

A. Organic Photovoltaics - Grand Ballroom

Section I - May 26, 2011 - 10:15 – 12:15

Chair: Christopher Bielawski - CST

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 Marks¹, Lin Chen², Luping Yu³, Mark Ratner⁴, and Robert Chang⁴¹*Northwestern U.*; ²*Argonne National Lab.*; ³*U. of Chicago*; ⁴*Northwestern U.***C. Solar Fuels and Biomass – Mt. Vernon Square**

Section I - May 26, 2011 - 10:35 – 12:15

Chair: Jenny Yang - CME

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 Bullock¹, Daniel L. DuBois¹, Michel Dupuis¹, James M. Mayer², Sharon Hammes-Schiffer³, Bruce A. Parkinson⁴, Jenny Y. Yang¹, Michael T. Mock¹, John A. S. Roberts¹, Simone Raugei¹, and Roger Rousseau¹¹*Pacific Northwest National Laboratory*; ²*Pacific Northwest National Laboratory*; ³*Pacific Northwest National Laboratory*;⁴*University of Washington*; ³*Pennsylvania State University*; 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***D. Energy Storage and Transmission - Congressional Hall A & B****Section I - May 26, 2011 - 10:15 – 12:15****Chair: Ashley Predith - NEES**

10:15 - 10:55

T-D01 - ELECTRODE REACTIONS IN LITHIUM ION BATTERIES - FUNDAMENTAL RESEARCH AT NECCES

[NECCES] Clare P. Grey¹, Anton Van Der Ven², Hui-Chia Yu², and Katsuyo Thornton²¹*Stony Brook University*; ²*University of Michigan*

10:55 - 11:15

T-D02 - COLLABORATIVE ENERGY FRONTIER RESEARCH: CONTROLLED SILICON NANOSTRUCTURES FOR LITHIUM STORAGE

[NEES] John Cumings¹ and S. T. Picraux²¹*University 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 Chan¹, Scott Kirklin², Hakim Iddir¹, Kah Chun Lau¹, Jishnu Bhattacharya², David Snyder², Jeff Greeley¹, Chris Wolverton², and Larry Curtiss¹¹*Argonne National Laboratory*; 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*

E. Energy Conservation and Efficiency - Renaissance Ballroom East

Section I - May 26, 2011 - 10:15 – 12:15

Chair: Rachel Goldman - CSTEC

10:15 - 10:55

T-E01 - HIGH PERFORMANCE NANOSTRUCTURED THERMOELECTRIC MATERIALS (NTHEM)

[RMSSEC] Mercouri Kanatzidis¹, Vidvuds Ozolins², David Seiman¹, Chris Wolverton¹, and Sergey Barabash²
¹Northwestern University; ²UCLA

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**G. Materials in Extreme Environments – Renaissance Ballroom West A**

Section I - May 26, 2011 - 10:15 – 12:15

Chair: Ellen Cerreta - CMIME

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 CeO₂[CMSNF] Peng Xu¹, Clarissa Yablinsky¹, Anthony Schulte¹, Todd Allen¹, Brent Heuser², Jian Gan²,
In-Wook Park³, John Moore³, and Jianliang Lin³
¹University of Wisconsin-Madison; ²Idaho National Laboratory; ³Colorado School of Mines

10:55 - 11:15

T-G03 - EFREE ACTIVITY AT THE SPALLATION NEUTRON SOURCE

[EFree] Guthrie Malcolm¹, Boehler Reini¹, Karotsis Georgios¹, Tulk Chris², dosSantos Antonio², Molaison Jamie²,
Pradhan Neelam², Somayazulu Maddury³, and Strobel Tim³
Carnegie Institution; Oak Ridge National Laboratory; and Carnegie Institution;

11:15 - 11:35

T-G04 - BENCHMARK PREDICTIONS OF STRUCTURAL MATERIALS: THE CASE OF ALUMINUM

[CDP] Randolph Q. Hood¹, P. R. C. Kent², and Fernando A. Reboledo³
Lawrence Livermore National Laboratory¹; Oak Ridge National Laboratory²; and Oak Ridge National Laboratory³

