Session A – Organic Photovoltaics - Grand Ballroom South

Parallel Scientific Session I - May 26, 2011
Grand Ballroom South

10:15 - 10:35
T-A01 - BOUNDLESS ENERGY: THE LIFE AND SCIENCE OF PAUL F. BARBARA
[CST] Xiaoyang Zhu and Jennifer Lyon
University of Texas at Austin

10:35 - 11:15
T-A02 - CHARGE SEPARATION AND TRANSFER AT ORGANIC SEMICONDUCTOR INTERFACES: FROM SINGLE MOLECULES TO SINGLE CRYSTALS
[CST] Xiaoyang Zhu, Peter J. Rossky, Loren Kaake, Adam Willard, Michael Bedard-Hearn, and Raluca Gearba
University of Texas at Austin

11:15 - 11:35
T-A03 - PLASTIC SOLAR CELLS: SELF-ASSEMBLY OF BULK HETEROJUNCTION NANO-MATERIALS BY SPONTANEOUS PHASE SEPARATION
[CEEM] Alan Heeger
University of California, Santa Barbara

11:35 - 11:55
T-A04 - UNDERSTANDING THE MORPHOLOGY OF ORGANIC PHOTOVOLTAICS
[PHaSE] Thomas Russell
University of Massachusetts Amherst

11:55 - 12:15
T-A05 - HIGH EFFICIENCY ORGANIC PHOTOVOLTAIC CELLS: MICROSTRUCTURAL, ELECTRONIC STRUCTURAL, AND INTERFACIAL MATERIALS DESIGN
[ANSER] Tobin Marks[1], Lin Chen[2], Luping Yu[3], Mark Ratner[4], and Robert Chang[4]
[1]Northwestern U.; [2]Argonne National Lab.; [3]U. of Chicago and [4]Northwestern U.

Parallel Scientific Session II – May 26, 2011
Grand Ballroom South

1:45 - 2:05
T-A06 - THE INTERFACE SCIENCE OF PHOTOVOLTAIC SOLAR ENERGY CONVERSION: CHARGE TRANSFER AT INORGANIC-ORGANIC AND INORGANIC-INORGANIC INTERFACES MODULATED BY HOLE- AND ELECTRON-SELECTIVE INTERLAYERS
[CISSEM] Neal Armstrong[1], Erin Ratcliff[1], Brian Zacher[1], Gordon MacDonald[1], Laura Schirra[1], Oliver Monti[1], Xerxes Steirer[1], Dana Olson[2], Jens Meyer[3], Antoine Kahn[3], Hyeunseok Cheun[4], and Bernard Kippelen[4]
[1]University of Arizona; [2]National Renewable Energy Laboratory; [3]Princeton University and [4]Georgia Institute of Technology

2:05 - 2:25
T-A07 - STRATEGIES TO CONTROL THE MORPHOLOGY OF ORGANIC PHOTOVOLTAICS
[PHaSE] Dhandapani Venkataraman
University of Massachusetts Amherst

2:25 - 2:45
T-A08 - MODIFYING THE WORK FUNCTION OF TRANSPARENT CONDUCTING OXIDES THROUGH INTERFACE CHEMISTRIES FOR INVERTED ARCHITECTURE ORGANIC-PHOTOVOLTAICS
[CISSEM] Bernard Kippelen, Yinhua Zhou, Hyeunseok Cheun, William Potscavage Jr., Canek Fuentes-Hernandez, Seth Marder, Jens Meyer, and Antoine Kahn
Georgia Institute of Technology

2:45 - 3:05
T-A09 - THE ROLE OF NANOSCALE ARCHITECTURE IN THE PERFORMANCE OF CONJUGATED POLYMER-BASED PHOTOVOLTAIC DEVICES
[MEEM] Benjamin Schwartz, Sarah Tolbert, Yves Rubin, Daniel Neuhauser, Nikos Kopidakis, Alex Ayzner, Stephanie Doan, Chris Tassone, Bertrand Tremolet de Villers, Krastina Petrova, and Daniel Kilbride
University of California, Los Angeles

3:05 - 3:45
T-A10 - MATERIALS AND DEVICES FOR ORGANIC PHOTOVOLTAIC DEVICES
[RPEMSC] Colin Nuckolls, Theanne Schiros, and Ioannis Kymissis
Columbia University

Parallel Scientific Session III – May 26, 2011
Grand Ballroom South

4:00 - 4:20
T-A11 - EXCITONIC ANTENNAS FOR SOLAR CELLS
[CE] Marc Baldo, Troy Van Voorhis, Jiye Lee, Priya Jadhav, Carmel Rotschild, and Phil Reusswig
MIT

4:20 - 4:40
T-A12 - EXCITON MANAGEMENT IN ORGANIC PHOTOVOLTAICS
[CEN] Mark Thompson[1], Barry C. Thompson[1], Stephen Bradforth[1], Sean Roberts[1], Matthew Whited[1], Robert McAnally[1], Beate Burkhart[1], Stephen Forrest[2], and Jeramy Zimmerman[2]
[1]University of Southern California and [2] University of Michigan

4:40 - 5:20
T-A13 - DYE-SENSITIZED PHOTOELECTROSYNTHESIS CELLS: FROM SYNTHESIS TO ASSEMBLY
[UNC] Javier Concepcion, Rene Lopez, and Kenneth Hanson
UNC

5:20 - 5:40
T-A14 - COMPUTATIONAL MOLECULAR ELECTROCATALYSIS: THE ROLE OF PROTON RELAYS IN H2 OXIDATION AND EVOLUTION CATALYSTS
[CME] Michel Dupuis[1], Simone Raugei[1], Roger Rousseau, Shentan Chen, M.H. Ho, R. Morris Bullock, Daniel L. DuBois, Jenny Y. Yang, Sharon Hammes-Schiffer[2], Alexander V. Soudackov[2], Samantha Horvath[2], and Laura E. Fernandez[2]
[1]Pacific Northwest National Laboratory and [2]Pennsylvania State University

5:40 - 6:00
T-A15 - A TWO-JUNCTION ARTIFICIAL LEAF: OPTIMIZING ARTIFICIAL ANTENNAS AND REACTION CENTERS FOR SOLAR-DRIVEN WATER TO HYDROGEN REDOX PROCESSES
[BISfuel] Ana L. Moore, Thomas A. Moore, Devens Gust, Antaeres' Antoniuk-Pablant, Jesse Bergkamp, Gerdenis Kodis, Matthieu Koepf, Jackson Megiatto, Dalvin Mendez, Smitha Pillai, Benjamin Sherman, and Yuichi Terazono
Arizona State University

Parallel Scientific Session IV – May 27, 2011
Grand Ballroom South

8:00 - 8:20
T-A16 - SYNTHESIS OF ORGANIC AND HYBRID MATERIALS FOR PHOTOVOLTAICS
[PHaSE] Todd Emrick
UMass-Amherst

8:20 - 8:40
T-A17 - NANOSCALE CHARACTERIZATION OF CHEMICALLY MODIFIED OXIDE SURFACES AND EARLY STUDIES OF THE DYNAMICS OF SMALL NUMBERS OF CHARGE CARRIERS IN NANOSCALE VOLUMES
[CISSEM] David Ginger[1], Bradley Macleod[1], Andreas Tillack[1], Matthew Gliboff[1], Kristina Knesting[1], Hong Li[2], Jean-Luc Bredas[2], Sergio Paniagua[2], Seth Marder[2], Matthew Schalnat[3], Jeanne Pemberton[3], and Mariola Macech[3]
[1]University of Washington ; [2]Georgia Institute of Technology and [3]University of Arizona

