notre Dame*

P-F-16: *IN-SITU* MEASUREMENTS OF DEFECT INTERACTION STRESSES USING 3D X-RAY MICROSCOPY
[CDP] Dhiraj Catoor[1], Hongbin Bei[1], Erik G. Herbert[2,1], Yanfei Gao[2,1], Eliot Specht[1], Bennett C. Larson[1], Michael J. Mills[3], George M. Pharr[2,1], Easo P. George[1,2]
[1]*Oak Ridge National Laboratory;* [2]*The University of Tennessee, Knoxville* [3]*The Ohio State University*

P-F-18: PERIODIC MESOSTRUCTURED MATERIALS AS PRECURSORS FOR HIGH PRESSURE SYNTHESIS
[EFree] Manik Mandal[1], Yingwei Fei[2] and Kai Landskron[1]
[1]*Department of Chemistry, Lehigh University, Bethlehem PA,* [2]*Geophysical Laboratory, Carnegie Institution of Washington, Washington DC*

P-F-20: ACTINIDE OXIDES AND ANALOGUE MATERIALS AT EXTREME CONDITIONS
[MSA] Maik Lang[1], Fuxiang Zhang[1], Cameron L. Tracy[1], Jiaming Zhang[1], and Rodney C. Ewing[1]
[1]*University of Michigan*

P-F-22: RECENT PROGRESS ON HIGH PRESSURE STUDIES OF UNCONVENTIONAL SUPERCONDUCTORS IN EFREE
[EFree] Xiao-jia Chen[1] and Viktor V. Struzhkin[1]
[1]*Geophysical Laboratory, Carnegie Institution of Washington, Washington DC*

P-F-24: HIGH-STRENGTH AND THERMALLY STABLE BULK NANOLAYERED COMPOSITES
[CMIME] Nathan A. Mara[1], Shijian Zheng[1], John S. Carpenter[1], Keonwook Kang[1], Jian Wang[1], Weizhong Han[1] and Irene Beyerlein[1]
[1]*Los Alamos National Laboratory.*

H. CATALYSIS

P-H-2: OPTIMIZING PROTON DELIVERY AND REMOVAL IN NICKEL CATALYSTS FOR HYDROGEN OXIDATION AND PRODUCTION
[CME] Molly O'Hagan[1], Jianbo Hou[1], John A.S. Roberts[1], Tianbio Liu[1], Elliott Hulley[1], Wendy J. Shaw[1], R. Morris Bullock[1]
[1]*Center for Molecular Electrocatalysis, Physical Sciences Division, Pacific Northwest National Laboratory, P.O. Box 999, K2-57, Richland, Washington 99352*

P-H-4: NANOCATALYST CHARACTERIZATION USING SMALL ANGLE X-RAY SCATTERING

[IACT] Tao Li,[1] Hong Xie,[2] Brandon O'Neill,[3] Soma Chattopadhyay,[4] Tomohiro Shibata,[4] Russell E. Cooks,[5] Sungsik Lee,[1] Byeongdu Lee,[1] Jeffrey Miller,[6] James Dumesic,[3] Kenneth Poeppelmeier,[2] Randall E. Winans[1]

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P-H-6: ADSORBED QUINONES AS MODEL PROTON COUPLED ELECTRON TRANSFER REACTANTS AT FLUID-SOLID INTERFACES

[FIRST] Z. Zhang[1], D.M. Anjos[1], G.M. Brown[1], Zili Wu[1], Yu Cai[2], M. Neurock[2] and S.H. Overbury[1]

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P-H-8: COMPUTATIONAL DESIGN OF BIMETALLIC SYNGAS CONVERSION CATALYSTS: HOW SURFACE DIFFUSION OF INTERMEDIATES IMPACTS PRODUCT DISTRIBUTIONS

[CALCD] Ming He[1], Jay McAliley[1] and David A. Bruce[1]

[1]Department of Chemical and Biomolecular Engineering, Clemson University, Clemson, SC 29634

P-H-10: RAPID, REVERSIBLE HETEROLYSIS OF H_2 AND THE DEVELOPMENT OF MANGANESE ELECTROCATALYSTS FOR H_2 OXIDATION

[CME] Elliott B. Hulley[1]; R. Morris Bullock[1]

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P-H-12: SYNTHETIC METHODS FOR THE CREATION OF SIZE SELECTIVE NANOCAVITIES BY ATOMIC LAYER DEPOSITION

