EFRC and DOE Research and Networking Poster Reception
Thursday, May 26, 2011, 6:00 – 7:30 pm

Department of Energy Programs
Thursday, May 26, 2011, 6:00 – 7:30 pm

P1-J1 Advanced Research Projects Agency – Energy (ARPA-E)
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Website: http://arpa-e.energy.gov/

P1-J2 Office of Energy Efficiency and Renewable Energy, Biomass Program
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P1-J4 Office of Environmental Management, Office of Technology Innovation & Development

P1-J5 Office of Fossil Energy
DIVISION OF ADVANCED ENERGY SYSTEMS
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P1-J6 National Nuclear Security Administration, Office of Inertial Confinement Fusion, Laboratory for Laser Energetics at the University of Rochester
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P1-J7 Office of Nuclear Energy, Fuel Cycle Technology
FUEL RESOURCES
Dr. Sheng Dai, National Technical Director, Dais@ornl.gov
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P1-J8 Office of Nuclear Energy, Office of Space and Defense Power Systems
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P1-J9 Office of Science, Advanced Scientific Computing Research
Contact: Barbara Helland, Barbara.Helland@science.doe.gov
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P1-J10 Office of Science, Basic Energy Sciences, Nanoscale Science Research Centers
CENTER FOR FUNCTIONAL NANOMATERIALS
Grace Webster, cfnuser@bnl.gov
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CENTER FOR INTEGRATED NANOTECHNOLOGIES
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CENTER FOR NANOPHASE MATERIALS SCIENCES
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CENTER FOR NANOSCALE MATERIALS
Katie Carrado Gregar, kcarrado@anl.gov
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THE MOLECULAR FOUNDRY
David Bunzow, dabunzow@lbl.gov
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P1-J11 Office of Science, Basic Energy Sciences, Electron-Beam Microcharacterization Centers
ELECTRON MICROSCOPY CENTER FOR MATERIALS RESEARCH (EMCMR)
Dean J. Miller, Director, miller@anl.gov
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NATIONAL CENTER FOR ELECTRON MICROSCOPY
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SHARED RESEARCH EQUIPMENT (SHARE) USER FACILITY
Karren More, Director, morekl1@ornl.gov
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P1-J12 Office of Science, Basic Energy Sciences, Neutron Scattering Facilities
LOS ALAMOS NEUTRON SCIENCE CENTER (LANSCE)
Kurt Schoenberg, kurts@lanl.gov
www.lansce.lanl.gov

SPALLATION NEUTRON SOURCE (SNS)
Judy Trimble, User Program Manager, trimblejl@ornl.gov
http://neutrons.ornl.gov/facilities/SNS/

HIGH FLUX ISOTOPE REACTOR (HFIR)
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P1-J13 Office of Science, Basic Energy Sciences, X-Ray Light Sources

ADVANCED LIGHT SOURCE (ALS) AT LAWRENCE BERKELEY NATIONAL LABORATORY
Scientific Contact: Roger Falcone, RFalcone@lbl.gov
User Program: Susan Bailey, sbailey2@lbl.gov
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ADVANCED PHOTON SOURCE (APS) AT ARGONNE NATIONAL LABORATORY
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LINAC COHERENT LIGHT SOURCE (LCLS) AT SLAC NATIONAL ACCELERATOR LABORATORY
Scientific Contact: Uwe Bergmann, bergmann@slac.stanford.edu
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NATIONAL SYNCHROTRON LIGHT SOURCE (NSLS) AT BROOKHAVEN NATIONAL LABORATORY
Scientific Contact: Qun Shen, qshen@bnl.gov
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STANFORD SYNCHROTRON RADIATION LIGHTSOURCE (SSRL) AT SLAC NATIONAL ACCELERATOR LABORATORY
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P1-J14 SunShot Initiative
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Website: http://www1.eere.energy.gov/solar/sunshot/
EFRC Research Posters
Thursday, May 26, 2011, 6:00 – 7:30 pm