8:40 - 9:00
T-A18 - SOLAR ABSORPTION EFFECTS WITH ORGANIC MACROMOLECULAR PHOTOVOLTAIC MATERIALS
[CSTEC] Theodore Goodson III
University of Michigan

9:00 - 9:20
T-A19 - FULLY PHASE-COHERENT MULTIDIMENSIONAL OPTICAL SPECTROSCOPY FOR MEASUREMENT OF EXCITON AND MULTIEXCITON DYNAMICS
[CE] Keith A Nelson
MIT

9:20 - 9:40
T-A20 - MEG TO MORPHOLOGY: THEORY APPLIED TO PHOTOVOLTAIC CONCEPTS
[RPEMSC] David Reichman, Ashraf Alam, and Mark Hybertsen
Columbia University; Purdue University and Brookhaven National Laboratories

A. Organic Photovoltaics Close-Out Panel - Grand Ballroom South
May 27, 2011: 11:30 – 12:30 PM

MODERATORS: Mark Spitler and Raul Miranda, *Department of Energy*

- David Ginley, *Center for Energy Efficient Materials*
- Peter Green, *Center for Solar and Thermal Energy Conversion*
- Tom Russell, *Polymer-Based Materials for Harvesting Solar Energy*
- Michael Wasielewski, *Argonne-Northwestern Solar Energy Research Center*

Session B – Inorganic Photovoltaics - Grand Ballroom Central

Parallel Scientific Session I – May 26, 2011
Grand Ballroom

10:15 - 10:35 (Joint with Session A)
T-B01 - BOUNDLESS ENERGY: THE LIFE AND SCIENCE OF PAUL F. BARBARA
[CST] Xiaoyang Zhu and Jennifer Lyon
University of Texas at Austin

Parallel Scientific Session II – May 26, 2011
Grand Ballroom Central

1:45 - 2:05
T-B02 - EXCITONICS IN NANOCRYSTAL QUANTUM DOTS
[CE] Moungi Bawendi
MIT

2:05 - 2:25
T-B03 - NANOSTRUCTURED COMPOUND SEMICONDUCTORS FOR SOLAR ENERGY CONVERSION: FROM INTERFACES TO INTERMEDIATE BAND ABSORPTION
[CSTEC] Rachel Goldman, Roy Clarke, Steve Forrest, Harley Johnson, Peicheng Ku, Cagliyan Kurdak, Joanna Millunchick, Xiaoqing Pan, Jamie Phillips, Vanessa Sih, Katsuyo Thornton, and Ctirad Uher
University of Michigan

2:25 - 2:45
T-B04 - SIMULATIONS OF OPTICAL ABSORPTION IN NANOWIRE ARRAYS FOR PHOTOVOLTAIC APPLICATIONS
[CEN] Chenxi Lin, Ningfeng Huang, and Michelle L. Povinelli
University of Southern California

2:45 - 3:05
T-B05 - NANOPHOTONICS FOR OPTIMAL SOLAR THERMOPHOTOVOLTAIC SYSTEMS
[S3TEC] Marin Soljacic
MIT

3:05 - 3:25
T-B06 - PHOTOPHYSICS OF SEMICONDUCTOR NANOSTRUCTURES IN RELATION TO PROBLEMS OF SOLAR ENERGY CONVERSION
[CASP] Victor I. Klimov
Los Alamos National Laboratory

Parallel Scientific Session III – May 26, 2011
Grand Ballroom Central

4:00 - 4:20
T-B07 - WHAT WENT WRONG WITH PAST EFFORTS TO USE EARTH ABUNDANT ABSORBERS SUCH AS FES2: THE DESIGN OF A MATERIAL FIX.
[CID] Douglas Keszler[1], John Wager[1], and Liping Yu[2]
[1]*Oregon State University and* [2]*NREL*

4:20 - 4:40
T-B08 - ADVANCED PHOTOELECTRODE ARCHITECTURES FOR EFFICIENT SOLAR ENERGY CONVERSION
[ANSER] Joseph Hupp
Northwestern University

4:40 - 5:00
T-B09 - LIGHT TRAPPING AND ABSORPTION BEYOND CLASSICAL LIMITS
[LMI] Harry Atwater
California Institute of Technology

5:00 - 5:20
T-B10 - ENGINEERING LIGHT-MATTER INTERACTION IN ENERGY CONVERSION DEVICES
[CNEEC] Mark Brongersma, Isabell Thomann, Chinmay Nivargi, Art Wangperawong, Steve Herron, Dong Rip Kim , Sang Moo Jeong, Vijay Parameshwaran, Xiaolin Zheng, Thomas Jaramillo, Stacey Bent, Bruce Clemens, Vardaan Chawla, Jonathan Bakke, and Carl Hagglund
Stanford

5:20 - 5:40
T-B11 - REACHING FOR THE LIMIT: THE NEW SCIENCE TO APPROACH THE SHOCKLEY-QUEISSER LIMIT
[LMI] Eli Yablonovitch, Owen Miller, and Vidya Ganapati
UC Berkeley

5:40 - 6:00
T-B12 - EMBEDDED PHOTONIC CRYSTALS FOR HIGHER EFFICIENCY LEDS AND PHOTOVOLTAICS
[CEEM] Claude Weisbuch and Elison Matioli
University of California, Santa Barbara and MIT

Parallel Scientific Session IV – May 27, 2011
Grand Ballroom Central

8:00 - 8:20
T-B13 - ADVANCED IN CHARGE MANIPULATION IN QUANTUM DOT ARRAYS AND ARCHITECTURES FOR 3RD GENERATION SOLAR CELLS
[CASP] Arthur J.Nozik
National Renewable Energy Laboratory

8:20 - 8:40
T-B14 - LIGHT CAPTURE IN SILICON MICROCELL PHOTOVOLTAICS
[LMI] John Rogers
UIUC

8:40 - 9:00
T-B15 - LIGHT HARVESTING WITH FRAMEWORK MATERIALS
[UNC] Wenbin Lin[1], Spiros Skourtis[2], Caleb A Kent[1], Demin Liu[1], Cheng Wang[1], Andre van Rynbach[2], Xiangqian Hu[2], Brian Mehl[1], Thomas Meyer[1], John Papanikolas[1], and David Beratan[2]
[1]University of North Carolina at Chapel Hill and [2]Duke University

9:00 - 9:20
T-B16 - DEVELOPMENT OF NOVEL NANOMATERIALS AS THE BUILDING BLOCKS FOR NEXT-GENERATION SOLAR CELLS
[CASP] Jeffrey M. Pietryga
Los Alamos National Laboratory

9:20 - 9:40
T-B17 - UNDERSTANDING CARRIER DOPING AND ELECTRICAL CONDUCTIVITY OF WIDE GAP OXIDES AS TRANSPARENT CONDUCTORS FOR SOLAR PHOTO CONVERSION.
[CID] Stephan Lany[1], Andriy Zakutayev[1], Thomas Mason[2], John Wager[3], Kenneth Poeppelmeier[2] , John Perkins[1], Joseph Berry[1], David Ginley[1], and Alex Zunger [1]
[1]NREL; [2]Northwestern University and [3]Oregon State University;

B. Inorganic Photovoltaics Close-Out Panel
May 27, 2011: 11:30 – 12:30 PM
Grand Ballroom Central

MODERATORS: Carol Bessel and Greg Fiechtner, *Department of Energy*

- Mark Baldo, *Center for Excitonics*
- Dan Dapkus, *Center for Energy Nanoscience*
- Victor Klimov, *Center for Advanced Solar Photophysics*