[IACT] Cassandra George[1], Natalie Ray[1], Christian Canalas[2], Justin Notestein[3], Rick Van Duyne[1], Peter Stair[1,2]

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P-H-14: DESIGNING A CONTINUUM OF ELECTROPHILIC TO NUCLEOPHILIC CATALYSTS AND MECHANISMS TO FUNCTIONALIZE NATURAL GAS AND PETROLEUM DERIVED HYDROCARBONS

[CCHF] Brian G. Hashiguchi[1], Steven M. Bischof[1], Kurtis M. Carsch[2,3], Mu-Jeng Cheng[2], Cody R. Freitag[3], Michael K. Konnick[1], Jiajun Mei[4], Erika M. Milczek[5], Robert J. Nielsen[2], Brooke M. Otten[3], Mark J. Pouy[4], Bruce M. Prince[3], Thomas R. Cundari[3], Daniel H. Ess[6], William A. Goddard, III[2], John T. Groves[5], Thomas B. Gunnoe[4], Roy A. Periana[1]

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P-H-16: RARE EARTH/TRANSITION METAL OXIDES FOR SYNGAS DESULFURIZATION AND TAR REFORMING

[CALCD] Kerry M. Dooley
Cain Department of Chemical Engineering, Louisiana State University, Baton Rouge, LA 70803

P-H-18: EXPERIMENTAL AND FIRST PRINCIPLE STUDY OF OXIDATION WITH O_2 OF LM(II)CH_3(OH_2)COMPLEXES (M=PT, PD) IN WATER

[CCHF] Wei-Guang Liu[1], Anna Sberegaeva[2], Robert J. Nielsen[1], William A. Goddard III[1], Andrei N. Vedernikov[2]
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I. PREDICTIVE THEORY AND MODELING

P-I-2: MODELING TRANSPORT PHENOMENA IN SUPERCAPACITORS

[MEEM] Hainan Wang[1], Anna D'Entremont, Alexander Thiele, and Laurent Pilon[1]
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P-I-4: COMPUTATIONAL APPROACH FOR SEARCHING NEW WATER SPLITTING SEMICONDUCTOR MATERIALS

[CID] Vladan Stevanovic,[1,2] Stephan Lany,[2] Jun-Wei Luo,[2] David S. Ginley,[2] William Tumas,[2] Alex Zunger[3]
[1]*Colorado School of Mines, Golden, CO, 80401, USA*, [2]*National Renewable Energy Laboratory, Golden, CO 80401, USA*, [3]*University of Colorado Boulder, CO 80309, USA*

P-I-6: Uncertainty Quantification and Propagation in Fundamental Reaction Kinetics and Detailed Kinetic Models

[CEFRC] Stephen J. Klippenstein,[1] Chih-Jen Sung,[2] Fokion N. Egolfopoulos,[3] Hai Wang[3]
[1]*Argonne National Laboratory,* [2]*University of Connecticut,* [3]*University of Southern California*

P-I-8: MOLECULAR MACHINE DESIGNS: FUNCTIONAL STRUCTURES AND RATCHET MECHANISMS

[NERC] Korosh Torabi[1] and George C. Schatz[1]
[1]*Department of Chemistry, Northwestern University, Evanston, IL*

P-I-10: FIRST PRINCIPLES SIMULATION OF PHONON AND THERMOELECTRIC TRANSPORT

[S3TEC] Bo Qiu[1], Bolin Liao[1], Zhiting Tian[1], Sangyeop Lee[1], Jivtesh Garg[1], Keivan Esfarjani[2], Jonathan M. Mendoza[1], Mona Zebarjadi,[2] Mildred S. Dresselhaus,[3] Gang Chen[1], David Parker[4], Xin Chen[4], David J. Singh[4], David Broido[5], Lucas Lindsay[6], Wu Li[7], Natalio Mingo[7], Derek Stewart[8], Chunhua Li[5], Olle Hellman[9]
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P-I-12: Insight into Proton-Coupled Electron Transfer Mechanisms and Theoretical Design of Ni-Based Molecular Electrocatalysts for H_2 Production.