11:35 - 11:55

T-G05 - COMPETING EFFECTS OF GRAIN BOUNDARIES IN RADIATION DAMAGE RESPONSE OF CU

[CMIME] Blas Uberuaga¹, Xian-Ming Bai², Richard Hoagland¹, Arthur Voter², and Mike Nastasi²
¹Los Alamos National Laboratory; ²Idaho National Laboratory

11:55 - 12:15

T-G06 - TOWARD A QUANTITATIVE UNDERSTANDING OF SINGLE DEFECT PHYSICS CONTROLLING MECHANICAL BEHAVIOR
 [CDP] George M. Pharr¹, Yanfei Gao¹, Easo P. George¹, K.S. Kumar², Michael J. Mills³, B.C. Larson⁴, Andrew M. Minor⁵, Ian M. Robertson⁶, and Eliot D. Specht⁷

¹University of Tennessee and Oak Ridge National Laboratory; ²University of Tennessee and Oak Ridge National Laboratory; ³Oak Ridge National Laboratory and University of Tennessee; ⁴Brown University; ⁵The Ohio State University; ⁶Oak Ridge National Laboratory; ⁷University of California Berkeley; ⁸University of Illinois; and ⁹Oak Ridge National Laboratory

H. Effective and Sustainable Materials Design: Integration of Computation, Theory and Experiment

Renaissance Ballroom West B

Section I - May 26, 2011 - 10:15 – 12:15

Chair: Frank DiSalvo - emc2

10:15 - 10:55

T-H01 - INTEGRATION OF NOVEL SYNTHESSES, EXPERIMENTS AND MOLECULAR MODELING REVEALS FUNDAMENTAL PROPERTIES OF ELECTRODE/ELECTROLYTE INTERFACES

[FIRST] David J. Wesolowski¹, Sheng Dai¹, and Peter T. Cummings²

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 Jayakumar¹, Rainer Kangas¹, Sounak Roy², Ashay Javadekar², Douglas J. Buttrey², John M. Vohs³, and Raymond J. Gorte³

¹University of Pennsylvania; ²University of Delaware; ³University 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 CO₂ TO METHANOL AT CU-BASED SURFACES

[CALCD] John Flake¹, Maoming Ren¹, Ziyu Zhang¹, Minh Le¹, Phillip Sprunger¹, Richard Kurtz¹, Gregory Griffin¹, Ullie Diebold², Susan Sinnott³, Aravind Asthagiri⁴, and Michael Janik⁵

Louisiana State University; ²Vienna University of Technology; ³University of Florida; ⁴Ohio State University; and ⁵Pennsylvania State University

11:55 - 12:15

T-H05 - HOMOGENEOUS AND HETEROGENEOUS METAL OXO INTERMEDIATES IN PHOTOCATALYTIC AND HIGH-TEMPERATURE HYDROCARBON FUNCTIONALIZATION CYCLES

[CCHF] William Goddard¹, Robert Bergman², Robert Crabtree³, Thomas Cundari⁴, John Groves⁵, Brent Gunnoe⁶, and Thomas Meyer⁷

¹California Institute of Technology; ²University of California at Berkeley; ³Yale University; ⁴University of North Texas; ⁵Princeton University; ⁶University of Virginia; and ⁷University of North Carolina

A. Organic Photovoltaics – Grand Ballroom South

Section II - May 26, 2011 - 1:45 – 3:45

Chair: Colin Nuckolls - RPEMSC

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 Armstrong¹, Erin Ratcliff¹, Brian Zacher¹, Gordon MacDonald¹, Laura Schirra¹, Oliver Monti¹, Xerxes Steirer¹, Dana Olson², Jens Meyer³, Antoine Kahn³, Hyeunseok Cheun⁴, and Bernard Kippelen⁴¹*University of Arizona*; ²*National Renewable Energy Laboratory*; ³*Princeton University*; 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***B. Inorganic Photovoltaics - Grand Ballroom Central**