C – Solar Fuels and Biomass – Mount Vernon Square/ Grand Ballroom North

Parallel Scientific Session I – May 26, 2011
Mount Vernon Square

10:15 - 10:35 (Joint with Session A in the Grand Ballroom)
T-C01 - BOUNDLESS ENERGY: THE LIFE AND SCIENCE OF PAUL F. BARBARA
[CST] Xiaoyang Zhu and Jennifer Lyon
University of Texas at Austin

10:35 - 10:55
T-C02 - NEW AVENUES TOWARDS THE DEVELOPMENT OF A BIO-INSPIRED ARTIFICIAL OXYGEN EVOLVING COMPLEX
[BISfuel] Petra Fromme, Hao Yan, Yan Liu, Giovanna Ghirlanda, James Allen, Kevin Redding, Don Seo, Raimund Fromme, Kim Rendek, Chad Simmons, Sandip Shinde, Mingui Liu, Justin Flory, Sudipta Biswas, Xixi Wei, Angelo Cereda, Matthieu Walter, Josifina Sarrou, Wang Dong, and Palash Dutta
Arizona State University

10:55 - 11:15
T-C03 - BIO-INSPIRED MOLECULAR MATERIALS FOR SOLAR FUELS
[ANSER] Michael R. Wasielewski
Northwestern University

11:15 - 11:35
T-C04 - UNDERSTANDING AND CONTROLLING PROTON MOVEMENT IN MOLECULAR ELECTROCATALYSIS
[CME] R. Morris Bullock[1], Daniel L. DuBois[1], Michel Dupuis[1], James M. Mayer[2], Sharon Hammes-Schiffer[3], Bruce A. Parkinson[4], Jenny Y. Yang[1], Michael T. Mock[1], John A. S. Roberts[1], Simone Raugei[1], and Roger Rousseau[1]
[1]Pacific Northwest National Laboratory; Pacific Northwest National Laboratory; Pacific Northwest National Laboratory; [2]University of Washington; [3]Pennsylvania State University and [4]University of Wyoming

11:35 - 11:55
T-C05 - DESIGN OF PEPTIDE-BASED CATALYSTS: DEVELOPMENT OF ARTIFICIAL HYDROGENASES
[BISfuel] Giovanna Ghirlanda, Anne K. Jones, Arnab Dutta, Anindya Roy, Sandip Shinde , and Mathieu Walther
Arizona State University;

11:55 - 12:15
T-C06 - MOLECULAR ELECTROCATALYSTS FOR PRODUCTION AND OXIDATION OF HYDROGEN
[CME] Daniel DuBois, Morris Bullock, Mary Rakowski DuBois, Wendy Shaw, Aaron Appel, Stuart Smith, Jenny Yang, John Roberts, Uriah Kilgore, Doug Pool, Simone Raugei, Michel Dupuis, Roger Rousseau, Molly O'Hagan, Michael Stewart, Shentan Chen, and Monte Helm
Pacific Northwest National Laboratory

Parallel Scientific Session II – May 26, 2011
Grand Ballroom North

1:45 - 2:05
T-C07 - ENGINEERING CATALYSTS AT THE NANO-SCALE FOR ENERGY CONVERSION REACTIONS
[CNEEC] Thomas F. Jaramillo, Zhebo Chen, Yelena Gorlin, Hee Joon Jung, Robert Sinclair, Jennifer Wilcox, Bruce M. Clemens, Mark Brongersma, Arthur Grossman, Fritz B. Prinz, Stacey F. Bent, and Jens K. Norskov
Stanford University

2:05 - 2:25
T-C08 - THE PHOTOSYNTHETIC ANTENNA RESEARCH CENTER: OVERVIEW AND NATURAL ANTENNAS
[PARC] Robert E. Blankenship and Himadri B. Pakrasi
Washington University in St. Louis

2:25 - 2:45
T-C09 - DESIGN, SYNTHESIS AND CHARACTERIZATION OF BIOHYBRID AND BIOINSPIRED LIGHT-HARVESTING SYSTEMS
[PARC] Dewey Holten and C Neil Hunter
Washington University in St. Louis and University of Sheffield

2:45 - 3:05
T-C10 - REDESIGNING METABOLIC FLUX FOR THE PRODUCTION OF ADVANCED BIOFUELS IN CAMELINA AND ALGAE
[CABS] Edgar Cahoon
University of Nebraska

3:05 - 3:25
T-C11 - COMBUSTION CHEMISTRY OF A NEW BIOFUEL: BUTANOL
[CEFRC] William Green[1], David Davidson[2], Fokion Egofopoulos[3], Nils Hansen[4], Michael Harper[1], Ron Hanson[2], Stephen Klippenstein[5], C.K.Ed Law[6], C.Jackie Sung[7], Donald Truhlar[8], and Hai Wang[3]
[1]MIT; [2]Stanford; [3]USC; [4]Sandia Livermore; [5]Argonne; [6]Princeton; [7]U. Connecticut and [8]U. Minnesota

3:25 - 3:45
T-C12 - INTERACTIONS OF CELLULOSE WITH MATRIX POLYSACCHARIDES
[CLSF] Yong Bum Park, Akira Tabuchi, Lian-Chao Li, and Daniel J. Cosgrove
The Pennsylvania State University

Parallel Scientific Session III – May 26, 2011
Grand Ballroom North

4:00 - 4:40
T-C13 - A ROADMAP FOR SELECTIVE DECONSTRUCTION OF LIGNOCELLULOSIC BIOMASS TO ADVANCED BIOFUELS AND USEFUL CO-PRODUCTS
[C3Bio] Maureen C McCann[1], Mahdi Abu-Omar[1], Joe Bozell[2], and Peter Ciesielski[3]
[1]Purdue University; [2]University of Tennessee and [3]NREL

4:40 - 5:00
T-C14 - PROBING THE STRUCTURE OF CELLULOSE SYNTHASE, A KEY PROTEIN WITHIN A REMARKABLE FIBRIL-SPINNING CELLULAR NANOMACHINE
[CLSF] Candace H. Haigler[1], Rami Alkhatib[1], Mark J. Grimson[2], James D. Kubicki[3], Le Li[1], Antonin Marek[1], Mohamed Naseer[3] Ali Mohamed[3], Tuyen Nguyen[1], Latsavongsakda Sethaphong[1], Abhishek Singh[1], Alex I. Smirnov[1], Maxim A. Voinov[1], and Yaroslava G. Yingling[1]
[1]North Carolina State University, North Carolina State University; [2]Texas Tech University and [3]The Pennsylvania State University

5:00 - 5:20
T-C15 - SELECTIVE TRANSFORMATION OF BIOMASS DERIVATIVES
[CCEI] Dion G. Vlachos
University of Delaware

5:20 - 5:40
T-C16 - IACT - GOALS AND PROGRESS IN BIOMASS REACTION MECHANISMS
[IACT] Christopher Marshall and Peter Stair
Argonne National Laboratory and Northwestern University

5:40 - 6:00
T-C17 - CATALYSIS FOR BIOMASS REFORMING
[CCEI] Michael Salciccioli, Weiting Yu, Mark Barteau, Jingguang Chen, and Dion Vlachos
University of Delaware