P1-A01 - POLARITON LASING BY INTRA-CAVITY PUMPING AND APPLICATIONS TO ULTRA-FAST OPTICAL MODULATION
[CE] Gleb Akselrod¹, Elizabeth Young¹, Scott Bradley¹, and Vladimir Bulovic¹
¹Massachusetts Institute of Technology

P1-A02 - NONDIABATIC QUANTUM MOLECULAR DYNAMICS SIMULATIONS OF RAPID ENERGY TRANSPORT IN LIGHT-HARVESTING MOLECULES
[CEN] Aiichiro Nakano¹, Rajiv. K. Kalia¹, and Priya Vashishta¹
¹University of Southern California

P1-A03 - PROBING NANOMETER-SCALE ENERGETICS AND ORIENTATION OF MOLECULES AT INTERFACES
[CISSEM] Bradley MacLeod¹, Matthew Schalnat², Dallas Matz², David Ginger¹, Jeanne Pemberton², Sergio Paniagua³, Seth Marder¹, Ajaya Sigdel¹, Joseph Berry¹, Mariola Macech³, Hong Li³, and Jean-Luc Bredas³
¹University of Washington; ²University of Arizona; ³Georgia Institute of Technology and ⁴National Renewable Energy Laboratory

P1-A04 - FULLERENE SELF-ASSEMBLY AS A MEANS TO CONTROL MORPHOLOGY IN POLYMER/FULLERENE BULK HETEROJUNCTION SOLAR CELLS
[MEEM] Christopher Tassone¹, Alexander Ayzner¹, Robert Kennedy¹, Yves Rubin¹, Benjamin Schwartz¹, and Sarah Tolbert¹
¹UCLA

P1-A05 - P3HT/PCBM BULK HETEROJUNCTION ORGANIC PHOTOVOLTAICS: CORRELATING EFFICIENCY AND MORPHOLOGY
[PHaSE] Dian Chen¹, Atsuhiro Nakahara², Dongguang Wei³, and Thomas P. Russell⁶
¹U Mass Amherst; ²Kurashiki Research Center; ³Carl Zeiss NTS LLC and ⁴U Mass Amherst

P1-A06 - SELF-ASSEMBLY OF MIXTURES OF NANORODS IN BINARY, PHASE-SEPARATING BLENDS
[PHaSE] Anna Balazs¹, Li-Tang Yan¹, Egor Maresov¹, and Gavin A Buxton²
¹Univ of Pittsburgh and ²Robert Morris University

P1-A07 - DESIGN, SYNTHESIS, AND CHARACTERIZATION OF CHEMICALLY TAILORED SEMICONDUCTOR NANOPARTICLES
[RPEMSC] Brandi Cossiart¹
¹Columbia University

P1-B01 - NEW TYPE OF SEMICONDUCTOR NANOCRYSTALS AND SEMICONDUCTOR-METAL NANOHYBRIDS FOR EFFICIENT CAPTURE OF SOLAR RADIATION
[CASP] Anshu Pandey¹, Liang Li¹, Bishnu P. Khanal¹, Hsihan Tsai¹, Hsing-Lin Wang¹, Jeffrey M. Pietryga¹, and Victor I. Klimov¹
¹Los Alamos National Laboratory

P1-B02 - CHEMICAL MODIFICATION OF PbSe QUANTUM DOT ARRAYS TO ENHANCE MULTIPLE EXCITON GENERATION AND IMPROVE DEVICE EFFICIENCY
[CASP] Octavi E. Semonin¹, Joseph M. Luther¹, Jianbo Gao¹, Sukgeun Choi¹, Matthew C. Beard¹, and Arthur J. Nozik⁷
¹National Renewable Energy Laboratory

P1-B03 - INGAN/GAN QUANTUM WELL SOLAR CELLS FOR MULTIJUNCTION CONCENTRATOR APPLICATION
[CEEM] Carl Neufeld¹, Samantha Cruz¹, Robert Farrell¹, Michael Iza¹, Stacia Keller¹, Shuji Nakamura¹, Steven DenBaars¹, James Speck¹, and Umesh Mishra¹
¹UCSB