Section II - May 26, 2011 - 1:45 - 3:25

Chair: Ken Poepelmeier - CID

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

C. Solar Fuels and Biomass – Grand Ballroom North

Section II - May 26, 2011 - 1:45 – 3:45

Chair: Xuemin (Sam) Wang - CABS

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. Nørskov

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 Green¹, David Davidson², Fokion Egoopoulos³, Nils Hansen⁴, Michael Harper¹, Ron Hanson², Stephen Klippenstein⁵, C.K. Ed Law⁶, C. Jackie Sung⁷, Donald Truhlar⁸, and Hai Wang³¹MIT; ²Stanford; ³USC; ⁴Sandia Livermore; ⁵Argonne; ⁶Princeton; ⁷U. Connecticut; ⁸U. Minnesota;

3:25 - 3:45

T-C12 - INTERACTIONS OF CELLULOSE WITH MATRIX POLYSACCHARIDES

[CLSIF] Yong Bum Park, Akira Tabuchi, Lian-Chao Li, and Daniel J. Cosgrove

The Pennsylvania State University

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

Section II - May 26, 2011 - 1:45 – 3:45

Chair: Ken Reifsnider - emc2

1:45 - 2:05

T-D06 - ELECTROCATALYTIC APPROACHES TO VIRTUAL HYDROGEN STORAGE

[CETM] Oana R. Luca¹, Steven J. Konezny¹, Jeremy Praetorius¹, Gary Yeager², Guillermo D. Zappi², David Simone², Grigori L. Soloveichik², John B. Kerr², Judith Stein³, Thomas Miebach², Chris E.D. Chidsey⁴, Victor S. Batista⁵, andRobert H. Crabtree⁵¹Yale University; ²GE Global Research; ³LBNL; ⁴Stanford University; ⁵Yale University

2:05 - 2:25

T-D07 - THERMODYNAMIC AND ELECTROCHEMICAL STUDIES ON ORGANIC FUELS

[CETM] Davide L. Simone¹, Thomas Miebach¹, Matthew Rainka¹, Robert H. Crabtree², and Grigori L. Soloveichik¹
¹GE Global Research; ²Yale University

2:25 - 2:45

T-D08 - NANOSCALE CONTROL OF THERMODYNAMIC POTENTIALS

[CNEEC] Bruce Clemens¹, Fritz Prinz¹, David Goldhaber-Gordon¹, Robert Sinclair¹, John Vajo², Ping Liu², Sung Chul Lee¹, Chia-Jung Chung¹, James Donough¹, Jang Wook Choi¹, Men Young Lee¹, James Williams¹, Phil Van Stockum¹, James Mack¹, Jun Liu², Adam Gross², Elena Sherman², and Sky Mahoney²
¹Stanford University; ²HRL Laboratories

2:45 - 3:05

T-D09 - EMC²: 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 Lynch¹, Min Kyu Song¹, Kevin Blinn¹, Lei Yang¹, Mostafa El-Sayed¹, Feng Liu², Andreas Heyden³, Anil Virkar², Ken Reifsnider³, and Meilin Liu¹
Ga Tech; ²University of Utah; ³USC; 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**E. Energy Conservation and Efficiency - Renaissance Ballroom East**

Section II - May 26, 2011 - 1:45 – 3:45

Chair: Michael Coltrin - SLS

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 Virkar¹, Wilson Chiu², Kenneth Reifsnider³, Prasun Majumder³, Fazole Rabbi³, MD. Raihan³, and Qianlong Liu³
¹University of Utah; ²University of Connecticut; ³University of South Carolina

2:25 - 2:45

T-E07 - UNDERSTANDING EFFICIENCY LIMITATIONS OF LEDs FOR SOLID-STATE LIGHTING

[SLS] Mary Crawford¹, Weng Chow¹, Daniel Koleske¹, Normand Modine¹, Andrew Armstrong¹, Tania Henry¹, Jeffrey Tsao¹, Qi Dai², Jaehee Cho², and E. Fred Schubert²
¹Sandia National Laboratories; ²Rensselaer 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***G. Materials in Extreme Environments – Renaissance Ballroom West A**