Parallel Scientific Session IV – May 27, 2011
Grand Ballroom North

8:00 - 8:20
T-C18 - COMPUTATIONAL AND ENABLING TECHNOLOGIES IN THE CENTER FOR ADVANCED BIOFUELS (CABS)
[CABS] Lisa Carey[1], Rahul Deshpande[1], David Gang[2] , Mahmoud Gargouri[2], Jeong-Jin Park[2], Leslie Hicks[3], Yair Shachar-Hill[1], Hongxia Wang[3], and Baichen Zhang[3]
[1]Michigan State University; [2]Washington State University and [3]Donald Danforth Plant Science Center

8:20 - 8:40
T-C19 - PYROPROBE/TANDEM MASS SPECTROMETRY PROVIDES INSIGHTS INTO FAST PYROLYSIS OF BIOMASS
[C3Bio] Piotr Gawecki, Andrew D. Smeltz, Matthew R. Hurt, David J. Borton II, Nelson R. Vinueza, Nicholas J. Nugent, Rakesh Agrawal, W. Nicholas Delgass, Hilkka I. Kenttamaa, William E. Anderson, and Fabio H. Ribeiro
Purdue University

8:40 - 9:00
T-C20 - MULTISCALE KINETIC KNOWLEDGE PROPAGATION - COMBUSTION CHEMISTRY OF SMALL HYDROCARBONS
[CEFRC] Hai Wang
University of Southern California

9:00 - 9:20
T-C21 - IDENTIFICATION OF NEW REGULATORY NETWORKS FOR INCREASING PLANT OIL ACCUMULATION
[CABS] Geliang Wang[1], Maoyin Li[1], Amanda Tawfall[1], Carlotta Peters[1], Brian Fanella[2] , and Xuemin (Sam) Wang[1]
[1]Donald Danforth Plant Science Center and [2]University of Missouri

9:20 - 9:40
T-C22 - DESIGN, ENGINEERING, AND PHOTOPHYSICAL CHARACTERIZATION OF ARTIFICIAL LIGHT-HARVESTING COMPLEXES USING SYNTHETIC CHLORINS AND MAQUETTES
[PARC] Goutham Kodali[1], Joseph W. Springer[2], Olga Mass[3], Lee A. Solomon[1], Tammer A. Farid[1], David F. Bocian[4], Christine Kirmaier[2], Jonathan S. Lindsey[3], Dewey Holten[2], Christopher C. Moser[1], and P. Leslie Dutton[1]
[1]University of Pennsylvania; [2]Washington University in St. Louis; [3]North Carolina State University and [4]University of California, Riverside

C. Solar Fuels and Biomass Close-Out Panel - Grand Ballroom North
May 27, 2011: 11:30 – 12:30 PM

MODERATORS: Gail McLean and Richard Greene, *Department of Energy*

- Dewey Holten, *Photosynthetic Antenna Frontier Research Center*
- Wenbin Lin, *Solar Fuels and Next Generation Photovoltaics*
- Maureen McCann, *Center for Direct Catalytic Conversion of Biomass to Biofuels*
- Ana Moore, *Center for Bio-Inspired Solar Fuel Production*

D – Energy Storage and Transmission - Congressional Hall A&B

Parallel Scientific Session I – May 26, 2011
Congressional Hall A&B

10:15 - 10:55
T-D01 - ELECTRODE REACTIONS IN LITHIUM ION BATTERIES - FUNDAMENTAL RESEARCH AT NECCES
[NECCES] Clare P. Grey[1], Anton Van Der Ven[2], Hui-Chia Yu[2], and Katsuyo Thornton[2]
[1]Stony Brook University and [2]University of Michigan

10:55 - 11:15
T-D02 - COLLABORATIVE ENERGY FRONTIER RESEARCH: CONTROLLED SILICON NANOSTRUCTURES FOR LITHIUM STORAGE
[NEES] John Cumings[1] and S. T. Picraux[2]
[1]Unversity of Maryland and [2]Los Alamos National Lab

11:15 - 11:35
T-D03 - UNDERSTANDING AND DESIGNING SURFACES AND INTERFACES IN LI-ION BATTERIES FROM FIRST PRINCIPLES
[CEES] Maria Chan[1], Scott Kirklin[2], Hakim Iddir[1], Kah Chun Lau[1], Jishnu Bhattacharya[2], David Snydacker[2], Jeff Greeley[1], Chris Wolverton[2], and Larry Curtiss[1]
[1]Argonne National Laboratory and [2]Northwestern University

11:35 - 11:55
T-D04 - UNDERSTANDING THE REACTION MECHANISM OF CONVERSION REACTION IN BATTERIES - A MULTIPRONGED EXPERIMENTAL AND THEORETICAL APPROACH
[NECCES] Glenn Amatucci
Rutgers University

11:55 - 12:15
T-D05 - ENABLING CONCEPTS FOR SAFE, SELF-HEALING LI-ION BATTERIES
[CEES] Jeffrey S. Moore
University of Illinois, Urbana-Champaign

Parallel Scientific Session II – May 26, 2011
Congressional Hall A&B

1:45 - 2:05
T-D06 - ELECTROCATALYTIC APPROACHES TO VIRTUAL HYDROGEN STORAGE
[CETM] Oana R. Luca[1], Steven J. Konezny[1], Jeremy Praetorius[1], Gary Yeager[2], Guillermo D. Zappi[2], David Simone[2], Grigorii L. Soloveichik[2], John B. Kerr[2], Judith Stein[3], Thomas Miebach[2], Chris E.D. Chidsey[4], Victor S. Batista[5], and Robert H. Crabtree[5]
[1]Yale University; [2]GE Global Research; [3]LBNL; [4]Stanford University and [5]Yale University

2:05 - 2:25
T-D07 - THERMODYNAMIC AND ELECTROCHEMICAL STUDIES ON ORGANIC FUELS
[CETM] Davide L. Simone[1], Thomas Miebach[1], Matthew Rainka[1], Robert H. Crabtree2, and Grigorii L. Soloveichik[1]
[1]GE Global Research and [2]Yale University

2:25 - 2:45
T-D08 - NANOSCALE CONTROL OF THERMODYNAMIC POTENTIALS
[CNEEC] Bruce Clemens[1], Fritz Prinz[1], David Goldhaber-Gordon[1], Robert Sinclair[1], John Vajo[2], Ping Liu[2], Sung Chul Lee[1], Chia-Jung Chung[1], James Donough[1], Jang Wook Choi[1], Men Young Lee[1], James Williams[1] , Phil Van Stockum[1], James Mack[1], Jun Liu[2], Adam Gross[2], Elena Sherman[2], and Sky Mahoney[2]
[1]Stanford University and [2]HRL Laboratories

2:45 - 3:05
T-D09 - EMC^2: OVERVIEW AND FUTURE PROJECTIONS
[EMC2] Hector Abruna
Cornell University

3:05 - 3:25
T-D10 - NANO-STRUCTURED SURFACES AND INTERFACES FOR EFFICIENT ENERGY STORAGE AND CONVERSION
[HeteroFoaM] Matt Lynch[1], Min Kyu Song[1], Kevin Blinn[1], Lei Yang[1], Mostafa El-Sayed[1], Feng Liu[2], Andreas Heyden[3], Anil Virkar[2], Ken Reifsnider[3], and Meilin Liu[1]
Ga Tech; [2]University of Utah; [3]USC and University of Utah

3:25 - 3:45
T-D11 - FUEL CELLS AND BATTERY MATERIALS: CHALLENGES AND PROGRESS
[EMC2] Frank Disalvo and Michael Lowe
Cornell University