[CME] Samantha Horvath,[1] Laura E. Fernandez,[2] Aaron M. Appel,[3] Sharon Hammes-Schiffer,[1]
[1]Department of Chemistry, University of Illinois at Urbana-Champaign, Urbana, IL 61801, [2]Department of Chemistry, Pennsylvania State University, University Park, PA 16802, [3]Pacific Northwest National Laboratory, P.O. Box 999, K2-57, Richland, WA 99352

P-I-14: Studies of Heterogeneous Catalysis of Biomass-derived Molecules by Zeolite and Metal Surfaces Using Density Functional Theory with Inclusion of Dispersion Interaction

[IACT] Lei Cheng, [1] Bin Liu,[2] Larry A. Curtiss[1,2] and Jeffrey Greeley[3]
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P-I-16: Artificial Bistable Catalytic Systems from Positive and Negative Feedback Loops

[NERC] Job Boekhoven,[1,2] José E. Betancourt-Borges,[2] Charles Rubert Pérez,[1] Amanda Worthy,[1] Samuel I. Stupp[1,2,3]
[1]Institute for BioNanotechnology in Medicine, Northwestern University, Chicago, IL, [2]Department of Chemistry, Northwestern University, Evanston, IL, [3]Departments of Materials Science and Biomedical Engineering, Northwestern University, Evanston, IL

P-I-18: Transport Rectification in Neutral Nanopores with Chemically Modified Outer Walls: Surface Charges Versus Polyelectrolyte Brushes

[NERC] Mario Tagliazucchi[1], Yitzhak Rabin[2], and Igal Szleifer[1]
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P-I-20: Molecular Insights into Energy-Relevant Fluid-Solid Interfaces

[FIRST] G. Feng,[1] S. Li,[1] H. Zhou,[2] E. W. Hagaman,[3] Yury Gogotsi,[4] and P. T. Cummings[1,5]
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P-I-22: First-Principle Studies of Fast Ion Intercalation in Nb_2O_5 and WO_3

[MEEM] Chi-Ping Liu[1] and Vidvuds Ozolins[1]
[1]University of California, Los Angeles

P-I-24: Inverse Design of a New d^5-Based p-Type Transparent Conducting Oxide: Li-doped Cr_2MnO_4 Spinel

[CID] Haowei Peng,[1] Andriy Zakutayev,[1] Stephan Lany,[1] Tula R. Paudel,[1] Mayeul d'Avezac,[1] Paul F. Ndione,[1] John D. Perkins,[1] David S. Ginley,[1] Arpun R. Nagaraja,[2] Nicola H. Perry,[2] Thomas O. Mason,[2] and Alex Zunger[3]
[1]*National Renewable Energy Laboratory, Golden, CO 80401, USA*, [2]*Northwestern University, Evanston, IL 60208, USA,* [3]*University of Colorado Boulder, CO 80309, USA*

P-I-26: THE NETWORK OF CHEMISTRY AND THE RISE OF AN AUTOMATIC CHEMIST

[NERC] Kyle Bishop

Department of Chemical Engineering, Pennsylvania State University, University Park, PA

P-I-28: CONTRIBUTIONS FROM THEORY TO BUTANOL AND BIODIESEL COMBUSTION MODELING

[CEFRC] Emily A. Carter,[1] Donald G. Truhlar,[2] William H. Green,[3] Chung K. Law,[1] Stephen J. Klippenstein,[4]

[1]Princeton University, [2]University of Minnesota, [3]Massachusetts Institute of Technology, [4]Argonne National Laboratory

P-I-30: FUNDAMENTAL REACTION MECHANISTIC STUDIES TOWARDS IMPROVED CATALYST DESIGN: A COMBINED THEORETICAL AND EXPERIMENTAL APPROACH

[IACT] Suyash Singh[1], Jessica Scaranto[1], Brandon O'Neill[1], Michael D. Detwiler[2], Luke Roling[1], Sha Li[1], Ronald Carrasquillo[1], Jeffrey Herron[1], Guowen Peng[1], Fabio H. Ribeiro[2], W. Nicholas Delgass [2], James A. Dumesic[1], Manos Mavrikakis[1]

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P-I-32: DETAILED UNDERSTANDING OF THE THERMAL TRANSPORT PROCESS IN NUCLEAR FUEL FROM THE ATOMISTIC SIMULATIONS

[CMSNF] Aleksandr Chernatynskiy[1], Bowen Deng[1], *Judy W.L. Pang[2]*, Bennett C. Larsen[2], Simon R. Phillpot[1],

[1]University of Florida, [2]Oak Ridge National Laboratory

P-I-34: LARGE ATOMISTIC SIMULATIONS OF NANOSTRUCTURE AND ORGANIC SOLAR CELLS

[CEN] Manaschai Kunaseth[1], Weiwei Mou[1], Zaoshi Yuan[1], Aiichiro Nakano[1]