Section II - May 26, 2011 - 1:45 – 3:45

Chair: Anter El-Azab - CMSNF

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 Beyerlein¹, Nathan Mara¹, Jian Wang¹, Jon Ledonne², Tony Rollett², Nhon Vo³, Pascal Bellon³, Bob Averback³, Ruifeng Zhang⁴, and Keonwook Kang⁴¹Los Alamos National Laboratory; ²Carnegie Mellon University; ³University of Illinois; ⁴Los 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 Pang¹, Alexandr Chernatynskiy², Bill Buyers³, Mark Lumsden⁴, Bennett Larson⁵, and Simon Phillpot²¹Oak Ridge National Laboratory; ²University of Florida; ³National Research Council; ⁴Chalk River Laboratories, Canada;

2:45 - 3:05

T-G10 - ENABLING ATOMIC-SCALE DESIGN OF RADIATION-RESISTANT NANOCOMPOSITES BY TAILORING INTERFACES

[CMIME] Michael Demkowcz¹, Amit Misra², Michael Nastasi², and Richard Hoagland²¹MIT; and ²Los Alamos National Laboratory

3:05 - 3:25

T-G11 - A NOVEL SUPERHARD SP³-BONDED NON-CRYSTALLINE CARBON ALLOTROPE[EFree] Yu Lin, Li Zhang¹, Ho-kwang Mao², Paul Chow³, Yuming Xiao³, Maria Baldini³, Jinfu Shu, and Wendy L. Mao¹¹Stanford University; ²Carnegie Institution of Washington; ³Carnegie Institution of Washington;**H. Effective and Sustainable Materials Design: Integration of Computation, Theory and Experiment****Renaissance Ballroom West B**

Section II - May 26, 2011 - 1:45 – 3:45

Chair: Roy Periana - CCHF

1:45 - 2:05

T-H06 - CHEMICAL NETWORKS: THE WIRED" UNIVERSE OF ORGANIC CHEMISTRY"

[NERC] Kyle J.M. Bishop¹, Aaron M. Drews¹, Mikolaj Kowalik¹, and Bartosz A. Grzybowski²¹Pennsylvania State University; ²Northwestern University

2:05 - 2:25

T-H07 - COMPUTATIONAL MODELING OF ACTINIDE COMPOUNDS: FROM CLUSTERS TO COMPLEX CRYSTAL STRUCTURES

[MSA] Mark Asta¹, Udo Becker², Laura Gagliardi³, Niels Gronbech-Jensen⁴, Ed Maginn², and William J. Weber⁵¹University of California, Berkeley and ²University of California, Davis; ³University of Michigan; ⁴University of Minnesota;²University of California, Davis; ⁵University 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 Goodman¹, Li Liu¹, Zihao Zhou¹, Feng Gao¹, Lymarie Semidey-Flecha², Ye Xu², Dieh Teng³, David Sholl³, Philip Sprunger⁴, and Ward Plummer⁴¹Texas A&M University; ²Oak Ridge National Laboratory ³Georgia Institute of Technology; *Georgia Institute of Technology*; ⁴Louisiana State University**A. Organic Photovoltaics – Grand Ballroom South****Section III - May 26, 2011 - 4:00 – 6:00****Chair: Morris Bullock - CME**

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 Thompson¹, Barry C. Thompson¹, Stephen Bradforth¹, Sean Roberts¹, Matthew Whited¹, Robert McAnally¹, Beate Burkhart¹, Stephen Forrest², and Jeremy Zimmerman²¹University of Southern California; ²University 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 Dupuis¹, Simone Raugei¹, Roger Rousseau, Shentan Chen, M.H. Ho, R. Morris Bullock, Daniel L. DuBois, Jenny Y. Yang, Sharon Hammes-Schiffer², Alexander V. Soudackov², Samantha Horvath², and Laura E. Fernandez²¹Pacific Northwest National Laboratory; ²Pennsylvania 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

B. Inorganic Photovoltaics – Grand Ballroom Central

Section III - May 26, 2011 - 4:00 – 6:00

Chair: Thomas Jaramillo - CNEEC

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 Keszler¹, John Wager¹, and Liping Yu²¹Oregon State University ²NREL