Parallel Scientific Session III – May 26, 2011
Congressional Hall A&B

4:00 - 4:20
T-D12 - PINCER METAL COMPLEXES AS ELECTROCATALYSTS
[CETM] Grigorii L. Soloveichik[1], Mark D. Doherty[1], Oltea Siclovan[1], Kenneth P. Zarnoch[1], Alex Usyatinsky[1], Guillermo D. Zappi[1], Oana R. Luca$_2$, Steven J. Konezny[2], Victor S. Batista[2], and Robert H. Crabtree[2]
[1]GE Global Research and [2]Yale University

4:20 - 4:40
T-D13 - CAPACITIVE ENERGY STORAGE
[MEEM] Bruce Dunn, Yunfeng Lu, Laurent Pilon, Sarah Tolbert, and Vidvuds Ozolins
UCLA

4:40 - 5:00
T-D14 - LITHOGRAPHICALLY PATTERNED MNO2 NANOWIRE ARRAYS
[NEES] Reginald Penner and Yan Wenbo
University of California, Irvine

5:00 - 5:20
T-D15 - ELECTRICAL ENERGY STORAGE: USE-INSPIRED BASIC RESEARCH
[CEES] Michael Thackeray
Argonne National Laboratory

5:20 - 6:00
T-D16 - CONTACT ELECTRIFICATION: SEARCHING FOR ANSWERS TO THE MILLENIA-OLD QUESTION
[NERC] H. T. Baytekin[1], A. I. Patashinski[1], M. Branicki[2], B. Baytekin[1], and B. A. Grzybowski[1]
[1]Northwestern University and [2]NYU

D. Energy Storage and Transmission Close-Out Panel - Congressional Hall A&B
May 27, 2011: 11:30 – 12:30 PM

MODERATORS: John Vetrano and Linda Horton, *Department of Energy*

- Hector Abruna, *Energy Materials Center at Cornell*
- Clare Grey, *Northeastern Center for Chemical Energy Storage*
- Harold Kung, *Center for Electrical Energy Storage*
- Grigorii Soloveichik, *Center for Electrocatalysis, Transport Phenomena and Materials for Innovative Energy Storage*

E – Energy Conservation and Efficiency - Renaissance Ballroom East

Parallel Scientific Session I – May 26, 2011
Renaissance Ballroom East

10:15 - 10:55
T-E01 - HIGH PERFORMANCE NANOSTRUCTURED THERMOELECTRIC MATERIALS (NTHEM)
[RMSSEC] Mercouri Kanatzidis[1], Vidvuds Ozolins[2], David Seiman[1], Chris Wolverton[1], and Sergey Barabash[2]
[1]Northwestern University and [2]UCLA

10:55 - 11:15
T-E02 - NEW THERMOELECTRIC MATERIALS USING RARE EARTH NANOPARTICLE FOR INCREASED SEEBECK COEFFICIENT
[CEEM] John Bowers, Art Gossard, Chris Palmstrom, Ali Shakouri, and Shuji Nakamura
University of California, Santa Barbara

11:15 - 11:55
T-E03 - SOLID-STATE SOLAR-THERMAL ENERGY CONVERSION CENTER, PHONON TRANSPORT AND SOLAR THERMOELECTRIC ENERGY CONVERSION
[S3TEC] Gang Chen, Keith Nelson, and Daniel Kraemer
Massachusetts Institute for Technology

11:55 - 12:15
T-E04 - HIGHLIGHTS OF THERMOELECTRIC RESEARCH AT THE UNIVERSITY OF MICHIGAN
[CSTEC] Ctirad Uher
University of Michigan

Parallel Scientific Session II – May 26, 2011
Renaissance Ballroom East

1:45 - 2:05
T-E05 - ELECTRONIC AND THERMAL TRANSPORT PROPERTY CHARACTERIZATION OF THERMOELECTRIC MATERIALS UNDER REVOLUTIONARY MATERIALS FOR SOLID STATE ENERGY CONVERSION-EFRC, AWARD NUMBER DE-SC001054
[RMSSEC] Ctirad Uher
University of Michigan

2:05 - 2:25
T-E06 - EFFECT OF ELECTRODE MORPHOLOGY AND MATERIALS CHEMISTRY ON POLARIZATION IN SOLID OXIDE FUEL CELLS
[HeteroFoaM] Anil Virkar[1], Wilson Chiu[2], Kenneth Reifsnider[3], Prasun Majumder[3], Fazle Rabbi[3], MD. Raihan[3], and Qianlong Liu[3]
[1]University of Utah; [2]University of Connecticut and [3]University of South Carolina

2:25 - 2:45
T-E07 - UNDERSTANDING EFFICIENCY LIMITATIONS OF LEDS FOR SOLID-STATE LIGHTING
[SSLS] Mary Crawford[1], Weng Chow[1], Daniel Koleske[1], Normand Modine[1], Andrew Armstrong[1], Tania Henry[1], Jeffrey Tsao[1], Qi Dai[2], Jaehee Cho[2], and E. Fred Schubert[2]
[1]Sandia National Laboratories and [2]Rensselaer Polytechnic Institute

2:45 - 3:05
T-E08 - NANOSTRUCTURES FOR ENERGY GENERATION AND CONSERVATION
[CEN] P. Daniel Dapkus, Ting-Wei Yeh, Chun Yung Chi, Hyung-Joon Chu, Yenting Lin, Anuj Madaria, Maoqing Yao, Ruijuan Li, and Chongwu Zhou
University of Southern California

3:05 - 3:25
T-E09 - BEYOND 2D: NANOWIRES FOR SOLID-STATE LIGHTING
[SSLS] George Wang
Sandia National Laboratories

3:25 - 3:45
T-E10 - LIGHT-MATTER INTERACTION IN SUBWAVELENGTH PHOTONIC STRUCTURES
[SSLS] Arthur J. Fischer, Ganapathi Subramania, Ting S. Luk, Weng W. Chow, Eric A. Shaner, Daniel D. Koleske, and Igal Brener
Sandia National Labs

Parallel Scientific Session III – May 26, 2011
Renaissance Ballroom East

4:00 - 4:20
T-E11 - SUPERCONDUCTIVITY AS AN ENERGY CARRIER
[CES] George Crabtree
Argonne National Laboratory and University of Illinois at Chicago

4:20 - 4:40 T-E12 - INTERPLAY OF SYNTHESIS, CALCULATION AND CHARACTERIZATION OF HETEROGENEOUS FUNCTIONAL MATERIALS
[HeteroFoaM] Emily Carter[1], Andreas Heyden[2], Hanno Zur Loye[2], Prasun Majumdar[2], Kyle Brinkman[2], and Fanglin Chen[2]
[1]Princeton University and [2]University of South Carolina

4:40 - 5:00
T-E13 - DEVELOPMENT OF KINETIC MODELS FOR METHYL-ESTER MOLECULES FOR BIODIESEL MODELING
[CEFRC] Pascal Divart[1], Stephen Dooley[1], Sang Hee Won[1], Frederick L. Dryer[1], Yiguang Ju[1], Emily A. Carter[1], Chung K. Law[1], Fokion Egolfpoulos[2], Ronald K. Hanson[3], Stephen J. Klippenstein[4], Nils Hansen[5], and Chih-Jen Sung[6]
[1]Princeton University; [2]University of Southern California; [3]Stanford University; [4]Argonne National Laboratory; [5]Sandia National Laboratories and [6]University of Connecticut

5:00 - 5:20
T-E14 - COMPARING IRON-BASED AND COPPER-BASED HIGH TEMPERATURE SUPERCONDUCTORS
[CES] J. C. Seamus Davis
Brookhaven National Laboratory