[1]University of Southern California

P-I-36: FIRST PRINCIPLES ELECTROCHEMISTRY WITH JOINT DENSITY-FUNCTIONAL THEORY

[emc^2] Kendra Letchworth-Weaver[1]; Deniz Gunceler[1]; Ravishankar Sundararaman[1]; Xin Huang[2]; Manuel Plaza[2]; Joel Brock[2]; Hector D. Abruña[3]; Tomás A. Arias[1]

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P-I-38: DESIGNING DISSIPATIVE SELF-ASSEMBLY

[NERC] Antonio F. Osorio Vivanco[1], Igal Szleifer[2], Monica Olvera de la Cruz[3], Sharon C. Glotzer[1,4]

[1]Materials Science and Engineering, University of Michigan, Ann Arbor, MI, [2]Biomedical Engineering, Northwestern University, Evanston, IL, [3]Materials Science and Engineering, Northwestern University, Evanston, IL, [4]Department of Chemical Engineering, University of Michigan, Ann Arbor, MI

Ten Hundred and One Word Challenge Entries

Entry	EFRC Acronym	Artists/Authors Names	Title of Submission
1	ANSER	Tejas Shastry	Soft Sun Cells
2	BISfuel	Anne Katherine Jones	Sunlight+Water=Tomorrow's Energy
3	C3Bio	Carl Huetteman, Pam Burroff-Murr and Sarah Anderson	The walk forward of sun-grown green-thing energy
4	CASP	Hunter McDaniel, Matthew C. Beard, Lance M. Wheeler, Jeffrey M. Pietryga	When small is better than BIG
5	CCEI	Nima Nikbin, Tyler Josephson, and Timothy Courtney	Rocks Filled with Tiny Spaces Can Turn Green Growing Things Into Stuff We Use Every Day
6	CCHF	Cecelia Cropley	Cleaner Energy for Cars
7	CDP	G. Malcolm Stocks, James Morris, Andrew Sproles, Priscilla Henson, Kathy Graham	Caught in the Act
8	CE	Joey Goodknight and Alan Aspuru-Guzik	Is The Same bit of Light Exciting Two (or more) Parts of a Thing at the Same Time?
9	CEEM	Leah Kuritzky and Jason Jewell	Making More Light with Less Energy
10	CEES	Oya Okman, Marta Baginska, Elizabeth MC Jones, Stephen J. Pety, Tae Wook Lim, Joshua A Kaitz, Hefei Dong, Daniel R. Vissers, Nancy R Sottos, Scott R White Jeffrey S Moore, Michael M. Thackery, Paul A Fenter, Lynn Trahey, Sana Sandler, Mark C Hersam, Aaron J Kapper	Not Your Normal Power Box
11	CEFRC	Chih-Jen Sung, Chung K. Law, Kyle Brady, Nicholas Curtis	Power to the People … Energy for Now and Later
12	CEN	P. Daniel "Dan" Dapkus and Michelle Povinelli	Using all the Energy from the Sun to Make Power
13	CES	Jon Rameau, George Crabtree, Laura Greene, Wai Kwok, Peter Johnson; Artist Alexei Tsvelik	Moving Energy
14	CFSES	Steve L Bryant, Tara R. Camacho-Lopez, Craig M. Tenney, Hongkyu Toon, Randall T. Cygan, Susan J. Altman	Make the World a Better Place