P1-B04 - THREE-DIMENSIONAL NANOJUNCTION DEVICE ARCHITECTURES FOR THIN-FILM PHOTOVOLTAICS
[CNEEC] Arpit Wangperawong¹ and Stacey F. Bent⁷
¹Stanford University
P1-B05 - GIANT ANHARMONIC PHONON SCATTERING IN PbTe: INELASTIC NEUTRON SCATTERING AND PHONON CALCULATIONS
[S3TEC] Olivier Delaire¹, Karol Marty¹, Jie Ma¹, Andrew May¹, Michael McGuire¹, Mao-Hua Du¹, David Singh¹, and Brian Sales¹
¹ORNL

P1-C01 - ULTRAFAST ELECTRON TRANSFER AND PHOTOCHEMICAL HYDROGEN PRODUCTION VIA COVALENT CHROMOPHORE-HYDROGENASE MODEL COMPLEX ASSEMBLIES
[ANSER] Samuel, Amanda P. S.², Co, Dick T.¹, Poddutoori, Premaladha¹, Vagnini, Michael T.¹, and Wasielewski, Michael R.¹
¹Northwestern University

P1-C02 - TAILORING THE ARCHITECTURE OF LIGNIFIED WALLS
[C3Bio] Jeong Im Kim¹, Joe Cox¹, Anna Olek¹, Nick Carpita¹, Maureen McCann¹, Dan Szymanski¹, and Clint Chapple¹
¹Purdue University

P1-C03 - REDUCTIVE ACTIVATION OF FATTY ACID SYNTHASE - A MECHANISM OF REGULATING FATTY ACID BIOSYNTHESIS
[CABS] Hui Chen¹, Huimin Man¹, Jinxia Wu¹, and Oliver Yu¹
¹Donald Danforth Plant Science Center

P1-C04 - USING COMBINED OMICS TOOLS TO INVESTIGATE REGULATION OF METABOLISM IN CHLAMYDOMONADAS
[CABS] Jeong-Jin Park¹, Mahmoud Gargouri¹, and David R. Gang¹
¹Washington State University

P1-C05 - POROUS ANTIMONY TIN OXIDE AS A CONDUCTIVE HOST FOR A FUNCTIONALIZED DNA NANOCAGE
[BISfuel] Chad R. Simmons¹, Xixi Wei¹, Alex Volosin¹, Dominik Schmitt¹, Dong-Kyun Seo¹, Yan Liu¹, and Hao Yan¹
¹Arizona State University

P1-C06 - TOWARDS BIO-INSPIRED MANGANESE-CALCIUM BIMETALLIC CENTERS FOR ELECTROCATALYTIC WATER OXIDATION
[BISfuel] Matthieu Koepf¹, Benjamin D. Sherman¹, Ana L. Moore¹, Devens Gust¹, and Thomas A. Moore¹
¹Arizona State University

P1-C07 - MOLECULAR SIEVE CATALYSTS AND ADSORBENTS FOR EFFICIENT SYNTHESIS AND PURIFICATION PROCESSES OF 5-HYDROXYMETHYL FURFURAL AND ITS ETHERS
[CCEI] Nafiseh Rajabbeigi¹ and Michael Tsapatsis¹
¹University of Minnesota

P1-C08 - ACCURATE COMPUTED THERMOCHEMISTRY AND KINETICS FOR THE REACTION BETWEEN N-BUTANOL AND THE HYDROPEROXYL RADICAL
[CEFRC] Ionut Alecu¹, Tao Yu¹, Jingjing Zheng¹, and Donald Truhlar¹
¹University of Minnesota

P1-C09 - NANOMECHANICAL IMAGING AND MAPPING OF PLANT CELL WALLS BY ATOMIC FORCE MICROSCOPY
[CLSF] Sahar Maghsoudy-Louyeh¹, Tian Zhang¹, Yong Bum Park¹, Daniel J. Cosgrove¹, and Bernhard R. Tittmann¹
¹The Pennsylvania State University