5:20 - 5:40
T-E15 - ENERGY FRONTIER RESEARCH UNDER HIGH PRESSURES
[EFree] Ho-kwang Mao
Carnegie Institution

5:40 - 6:00
T-E16 - CES HIGH TEMPERATURE SUPERCONDUCTING MATERIALS RESEARCH, PRESENT AND FUTURE
[CES] Peter Abbamonte
University of Illinois at Urbana-Champaign

E. Energy Conservation and Efficiency Close-Out Panel, Renaissance Ballroom East
May 27, 2011: 11:30 – 12:30 PM

MODERATORS: Michael Casassa and Jim Horwitz*, Department of Energy*

- Gang Chen, *Solid-State Solar-Thermal Energy Conversion Center*
- George Crabtree, *Center for Emergent Superconductivity*
- Don Morelli, *Revolutionary Materials for Solid State Energy Conversion*
- Jeff Tsao, *EFRC for Solid State Lighting Science*

F – Carbon Capture and Sequestration - Renaissance Ballroom West A

Parallel Scientific Session III - May 26, 2011
Renaissance Ballroom West A

4:00 - 4:20
T-F01 - COMPUTATIONAL CARBON CAPTURE
[CGS] Berend Smit[1], Joe Swisher[1], Maciej Haranczyk[2], Jeff Neaton[2], Roberta Poloni[1], Giullia Galli[3], Laura Gagliardi[4], Allison Dzubak[4], Jihan Kim[5], and Richard Martin[5]
[1]UC Berkeley [2]LBNL; [3]UC Davis and [4]U Minnesota [5]LBNL

4:20 - 4:40
T-F02 - CARBONATE MINERAL NUCLEATION PATHWAYS
[NCGC] A. Fernandez-Martinez[1], A. Radha[2], A.G. Stack[3], L. Hedges[1], Y. Hu[4], A. Loulier[4], L. J. Banuelos[3], G. Rother[3], Y.S. Jun[4], S. Whitelam[1], D. R. Cole[5], A. Navrotsky[2], G.A. Waychunas[1], and J.J. DeYoreo[1]
[1]Lawrence Berkeley National Laboratory; [2]University of California, Davis; [3]Oak Ridge National Laboratory; [4]Washington University in St. Louis and [5]Ohio State University

4:40 - 5:00
T-F03 - MOLECULAR, CHEMICAL AND PHYSICAL PROPERTIES OF CO_2-H_2O - ELECTROLYTE-MINERAL SYSTEM
[CFSES] Philip Bennett[1], Susan Altman[2], Bayani Cardenas[1], Randall Cygan[2], Eugenio Santillan[1], Matthew Kirk[2], Molly Kent[1], Kuldeep Chaudhary[1] and Wen Deng[1]
[1]University of Texas at Austin and [2]Sandia National Laboratories

5:00 - 5:20
T-F04 - NANOPORE PROCESSES IN SEALING CAP ROCKS OF CARBON DIOXIDE STORAGE REPOSITORIES
[NCGC] Ian Bourg
Lawrence Berkeley National Laboratory

5:20 - 5:40
T-F05 - MULTISCALE SIMULATION OF CO_2 SEQUESTRATION IN SUBSURFACE MEDIA
[CFSES] Steven Bryant[1], Matt Balhoff[1], David DiCarlo[1], Sanjay Srinivasan[1], Tom Dewers[2], Hongkyu Yoon[2], Peter Eichhubl[1], Behdad Aminizadeh-Goharrizi[1], Tie Sun[1], Yashar Mehmani[1], Matt Roberts[1], and Valentina Prigiobbe[1]
[1]University of Texas at Austin and [2]Sandia National Laboratories

5:40 - 6:00
T-F06 - APPROACHES TO IMPROVING CARBON DIOXIDE ADSORPTION IN MULTIVARIATE METAL-ORGANIC FRAMEWORKS
[CGS] Omar M. Yaghi
UCLA

Parallel Scientific Session IV - May 27, 2011
Renaissance Ballroom West A

8:00 - 8:20
T-F07 - BASIC SCIENCE FOUNDATIONS FOR SUBSURFACE ENERGY SECURITY
[CFSES] Marianne Walck, Gary Pope, Susan Altman, and Mojdeh Delshad
Sandia National Laboratories; University of Texas at Austin; Sandia National Laboratories and University of Texas at Austin

8:20 - 8:40
T-F08 - PROBING CO_2-RICH FLUID INTERACTIONS WITH RESERVOIR ROCKS: FROM ATOMIC TO PORE SCALES
[NCGC] Gernot Rother[1], Larry Anovitz[1], Ariel Chialvo[1], David Cole[2], Mirek Gruszkiewicz[1], Andrew Stack[1], Lukas Vlcek[1], and Garrison Sposito[3]
[1]Oak Ridge National Laboratory; [2]Ohio State University and [3]Lawrence Berkeley National Laboratory

8:40 - 9:00
T-F09 - SYNTHESIS OF ZEOLITIC IMIDAZOLATE FRAMEWORKS AND THEIR GAS ADSORPTION
[MEEM] Omar M. Yaghi
UCLA

9:00 - 9:20
T-F10 - TOWARD MOLECULARLY DEFINED POROUS MEMBRANE
[CGS] Ting Xu
University of California, Berkeley

F. Carbon Capture and Sequestration Close-Out Panel. Renaissance Ballroom West A
May 27, 2011: 11:30 – 12:30 PM

MODERATORS: Thiyaga Thiyagarajan and Nick Woodward*, Department of Energy*

- Don DePaolo, *Center for Nanoscale Control of Geologic CO_2*
- Gary Pope, *Center for Frontiers of Subsurface Energy Security*
- Berend Smit, *Center for Gas Separations Relevant to Clean Energy Technologies*
- Dave Wesolowski, *Fluid Interface Reactions, Structures and Transport Center*

G – Materials in Extreme Environments - Renaissance Ballroom West A

Parallel Scientific Session I - May 26, 2011
Renaissance Ballroom West A

10:15 - 10:35
T-G01 - WHAT SUB-PICOSECOND X-RAY DIFFRACTION WILL TELL US ABOUT THE STRUCTURAL DYNAMICS OF DISPLACEMENT CASCADES
[CDP] Ben Larson, Jon Tischler, Roger Stoller, Yuri Osetskiy, Rad Radhakrishnan, Haixuan Xu, and Don Nicholson
Oak Ridge National Laboratory

10:35 - 10:55
T-G02 - THE EFRC MICROSTRUCTURAL CHARACTERIZATION OF ION IRRADIATED CeO_2
[CMSNF] Peng Xu[1], Clarissa Yablinsky[1] , Anthony Schulte[1], Todd Allen[1], Brent Heuser[2], Jian Gan[2], In-Wook Park[3], John Moore[3], and Jianliang Lin[3]
[1]University of Wisconsin-Madison; [2]University of Illinois; [2]Idaho National Laboratory and [3]Colorado School of Mines

10:55 - 11:15
T-G03 - EFREE ACTIVITY AT THE SPALLATION NEUTRON SOURCE
[EFree] Guthrie Malcolm[1], Boehler Reini[1], Karotsis Georgios[1], Tulk Chris[2], dosSantos Antonio[2], Molaison Jamie[2], Pradhan Neelam[2], Somayazulu Maddury[3], and Strobel Tim[3]
[1]Carnegie Institution; [2]Oak Ridge National Laboratory and [3]Carnegie Institution