Entry	EFRC Acronym	Artists/Authors Names	Title of Submission
15	CID	Lawrence Kazmerski, Don Gwinner, Al Hicks	Our On-Its-Head-and-In-Your-Dreams Approach Leads to Clean Energy
16	CISSEM	Dawn Moseke, Robin Richards, Daniel Moseke	Sun-to-power cells layer by layer
17	CLSF	Daniel Cosgrove, Nicole Brown and Sarah Kiemle	Powering your car with sun light
18	CME	Jonathan M. Darmon, Charles J. Weiss, Elliott B. Hulley, Monte L. Helm, R. Morris Bullock	A Better Way to Store Energy for Less Cost
19	CMSNF	Xianming Bai, Lingfeng He, Marat Khafizov, Jianguo Yu, Aleksandr Chernatynskiy	How are the energy waves blocked on the way from hot to cold?
20	CNEEC	Joseph Montoya	Small
21	CST	All EFRC effort	Stuff Moving Through Other Stuff - For Energy
22	CSTEC	Anton Li, David Bilby, Adam Barito, Brenda Vyletel	Building a Road from Light to Energy
23	EMC2	Paul F. Mutolo, David Muller, James O'Dea, Héctor D. Abruña, Alice Muhlback/Spirit and Kitsch	A boy asked his Mom about energy
24	LMI	Carrie Hoffman, Dennis Callahan, Carissa Eisler, Bryce Sadtler, Cris Flowers, Chris Corcoran, Matt Goodman	Controlling Light to Make the Most Energy From the Sun
25	MEEM	Veronica Augustyn, Jesse Ko and Iris Rauda	How to Store Energy Fast
26	MSA	Sally Steuterman, Alicia Czarnecki, Paul Hurley, Kathryn Peruski, Alejandra Cartegena-Sierra, Alexis Guzman, Isaac Evans	Using Left Overs to Make Energy
27	NCGC	Andrew Stack	The Big Group of People Looking at How to Control Putting the Parts of the Air That Are the Same as What You Breathe Out Into Small Spaces in Rocks
28	NECCES	Karena Chapman	Putting more power in your pocket
29	S3TEC	Marianne Epstein, Maria Luckyanova, and Kara Manke	The Sun Makes You Number One!
30	SSLS	Nicole Wilber, Krista Houmpheng, Mike Coltrin	Lighting the World in a Different Way
31	UNC	Chuanqi Jiang, Yan Liang (l2xy2.com), Lars Sah	Energy from the Sun

Graduate Student and Postdoctoral Researcher Finalists

Graduate Student

B-I-4: HIGH-RATE ELECTROCHEMICAL ENERGY STORAGE WITH NB_2O_5

[MEEM] Veronica Augustyn[1], Jeremy Come[2], Michael A. Lowe[3], Jong Wuong Kim[1], Pierre-Louis Taberna[2], Sarah H. Tolbert[4], Hector D. Abruña[3], Patrice Simon[2], and Bruce Dunn[1]

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Postdoctoral Researcher

Ib-IV-1: NEW TERNARY MATERIALS DISCOVERED BY INVERSE DESIGN

[CID] Romain Gautier,[1] Xiuwen Zhang,[2] Andriy Zakutayev,[2] Arpun R. Nagaraja,[1] Feng Yang,[1] Liping Yu,[3] Stephan Lany,[2] David S. Ginley,[2] Thomas O. Mason,[1] Kenneth R. Poeppelmeier,[1] Alex Zunger[3]

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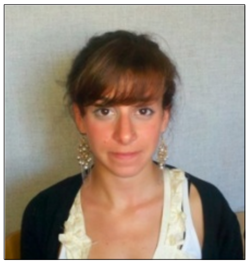
[2]National Renewable Energy Laboratory, Golden, CO 80401, USA
[3]University of Colorado, Boulder, CO 80309, USA

Postdoctoral Researcher

F-I-1: MICROSTRUCTURAL INVESTIGATIONS OF KR AND XE IRRADIATED UO_2

[CMSNF] Lingfeng He[1], Mahima Gupta[1], Billy Valderrama[2]. Hunter B. Henderson[2], Abdel-Rahman Hassan[3], Janne Pakarinen[1], Jian Gan[4], Marquis A. Kirk[5], Michele V. Manuel[2]. Anter A. El-Azab[3], Todd R. Allen[1,3]

[1]University of Wisconsin at Madison, [2]University of Florida, [3]Purdue University, [4]Idaho National Laboratory, [5]Argonne National Laboratory



Graduate Student

G-II-5: SOLID, POROUS MATERIAL FOR IMPROVED EFFICIENCY OF GASOLINE PRODUCTION AND LOW-COST AND NON-TOXIC ENHANCEMENT OF GASOLINE QUALITY

[CGS] Zoey R. Herm,[1] Brian M. Wiers,[1] Jarad A. Mason,[1] Jasper M. van Baten,[2] Norberto Masciocchi,[3] Rajamani Krishna,[2] Jeffrey R. Long[1]

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Graduate Student

F-II-3: REACTION DYNAMICS OF A NANOMETER-SIZED URANYL CLUSTER IN SOLUTION

[MSA] Rene L. Johnson;[1] C. André Ohlin;[2] Kristi L. Pellegrini;[3] Peter. C. Burns;[3,4] William H. Casey[1,5]

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Graduate Student

B-III-1: NANO-ENGINEERING OF SILICON NANOSTRUCTURES FOR LITHIUM-ION BATTERIES AND ENERGY STORAGE DEVICES

[NEES] Khim Karki[1], Chuanfu Sun[2], Eric Epstein[1], Jeong-Hyun Cho[3], Zheng Jia[4], Yujie Zhu[5] Teng Li[4], Yue Qi[6], Tom Picraux[3], Gary Rubloff[1], Chunsheng Wang[5], YuHuang Wang[2], and John Cumings[1]