P1-C10 - MOLECULAR ELECTROCATALYSTS FOR HYDROGEN PRODUCTION AND OXIDATION
[CME] Jenny Y. Yang¹, Uriah J. Kilgore¹, Monte Helm¹, Stuart E. Smith¹, John A. Roberts¹, Michael P. Stewart¹, Douglas P. Pool¹, Daniel L. DuBois¹, Mary Rakowski DuBois¹, and R. Morris Bullock¹
¹Pacific Northwest National Laboratory

P1-C11 - Ni(II) COMPLEXES FOR HYDROGEN OXIDATION AND HYDROGEN PRODUCTION: AN AB-INITIO MOLECULAR DYNAMICS INVESTIGATION
[CME] Raugei Simone¹, Chen Shentan¹, Ho Ming-Hsun¹, Rousseau Roger¹, Dupuis Michel¹, DuBois Daniel, and Bullock R. Morris
¹Pacific Northwest National Laboratory
P1-C12 - TEMPERATURE AND IONIC STRENGTH EFFECTS ON THE CHLOROSOME LIGHT-HARVESTING ANTENNA COMPLEX
[PARC] Joseph K.-H. Tang1, Liying Zhu1, Volker S. Urban2, Aaron M. Collins1, Pratim Biswas1, and Robert E. Blankenship1
1Washington University in St. Louis and 2Oak Ridge National Laboratory

P1-C13 - SYNTHESIS AND CHARACTERIZATION OF NANO-BIOHYBRID LIGHT HARVESTING COMPLEXES FOR SOLAR UTILIZATION
[PARC] Woo-Jin An1, Joseph K.H. Tang1, Robert E. Blankenship1, and Pratim Biswas1
1Washington University in St. Louis

P1-C14 - STRUCTURE-PROPERTY RELATIONSHIPS OF PHOSPHONATE-BASED RUTHENIUM(II) BIPYRIDINE DYES ON NANOCRYSTALLINE TiO2 IN AN AQUEOUS ENVIRONMENT
[UNC] Kenneth Hanson1, M. Kyle Brennanman1, Hanliu Luo1, Mike Norris1, Christopher Glasson1, Javier J. Concepcion1, Wenjing Song1, and Thomas J. Meyer1
1UNC

P1-D01 - AUTONOMIC PROTECTION, REPAIR, AND SHUTDOWN OF LI-ION BATTERIES
[CEES] B. Blaiszik1, M. Baginska1, S. Odom1, E. Jones1, S. Kang1, A. Abouimrane2, W. Weng2, Z. Zhang2, J. Moore1, S. White1, N. Sottos1, and K. Amine1
1University of Illinois Urbana Champaign and 2Argonne National Laboratory

P1-D02 - CENTER FOR ELECTRICAL ENERGY STORAGE: AN OVERVIEW
[CEES] M. Thackeray1, P. Fenter1, J. Elam1, L. Curtiss1, H. Kung1, M. Hersam2, A. Gewirth3, and J. Moore3
1Argonne National Laboratory; 2Northwestern University and 3University of Illinois Urbana Champaign

P1-D03 - 'CLICK' IMMOBILIZATION OF CATALYSTS ON ELECTRODES
[CETM] Christopher E. D. Chidsey1, Vadim R. Ziatdinov1, and Ali Hosseini1
1Stanford University

P1-D04 - SURFACE-MODIFIED SILICON NANOSTRUCTURES FOR ENHANCED ENERGY STORAGE
[CST] Justin T. Harris1, Sankaran Murugesan1, Anthony Dylla1, Aaron M. Chockla1, Keith J. Stevenson1, and Brian A. Korgel1
1University of Texas at Austin

P1-D05 - COMPUTATIONAL MODELING OF CAPACITIVE CHARGE STORAGE IN NANOSTRUCTURED OXIDES
[MEEM] Fei Zhou1 and Vidvuds Ozolins1
1UCLA