11:15 - 11:35
T-G04 - BENCHMARK PREDICTIONS OF STRUCTURAL MATERIALS: THE CASE OF ALUMINUM
[CDP] Randolph Q. Hood[1], P. R. C. Kent[2], and Fernando A. Reboredo[3]
[1]Lawrence Livermore National Laboratory; [2]Oak Ridge National Laboratory and [3]Oak Ridge National Laboratory

11:35 - 11:55
T-G05 - COMPETING EFFECTS OF GRAIN BOUNDARIES IN RADIATION DAMAGE RESPONSE OF CU
[CMIME] Blas Uberuaga[1], Xian-Ming Bai[2], Richard Hoagland[1], Arthur Voter[2], and Mike Nastasi[2]
[1]Los Alamos National Laboratory and [2]Idaho National Laboratory

11:55 - 12:15
T-G06 - TOWARD A QUANTITATIVE UNDERSTANDING OF SINGLE DEFECT PHYSICS CONTROLLING MECHANICAL BEHAVIOR
[CDP] George M. Pharr[1], Yanfei Gao[1], Easo P. George[1], K.S. Kumar[2], Michael J. Mills[3], B.C. Larson[4], Andrew M. Minor[5], Ian M. Robertson[6], and Eliot D. Specht[7]
[1]University of Tennessee and Oak Ridge National Laboratory; University of Tennessee and Oak Ridge National Laboratory; Oak Ridge National Laboratory and University of Tennessee ; [2]Brown University; [3]The Ohio State University; [4]Oak Ridge National Laboratory; [5]University of California Berkeley; [6]University of Illinois and [7]Oak Ridge National Laboratory

Parallel Scientific Session II - May 26, 2011
Renaissance Ballroom West A

1:45 - 2:05
T-G07 - ACTINIDE MATERIALS UNDER THE EXTREME CONDITIONS OF TEMPERATURE, PRESSURE AND INTENSE RADIATION FIELDS
[MSA] Maik Lang
University of Michigan

2:05 - 2:25
T-G08 - CHARACTERISTIC INTERFACES IN METALLIC COMPOSITES SYNTHESIZED BY SEVERE PLASTIC DEFORMATION
[CMIME] Irene Beyerlein[1], Nathan Mara[1], Jian Wang[1], Jon Ledonne[2], Tony Rollett[2], Nhon Vo[3], Pascal Bellon[3], Bob Averback[3], Ruifeng Zhang[4], and Keonwook Kang[4]
[1]Los Alamos National Laboratory [2]Carnegie Mellon University; [3]University of Illinois; [4]Los Alamos National Laboratory and Los Alamos National Laboratory

2:25 - 2:45
T-G09 - NUCLEAR FUEL THERMAL CONDUCTIVITY INSIGHTS FROM PHONONS IN UO2
[CMSNF] Judy Pang[1], Alexsandr Chernatynskiy[2] , Bill Buyers[3] , Mark Lumsden[4] , Bennett Larson[5] , and Simon Phillpot[2]
[1]Oak Ridge National Laboratory; [2]University of Florida ; [3]National Research Council, [4]Chalk River Laboratories, Canada

2:45 - 3:05
T-G10 - ENABLING ATOMIC-SCALE DESIGN OF RADIATION-RESISTANT NANOCOMPOSITES BY TAILORING INTERFACES
[CMIME] Michael Demkowcz[1], Amit Misra[2], Michael Nastasi[2], and Richard Hoagland[2]
[1]MIT and [2]Los Alamos National Laboratory

3:05 - 3:25
T-G11 - A NOVEL SUPERHARD SP3-BONDED NON-CRYSTALLINE CARBON ALLOTROPE
[EFree] Yu Lin, Li Zhang[1] , Ho-kwang Mao[2], Paul Chow[3], Yuming Xiao[3], Maria Baldini[3], Jinfu Shu, and Wendy L. Mao[1]
[1]Stanford University; [2]Carnegie Institution of Washington and [3]Carnegie Institution of Washington

G. Materials in Extreme Environments Close-Out Panel
May 27, 2011: 9:00 – 10:00 AM
Renaissance Ballroom East

MODERATORS: John Vetrano and John Miller, *Department of Energy*

- Malcolm Stocks, *Center for Defect Physics in Structural Materials*
- Rus Hemley, *Center for Energy Frontier Research in Extreme Environments*
- Mike Demkowicz, *Center for Materials at Irradiation and Mechanical Extremes*
- Todd Allen, *Center for materials Science of Nuclear Fuel*

H – Effective and Sustainable Materials Design: Integration of Computation, Theory and Experiment
Renaissance Ballroom West A

Parallel Scientific Session I - May 26, 2011
Renaissance Ballroom West A

10:15 - 10:55
T-H01 - INTEGRATION OF NOVEL SYNTHESES, EXPERIMENTS AND MOLECULAR MODELING REVEALS FUNDAMENTAL PROPERTIES OF ELECTRODE/ELECTROLYTE INTERFACES
[FIRST] David J. Wesolowski[1], Sheng Dai[1], and Peter T. Cummings[2]
Oak Ridge National Laboratory and Vanderbilt University

10:55 - 11:15
T-H02 - POWER GENERATION FROM SOLID FUELS IN SOLID OXIDE FUEL CELL WITH MOLTEN ANTIMONY ANODE
[CCEI] Abhimanyu Jayakumar[1], Rainer Kangas[1], Sounak Roy[2], Ashay Javadekar[2], Douglas J. Buttrey[2], John M. Vohs[3], and Raymond J. Gorte[3]
[1]University of Pennsylvania; [2]University of Delaware and [3]University of Pennsylvania

11:15 - 11:35
T-H03 - MODELING LI^+ DIFFUSION IN BATTERY MATERIALS
[CST] Graeme Henkelman, Phani Dathar, Penghao Xiao, Keith J. Stevenson, Arumugam Manthiram, and John B. Goodenough
University of Texas at Austin

11:35 - 11:55
T-H04 - ELECTROCATALYTIC REDUCTION OF CO_2 TO METHANOL AT CU-BASED SURFACES
[CALCD] John Flake[1], Maoming Ren[1], Ziyu Zhang[1], Minh Le[1], Phillip Sprunger[1], Richard Kurtz[1], Gregory Griffin[1], Ullie Diebold[2], Susan Sinnott[3], Aravind Asthagiri[4], and Michael Janik[5]
Louisana State University; [2]Vienna University of Technology; [3]University of Florida; [4]Ohio State University and [5]Pennsylvania State University

11:55 - 12:15
T-H05 - HOMOGENEOUS AND HETEROGENEOUS METAL OXO INTERMEDIATES IN PHOTOCATALYTIC AND HIGH-TEMPERATURE HYDROCARBON FUNCTIONALIZATION CYCLES
[CCHF] William Goddard[1], Robert Bergman[2], Robert Crabtree[3], Thomas Cundari[4], John Groves[5], Brent Gunnoe[6], and Thomas Meyer[7]
[1]California Institute of Technology; [2]University of California at Berkeley; [3]Yale University; [4]University of North Texas; [5]Princeton University; [6]University of Virginia and [7]University of North Carolina

Parallel Scientific Session II - May 26, 2011
Renaissance Ballroom West A

1:45 - 2:05
T-H06 - CHEMICAL NETWORKS: THE WIRED" UNIVERSE OF ORGANIC CHEMISTRY"
[NERC] Kyle J.M. Bishop[1], Aaron M. Drews[1], Mikolaj Kowalik[1], and Bartosz A. Grzybowski[2]
[1]Pennsylvania State University and [2]Northwestern University