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, MIT

C. Solar Fuels and Biomass – Grand Ballroom North

Section III - May 26, 2011 - 4:00 – 6:00

Chair: Candace Haigler - CLSF

4:00 - 4:40

T-C13 - A ROADMAP FOR SELECTIVE DECONSTRUCTION OF LIGNOCELLULOSIC BIOMASS TO ADVANCED BIOFUELS AND USEFUL CO-PRODUCTS

[C3Bio] Maureen C McCann¹, Mahdi Abu-Omar¹, Joe Bozell², and Peter Ciesielski³¹Purdue University; ²University of Tennessee; ³NREL

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. Haigler¹, Rami Alkhatib¹, Mark J. Grimson², James D. Kubicki³, Le Li¹, Antonin Marek¹, Mohamed Naseer³, Ali Mohamed³, Tuyen Nguyen¹, Latsavongsakda Sethaphong¹, Abhishek Singh¹, Alex I. Smirnov¹, Maxim A. Voinov¹, and Yaroslava G. Yingling¹¹North Carolina State University, ²North Carolina State University; ³Texas Tech University; ³The 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 Saliccioli, Weiting Yu, Mark Barteau, Jingguang Chen, and Dion Vlachos*University of Delaware***D. Energy Storage and Transmission – Congressional Hall A & B**

Section III - May 26, 2011 - 4:00 - 6:00

Chair: Andrew Gewirth - CEES

4:00 - 4:20

T-D12 - Pincer Metal Complexes as Electrocatalysts

[CETM] Grigori L. Soloveichik¹, Mark D. Doherty¹, Oltea Siclovan¹, Kenneth P. Zarnoch¹, Alex Usyatinsky¹, Guillermo D. Zappi¹, Oana R. Luca², Steven J. Konezny², Victor S. Batista², and Robert H. Crabtree²¹GE Global Research; ²Yale 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 MILLENNIA-OLD QUESTION

[NERC] H. T. Baytekin¹, A. I. Patashinski¹, M. Branicki², B. Baytekin¹, and B. A. Grzybowski¹¹Northwestern University; ²NYU**E. Energy Conservation and Efficiency – Renaissance Ballroom East**

Section III - May 26, 2011 - 4:00 - 6:00

Chair: Laura Greene - CES

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 Carter¹, Andreas Heyden², Hanno Zur Loye², Prasun Majumdar², Kyle Brinkman², and Fanglin Chen²¹Princeton University; ²University of South Carolina

4:40 - 5:00

T-E13 - DEVELOPMENT OF KINETIC MODELS FOR METHYL-ESTER MOLECULES FOR BIODIESEL MODELING

[CEFRC] Pascal Divart¹, Stephen Dooley¹, Sang Hee Won¹, Frederick L. Dryer¹, Yiguang Ju¹, Emily A. Carter¹, Chung K. Law¹, Fokion Egolfopoulos², Ronald K. Hanson³, Stephen J. Klippenstein⁴, Nils Hansen⁵, and Chih-Jen Sung⁶¹Princeton University; ²University of Southern California; ³Stanford University; ⁴Argonne National Laboratory; ⁵Sandia National Laboratories; and ⁶University 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***F. Carbon Capture and Sequestration – Renaissance Ballroom West A**

Section III - May 26, 2011 - 4:00 – 6:00

Chair: Alexander Navrotsky - MSA

4:00 - 4:20

T-F01 - COMPUTATIONAL CARBON CAPTURE

[CGS] Berend Smit¹, Joe Swisher¹, Maciej Haranczyk², Jeff Neaton², Roberta Poloni¹, Giulia Galli³, Laura Gagliardi⁴, Allison Dzubak⁴, Jihan Kim⁵, and Richard Martin⁵¹UC Berkeley ²LBNL; ³UC Davis; ⁴U Minnesota ⁵LBNL