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Postdoctoral Researcher

A-III-3: PROBING LIGHT HARVESTING AND PHOTOSYNTHETIC PRODUCTIVITY IN CYANOBACTERIA

[PARC] Michelle Liberton[1], Lawrence Page[1*], Aaron M. Collins[2], William B. O'Dell[3], Hugh O'Neill[3], Volker S. Urban[3], Jerilyn A. Timlin[2], and Himadri B. Pakrasi[1]

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Graduate Student

Ib-IV-2: PREVENTING HELIUM-INDUCED DAMAGE THROUGH INTERFACE ENGINEERING

[CMIME] Abishek Kashinath[1], Michael J. Demkowicz[1]

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Graduate Student

A-I-3: UNDERSTANDING CRYSTALLINE CELLULOSE MICROFIBRILS ASSEMBLY IN PLANT CELL WALLS USING SUM-FREQUENCY-GENERATION (SFG) VIBRATION SPECTROSCOPY

[CLSF] Christopher M. Lee[1], Kabindra Kafle[1], Yong Bum Park[2], James D. Kubicki[3], Daniel Cosgrove[2], Candace Haigler[4] and Seong H. Kim[1]

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Graduate Student

E-II-2: COHERENT PHONON HEAT CONDUCTION IN SUPERLATTICES

[S3TEC] Maria N. Luckyanova[1]; Jivtesh Garg[1]; Keivan Esfarjani[1]; Adam Jandl[2]; Zhiting Tian[1]; Bo Qiu[1]; Mayank T. Bulsara[2]; Aaron J. Schmidt[3]; Austin J. Minnich[4]; Shuo Chen[5]; Mildred S. Dresselhaus[6]; Zhifeng Ren[5]; Eugene A. Fitzgerald[2]; Gang Chen[1]

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Graduate Student

A-II-1: ELECTROCATALYSIS OF TOTAL WATER SPLITTING ON PEROVSKITE OXIDES AND OXYNITRIDES

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Graduate Student

H-III-4: STABILIZATION BY ATOMIC LAYER DEPOSITION OF COPPER CATALYSTS FOR LIQUID PHASE REACTIONS

[IACT] Brandon J. O'Neill[1], David H. K. Jackson[2], Anthony J. Crisci[1,3], Carrie A. Farberow[1], Fengyuan Shi[2], Junling Lu[4], Paul J. Dietrich[5], Xiangkui Gu[5],Christopher L. Marshall[6], Peter C. Stair[6,7], Jeffrey W. Elam[8], Jeffrey T. Miller[6], Fabio H. Ribeiro[5], Paul M. Voyles[2], Jeffrey Greeley[5], Manos Mavrikakis[1], Susannah L. Scott[3,9], Thomas F. Kuech[1,2], and James A. Dumesic[1]

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Postdoctoral Researcher

H-I-4: ADSORBATE INDUCED ADATOM MOBILITY IN A MODEL CATALYST: PD/Fe_3O_4

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Postdoctoral Researcher

C-III-4: NANOSCALE ATOMS IN SOLID-STATE CHEMISTRY

[RPEMSC] Xavier Roy[1], Chul-Ho Lee[1,2], Andrew C. Crowther[3], Christine L. Schenck[1], Tiglet Besara[4], Roger A. Lalancette[6], Theo Siegrist[4,5], Peter W. Stephens[7], Louis E. Brus[1], Philip Kim[2], Michael L. Steigerwald[1], Colin Nuckolls[1]

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Postdoctoral Researcher

D-III-2: PHOTOTROPIC GROWTH CONTROL OF NANOSCALE PATTERN FORMATION IN PHOTOELECTRODEPOSITED SE–TE FILMS

[LMI] Bryce Sadtler[1]; Stanley P. Burgos[2]; Nicolas A. Batara[2]; Joseph A. Beardslee[1]; Harry A. Atwater[2,3]; Nathan S. Lewis[1,3,4]

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Graduate Student

C-I-2: CONCERTED PROCESSES IN ORGANIC PHOTOVOLTAICS: THE RELATED CHALLENGES OF GENERATING AND COLLECTING CHARGE IN A DISORDER ENVIRONMENT.