2:05 - 2:25
T-H07 - COMPUTATIONAL MODELING OF ACTINIDE COMPOUNDS: FROM CLUSTERS TO COMPLEX CRYSTAL STRUCTURES
[MSA] Mark Asta[1], Udo Becker[2], Laura Gagliardi[3], Niels Gronbech-Jensen[4], Ed Maginn[2], and William J. Weber[5]
[1]University of California, Berkeley and [2]University of California, Davis; [3]University of Michigan; [4]University of Minnesota; [2]University of California, Davis and [5]University of Notre Dame

2:25 - 2:45
T-H08 - CAN MATERIALS BE DESIGNED FOR SPECIFIC TARGET PROPERTIES?
[CID] Alex Zunger, David Ginley, and Larry Kazmerski
NREL

2:45 - 3:05
T-H09 - ETHANOL SYNTHESIS FROM SYN-GAS: HOW SURFACE DIFFUSION OF INTERMEDIATES IMPACTS THE PRODUCT DISTRIBUTIONS PREDICTED FOR BIMETALLIC CATALYSTS
[CALCD] David Bruce, Ming He, and James McAliley
Clemson University

3:05 - 3:25
T-H10 - IACT - COMPUTATION AND THEORY FOR CATALYST DESIGN
[IACT] Linda Broadbelt
Northwestern

3:25 - 3:45
T-H11 - EXPLORING GRAPHENE MOIRE-SUPPORTED CLUSTERS AS A NEW CATALYTIC MATERIAL PLATFORM
[CALCD] D. Wayne Goodman[1], Li Liu[1], Zihao Zhou[1], Feng Gao[1], Lymarie Semidey-Flecha[2], Ye Xu[2], Dieh Teng[3], David Sholl[3], Philip Sprunger[4], and Ward Plummer[4]
[1]Texas A&M University; [2]Oak Ridge National Laboratory [3]Georgia Institute of Technology; Georgia Institute of Technology and [4]Louisiana State University

H. Effective and Sustainable Materials Design: Integration of Computation, Theory and Experiment Close-Out Panel
May 27, 2011: 8:00 – 9:00 AM
Renaissance Ballroom East

MODERATORS: Mark Pederson and Andy Schwartz*, Department of Energy*

- Chris Marshall, *Institute for Atom-efficient Chemical Transformations*
- Jerry Spivey, *Center for Atomic-Level Catalyst Design*
- Xiayang Zhu, *Understanding Charge Separation and Transfer at Interfaces in Energy Materials*
- Vidvuds Ozolins, *Molecularly Engineered Energy Materials*

I – New Tools and Methods for Materials Synthesis and Characterization
Renaissance Ballroom West B

Parallel Scientific Session III - May 26, 2011
Renaissance Ballroom West B

4:00 - 4:20
T-I01 - MODULATING THE REACTIVITY OF MOLECULAR CATALYSTS FOR CH FUNCTIONALIZATION BY PROTON TRANSFER WITH NON-INNOCENT LIGANDS
[CCHF] Roy A. Periana[1], Brian G. Hasihiguchi[1], Steven M. Bischof[1], Kapil S. Lokare[1], Claas H. Hovelmann[1], Robert J. Nielsen[2], Kenneth J. H. Young[3], and William A. Goddard, III[2]
[1]The Scripps Research Institute; [2]California Institute of Technology and [3]University of Southern California

4:20 - 4:40
T-I02 - SYNTHESIS OF NANOSTRUCTURED CATALYSTS FOR BIOMASS CONVERSION
[IACT] Christopher Marshall[1], Eric Stach[2], Fabio Ribeiro[3], Jeffrey Greeley[1], Justin Notestein[4], Kenneth Poeppelmeier[1], Larry Curtiss[1], Mayfair Kung[4], Peter Stair[4], Randy Winans[4], SonBinh Nguyn[4], and Jeffrey Elam[1]
[1]Argonne; [2]BNL; [3]Purdue; Argonne and [4]Northwestern

4:40 - 5:00
T-I03 - DEVELOPMENT OF CATALYSTS FOR SELECTIVE FUNCTIONALIZATION OF HYDROCARBONS
[CCHF] T. Brent Gunnoe[1], Jeremy Andreatta[1], Bradley A. McKeown[1], Victor S.-Y. Lin[2], Brian G. Trewyn[2], Hung-Ting Chen[2], and Thomas R. Cundari[3]
[1]University of Virginia; [2]Iowa State University and [3]University of North Texas

5:00 - 5:20
T-I04 - SEEING CELLULOSE IN PLANT CELL WALLS AND LIGNOCELLULOSIC BIOMASS -- SUM-FREQUENCY-GENERATION (SFG) VIBRATION SPECTROSCOPY STUDY
[CLSF] Seong H. Kim[1], Christopher Lee[1], Anna L. Barnette[1], Yong Bum Park[1], Daniel J. Cosgrove[1], Jin Gu[1], Jeffrey M. Catchmark[1], Sunkyu Park[1], Candace Haigler[2] and Eric Roberts[3]
1The Pennsylvania State University [2]North Carolina State University and [3]Rhode Island College

5:20 - 5:40
T-I05 - DYNAMICS OF VOID GROWTH IN IRRADIATION
[CMSNF] Thomas Hochrainer[1], Abdel-Rahman Hassan[1], Peng Xu [2], Todd Allen[2] , and Anter El-Azab[1]
[1]Florida State University; [2]University of Wisconsin-Madison and [3]Florida State University

5:40 - 6:00
T-I06 - NDTB-1: A SUPERTETRAHEDRAL CATIONIC FRAMEWORK MATERIAL FOR SELECTIVE TRAPPING OF RADIOISOTOPES
[MSA] Shauo Wang[1], Evgeny V. Alekseev[2], Juan Diwu[1], William H. Casey[3], Brian L. Phillips[4], Wulf Depmeier[2] and Thomas E. Albrecht-Schmitt[1]
[1]University of Notre Dame; [2]University of Kiel and University of Notre Dame; [3]University of California, Davis and [4]SUNY-Stony Brook

Parallel Scientific Session IV - May 27, 2011
Renaissance Ballroom West B

8:00 - 8:20
T-I07 - ELECTROCHEMICAL STRAIN MICROSCOPY: A NEW PROBE OF LI-ION DYNAMICS IN ELECTRODE MATERIALS
[FIRST] Nina Balke, Leslie Adamczyk, Nancy Dudney, and Sergei Kalinin
Oak Ridge National Laboratory

8:20 - 8:40
T-I08 - NANOSCALE STUDIES OF BATTERY ELECTROCHEMISTRY: IN-SITU TEM AND SPM AND ATOMISTIC MODELING
[NEES] John Sullivan, Jian Yu Huang, Kevin Zavadil, Kevin Leung, Xiao Hua Liu, Arunkumar Subramanian, NIcholas Hudak, and Yang Liu
Sandia National Labs

8:40 - 9:00
T-I09 - COMPLEX OXIDES AND COMPUTATIONAL STUDIES
[EMC2] Joel Brock, Kendra Weaver, Ravishankar Sundararaman, and Tomas Arias
Cornell University

I. New Tools and Methods for Materials Synthesis and Characterization Close-Out Panel
Renaissance Ballroom West B
May 27, 2011: 9:00 – 10:00 AM

MODERATORS: Jeff Krause and Helen Kerch, *Department of Energy*

- Nina Balke, *Fluid Interface Reactions, Structures and Transport Center*
- Peter Burns, *Materials Science of Actinides*
- Bartosz Grybkowski, *Non-equilibrium Energy Research Center*
- Michael Toney, *Center for Inverse Design*