4:20 - 4:40

T-F02 - CARBONATE MINERAL NUCLEATION PATHWAYS

[NCGC] A. Fernandez-Martinez¹, A. Radha², A.G. Stack³, L. Hedges¹, Y. Hu⁴, A. Loulier⁴, L. J. Banuelos³, G. Rother³, Y.S. Jun⁴, S. Whitlam¹, D. R. Cole⁵, A. Navrotsky², G.A. Waychunas¹, and J.J. DeYoreo¹¹Lawrence Berkeley National Laboratory; ²University of California, Davis; ³Oak Ridge National Laboratory; ⁴Washington University in St. Louis; ⁵Ohio State University

4:40 - 5:00

T-F03 - MOLECULAR, CHEMICAL AND PHYSICAL PROPERTIES OF CO₂-H₂O- ELECTROLYTE-MINERAL SYSTEM[CFSES] Philip Bennett¹, Susan Altman², Bayani Cardenas¹, Randall Cygan², Eugenio Santillan¹, Matthew Kirk², Molly Kent¹, Kuldeep Chaudhary¹ and Wen Deng¹¹University of Texas at Austin; ²Sandia 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 CO₂ SEQUESTRATION IN SUBSURFACE MEDIA[CFSES] Steven Bryant¹, Matt Balhoff¹, David DiCarlo¹, Sanjay Srinivasan¹, Tom Dewers², Hongkyu Yoon², Peter Eichhubl¹, Behdad Aminizadeh-Goharrizi¹, Tie Sun¹, Yashar Mehmani¹, Matt Roberts¹, and Valentina Prigiobbe¹¹University of Texas at Austin; ²Sandia National Laboratories

5:40 - 6:00

T-F06 - APPROACHES TO IMPROVING CARBON DIOXIDE ADSORPTION IN MULTIVARIATE METAL-ORGANIC FRAMEWORKS

[CGS] Omar M. Yaghi

UCLA

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

Section III - May 26, 2011 - 4:00 – 6:00

Chair: *Jingguang Chen - CCEI*

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. Periana¹, Brian G. Hasihiguchi¹, Steven M. Bischof¹, Kapil S. Lokare¹, Claas H. Hovelmann¹, Robert J. Nielsen², Kenneth J. H. Young³, and William A. Goddard, III²¹The Scripps Research Institute; ²California Institute of Technology; ³University of Southern California;

4:20 - 4:40

T-I02 - SYNTHESIS OF NANOSTRUCTURED CATALYSTS FOR BIOMASS CONVERSION

[IACT] Christopher Marshall¹, Eric Stach², Fabio Ribeiro³, Jeffrey Greeley¹, Justin Notestein⁴, Kenneth Poepelmeier¹, Larry Curtiss¹, Mayfair Kung⁴, Peter Stair⁴, Randy Winans⁴, SonBinh Nguyn⁴, and Jeffrey Elam¹¹Argonne; ²BNL; ³Purdue; ⁴Northwestern;

4:40 - 5:00

T-I03 - DEVELOPMENT OF CATALYSTS FOR SELECTIVE FUNCTIONALIZATION OF HYDROCARBONS

[CCHF] T. Brent Gunnoe¹, Jeremy Andreatta¹, Bradley A. McKeown¹, Victor S.-Y. Lin², Brian G. Trewyn², Hung-Ting Chen², and Thomas R. Cundari³¹University of Virginia; ²Iowa State University; ³University 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. Kim¹, Christopher Lee¹, Anna L. Barnette¹, Yong Bum Park¹, Daniel J. Cosgrove¹, Jin Gu¹, Jeffrey M. Catchmark¹, Sunkyu Park¹, Candace Haigler² and Eric Roberts³¹The Pennsylvania State University ²North Carolina State University; ³Rhode Island College

5:20 - 5:40

T-I05 - DYNAMICS OF VOID GROWTH IN IRRADIATION

[CMSNF] Thomas Hochrainer¹, Abdel-Rahman Hassan¹, Peng Xu², Todd Allen², and Anter El-Azab¹¹Florida State University; ²University of Wisconsin-Madison; ³Florida State University