[ANSER] Brett M. Savoie[1]; Henry Heitzer[1]; Brian S. Rolczynszki[1]; Bijan Movaghar[1]; Stephen Loser[1]; Sylvia Lou[1]; Luping Yu[1,2]; Lin X. Chen[1,3]; Tobin J. Marks[1]; Mark A. Ratner[1]

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Postdoctoral Researcher

E-III-1: FIRST-PRINCIPLES STUDIES OF LOSS MECHANISMS IN LIGHT-EMITTING DIODES

[CEEM] Daniel Steiauf[1], Qimin Yan[2], Emmanouil Kioupakis[3], and Chris G. Van de Walle[1]

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Postdoctoral Researcher

B-IV-3: DEVELOPMENT OF *IN SITU* MAGNETIC RESONANCE TECHNIQUES TO STUDY LI METAL BATTERIES AND SUPERCAPACITORS IN REAL TIME

[NECCES] Nicole M. Trease[1], Hee Jung Chang[1], Andrew J. Ilott[2], S. Chandrashekar[1,2], Hao Wang[1,3], Thomas J.-K. Köster[3], Lin-Shu Du[1], Alexej Jerschow[2], and Clare P. Grey[1,3]

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Graduate Student

D-IV-1: HYPERVALENT SURFACE INTERACTIONS FOR COLLOIDAL STABILITY AND DOPING OF SILICON NANOCRYSTALS

[CASP] Lance M. Wheeler[1], Nathan R. Neale[2], Ting Chen[1], Uwe R. Kortshagen[1]

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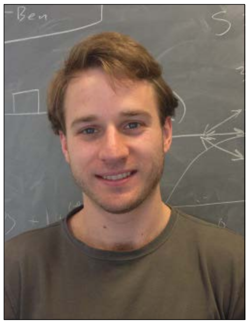

Postdoctoral Researcher

C-II-3: PREDICTING AND UNDERSTANDING THE SINGLET FISSION RATE: A COMBINED THEORETICAL AND EXPERIMENTAL EFFORT

[CE] Shane R. Yost[1], Jiye Lee[2], Mark W. B. Wilson[1], David P. McMahon[1], Rebecca R. Parkhurst[1], Nicholas J. Thompson[2], Akshay Rao[3], Kerr Johnson[3], Matthew Y. Sfeir[4], Moungi Bawendi[1], Timothy M. Swager[1], Richard H. Friend[3], Marc A. Baldo[2], and Troy Van Voorhis[1]

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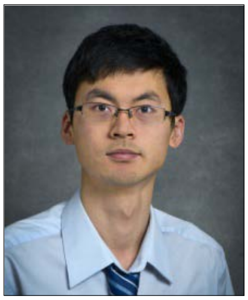

Graduate Student

G-II-4: CONTROLS ON MINERALIZATION IN VOLCANOGENIC RESERVOIR ROCKS

[NCGC] Shuo Zhang[1,2], Donald J. DePaolo[2], Tianfu Xu[2], Marco Voltolini[2]

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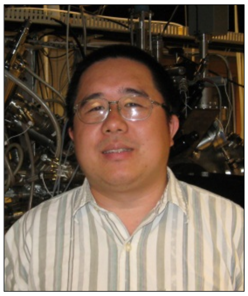

Graduate Student

E-I-1: GROWTH OF NOVEL SUPERCONDUCTORS BY ATOMIC LAYER BY LAYER MOLECULAR BEAM EPITAXY

[CES] Mao Zheng[1], Can Zhang[1], Brian Mulcahy[1], Xiaoxiao Wang[1], Hefei Hu[2], Han Zhang[1], Hamood Z. Ahram[1], Ying Jia[3], Ulrich Welp[3], Alexey Koshelev[3], Jian-Min Zuo[1], Laura Greene[1], James N. Eckstein[1]

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List of EFRC Acronyms

(ANSER) Argonne-Northwestern Solar Energy Research Center
Michael R. Wasielewski, Northwestern University

(BISfuel) Center for Bio-Inspired Solar Fuel Production
Devens Gust, Arizona State University

(C3Bio) Center for Direct Catalytic Conversion of Biomass to Biofuels
Maureen McCann, Purdue University

(CABS) Center for Advanced Biofuel Systems
Jan Jaworski, Donald Danforth Plant Science Center

(CALCD) Center for Atomic-Level Catalyst Design
James Spivey, Louisiana State University

(CASP) Center for Advanced Solar Photophysics
Victor I. Klimov, Los Alamos National Laboratory