5:40 - 6:00

T-I06 - NDTB-1: A SUPERTETRAHEDRAL CATIONIC FRAMEWORK MATERIAL FOR SELECTIVE TRAPPING OF RADIOISOTOPES

[MSA] Shao Wang¹, Evgeny V. Alekseev², Juan Diwu¹, William H. Casey³, Brian L. Phillips⁴, Wulf Depmeier² and Thomas E. Albrecht-Schmitt¹¹University of Notre Dame; ²University of Kiel and University of Notre Dame; ³University of California, Davis; ⁴SUNY-Stony Brook**A. Organic Photovoltaics – Grand Ballroom South**

Section IV - May 27, 2011 - 8:00 – 9:40

Chair: *Paul Lahti - PHaSE*

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 Ginger¹, Bradley Macleod¹, Andreas Tillack¹, Matthew Gliboff¹, Kristina Knesting¹, Hong Li², Jean-Luc Bredas², Sergio Paniagua², Seth Marder², Matthew Schalnat³, Jeanne Pemberton³, and Mariola Macech³¹University of Washington ; ²Georgia Institute of Technology; ³University 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

B. Inorganic Photovoltaics – Grand Ballroom Central**Section IV - May 27, 2011 - 8:00 – 9:40****Chair: Paul Braun - LMI**

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 Lin¹, Spiros Skourtis², Caleb A Kent¹, Demin Liu¹, Cheng Wang¹, Andre van Rynbach², Xiangqian Hu², Brian Mehl¹, Thomas Meyer¹, John Papanikolas¹, and David Beratan²¹University of North Carolina at Chapel Hill; ²Duke 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 Lany¹, Andriy Zakutayev¹, Thomas Mason², John Wager³, Kenneth Poeppelmeier², John Perkins¹, Joseph Berry¹, David Ginley¹, and Alex Zunger¹¹NREL; ²Northwestern University; ³Oregon State University;

C. Solar Fuels and Biomass – Grand Ballroom North

Section IV - May 27, 2011 - 8:00 – 9:40

Chair: *Nicholas Carpita - C3Bio*

8:00 - 8:20

T-C18 - COMPUTATIONAL AND ENABLING TECHNOLOGIES IN THE CENTER FOR ADVANCED BIOFUELS (CABS)

[CABS] Lisa Carey¹, Rahul Deshpande¹, David Gang², Mahmoud Gargouri², Jeong-Jin Park², Leslie Hicks³, Yair Shachar-Hill¹, Hongxia Wang³, and Baichen Zhang³¹Michigan State University; ²Washington State University ³Donald 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 Wang¹, Maoyin Li¹, Amanda Tawfall¹, Carlotta Peters¹, Brian Fanella², and Xuemin (Sam) Wang¹¹Donald Danforth Plant Science Center; ²University 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 Kodali¹, Joseph W. Springer², Olga Mass³, Lee A. Solomon¹, Tammer A. Farid¹, David F. Bocian⁴, Christine Kirmaier², Jonathan S. Lindsey³, Dewey Holten², Christopher C. Moser¹, and P. Leslie Dutton¹¹University of Pennsylvania; ²Washington University in St. Louis; ³North Carolina State University; ⁴University of California, Riverside;**F. Carbon Capture and Sequestration – Renaissance Ballroom West A**

Section IV - May 27, 2011 - 8:00 – 9:20

Chair: *Susan Altman - CFSES*

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 CO₂-RICH FLUID INTERACTIONS WITH RESERVOIR ROCKS: FROM ATOMIC TO PORE SCALES[NCGC] Gernot Rother¹, Larry Anovitz¹, Ariel Chialvo¹, David Cole², Mirek Gruskiewicz¹, Andrew Stack¹, Lukas Vlcek¹, and Garrison Sposito³¹Oak Ridge National Laboratory; ²Ohio State University; and ³Lawrence 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

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

Section IV - May 27, 2011 - 8:00 – 9:00

Chair: Jason Graetz - NECCES

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

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

G – Materials in Extreme Environments Closeout Panel – *Renaissance Ballroom East***May 27, 2011: 9:00 – 10:00 AM**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*

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*

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*

B – Inorganic Photovoltaics Close-out Panel – *Grand Ballroom Central***May 27, 2011: 11:30 – 12:30 PM**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 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 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 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 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 CO₂*
- 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*