(CCEI) Catalysis Center for Energy Innovation
Dion Vlachos, University of Delaware

(CCHF) Center for Catalytic Hydrocarbon Functionalization
T. Brent Gunnoe, University of Virginia

(CDP) Center for Defect Physics in Structural Materials
G. Malcolm Stocks, Oak Ridge National Laboratory

(CE) Center for Excitonics
Marc Baldo, Massachusetts Institute of Technology

(CEEM) Center for Energy Efficient Materials
John Bowers, University of California, Santa Barbara

(CEES) Center for Electrical Energy Storage
Michael Thackeray, Argonne National Laboratory

(CEFRC) Combustion Energy Frontier Research Center
Chung K. Law, Princeton University

(CEN) Center for Energy Nanoscience
P. Daniel Dapkus, University of Southern California

(CES) Center for Emergent Superconductivity
J. C. Séamus Davis, Brookhaven National Laboratory

(CETM) Center for Electrocatalysis, Transport Phenomena and Materials for Innovative Energy Storage
Grigorii Soloveichik, General Electric Global Research

(CFSES) Center for Frontiers of Subsurface Energy Security
Steven Bryant, University of Texas at Austin

(CGS) Center for Gas Separations Relevant to Clean Energy Technologies
Berend Smit, University of California, Berkeley

(CID) Center for Inverse Design
William Tumas, National Renewable Energy Laboratory

(CISSEM) Center for Interface Science: Solar Electric Materials
Neal R. Armstrong, University of Arizona

(CLSF) Center for Lignocellulose Structure and Formation
Daniel Cosgrove, Pennsylvania State University

(CME) Center for Molecular Electrocatalysis
R. Morris Bullock, Pacific Northwest National Laboratory

(CMIME) Center for Materials at Irradiation and Mechanical Extremes
Amit Misra, Los Alamos National Laboratory

(CMSNF) Center for Materials Science of Nuclear Fuel
Todd Allen, Idaho National Laboratory

(CNEEC) Center on Nanostructuring for Efficient Energy Conversion
Stacey Bent and Fritz Prinz, Stanford University

(CST) Understanding Charge Separation and Transfer at Interfaces in Energy Materials
Peter J. Rossky, University of Texas at Austin

(CSTEC) Center for Solar and Thermal Energy Conversion
Peter F. Green, University of Michigan

(Efree) Center for Energy Frontier Research in Extreme Environments
Ho-kwang Mao, Carnegie Institution of Washington

(emc^2) Energy Materials Center at Cornell
Héctor D. Abruña, Cornell University

(FIRST) Fluid Interface Reactions, Structures and Transport Center
David J. Wesolowski, Oak Ridge National Laboratory

(HeteroFoaM) Heterogeneous Functional Materials Center
Kenneth Reifsnider, University of South Carolina

(IACT) Institute for Atom-efficient Chemical Transformations
Christopher L. Marshall, Argonne National Laboratory

(LMI) Light-Material Interactions in Energy Conversion
Harry Atwater, California Institute of Technology

(MEEM) Molecularly Engineered Energy Materials
Vidvuds Ozolins, University of California, Los Angeles

(MSA) Materials Science of Actinides
Peter C. Burns, University of Notre Dame

(NCGC) Center for Nanoscale Control of Geologic CO_2
Donald J. DePaolo, Lawrence Berkeley National Laboratory

(NECCES) Northeastern Center for Chemical Energy Storage
M. Stanley Whittingham, Stony Brook University

(NEES) Nanostructures for Electrical Energy Storage
Gary Rubloff, University of Maryland

(NERC) Non-equilibrium Energy Research Center
Bartosz A. Grzybowski, Northwestern University

(PARC) Photosynthetic Antenna Frontier Research Center
Robert E. Blankenship, Washington University in St. Louis

(PHaSE) Polymer-Based Materials for Harvesting Solar Energy
Paul Lahti & Thomas Russell, University of Massachusetts, Amherst

(RMSSEC) Revolutionary Materials for Solid State Energy Conversion
Donald T. Morelli, Michigan State University

(RPEMSC) Re-Defining Photovoltaic Efficiency Through Molecule Scale Control
James Yardley, Columbia University

(S3TEC) Solid-State Solar-Thermal Energy Conversion Center
Gang Chen, Massachusetts Institute of Technology

(SSLS) EFRC for Solid State Lighting Science
Michael E. Coltrin, Sandia National Laboratories (NM)

(UNC) Center for Solar Fuels
Thomas J. Meyer, University of North Carolina