P1-D06 - EXPLORING ELECTROCHEMICAL PROCESSES OF METAL FLUORIDE/OXYFLUORIDE NANOCOMPOSITES AS CATHODE MATERIALS FOR LI ION BATTERIES
[NECGES] Lin-Shu Du1, James P. Pastore1, Clare P. Grey1, Feng Wang2, Yimei Zhu2, Jason Graetz2, Andrew Gmitter3, Nathalie Pereira1, Glenn G. Amatucci3, Olaf Borkiewicz2, Karena W. Chapman1, and Peter J. Chupas1
1Stony Brook University; 2Brookhaven National Laboratory and 3Rutgers University

P1-E01 - HIGH EFFICIENCY NONPOLAR AND SEMIPOLAR InGaN LEDs
[CEEM] James Speck1, Ravi Shivaraman1, Elison Matioli1, Dobri Simenov1, Steve DenBaars1, Shuji Nakamura1, and Claude Weisbuch1
1UCSB

P1-E02 - TOWARDS ACCURATE THERMOCHEMICAL KINETICS OF BIODIESEL COMBUSTION FROM MULTIREFEERENCE CONFIGURATION INTERACTION CALCULATIONS
[CEFRC] Victor Oyeyemi1, Ting Tan1, Michele Pavone1, and Emily A. Carter1
1Princeton University

P1-E03 - THERMAL ANALYSIS OF HIGH INTENSITY OLEDs USING A TRANSMISSION MATRIX APPROACH
[CEN] Xiangfei Qi1 and Stephen Forrest1
1University of Michigan
P1-E04 - PAIRS AND VORTICES ABOVE AND BELOW TC
[CES] Wai-Kwong Kwok1, Ulrich Welp1, George Crabtree1, Mike Norman1, Juan Atkinson1, Dale Van Harlingen2, Raffi Budakian1, Gregory Polshyn1, Peter Johnson1, and Seamus Davis3,4
1Argonne National Laboratory; 2University of Illinois at Urbana-Champaign; 3Brookhaven National Laboratory and 4Cornell University

P1-E05 - NEW SUPERCONDUCTORS BY DESIGN
[CES] Wai Kwon Kwok1, Tony Leggett2, Laura Greene2, Philip Phillips2, Cedomir Petroic3, Ivan Bozovic3, Peter Abbamonte2, Mao Zheng2, Weicheng Lee2, Yize Li2, James Lee2, and Jim Eckstein2
1Argonne National Lab; 2University of Illinois, Urbana-Champaign and 3Brookhaven National Lab

P1-E06 - ATOMIC CONFIGURATION STUDIES IN CUBIC AND TETRAGONAL YTTRIA-STABILIZED ZIRCONIA
[HeteroFoaM] Hepeng Ding1 and Feng Liu1
1University of Utah

P1-E07 - SOLID-STATE LIGHTING: AN ENERGY ECONOMICS PERSPECTIVE
[SSLS] JY Tsao1, HD Saunders2, JR Creighton1, ME Coltrin1, and JA Simmons1
1Sandia National Laboratories and 2Decision Processes Incorporated

P1-E08 - ON THE SYMMETRY OF EFFICIENCY-VERSUS-CARRIER-CONCENTRATION CURVES IN GAInN/GaN LIGHT-EMITTING DIODES AND RELATION TO DROOP-CAUSING MECHANISMS
[SSLS] Qi Dai1, Qifeng Shan1, Jaehee Cho1, E. Fred Schubert1, Mary H. Crawford2, and Daniel D. Koleske2
1Rensselaer Polytechnic Institute and 2Sandia National Laboratories

P1-F01 - MULTISCALE NUMERICAL METHODS FOR MODELING THE EARTH'S SUBSURFACE
[CFSES] Benjamin Ganis1, Gergina Pencheva1, Mary Wheeler1, Todd Arbogast1, Hailong Xiao1, Guangri Xue1, Mojdeh Delshad1, and Xianhui Kong1
1University of Texas at Austin

P1-F02 - THE COUPLED EFFECTS OF MICROBIAL AND PHYSIC-CHEMICAL PROCESSES ON GEOLOGICAL CARBON STORAGE
[CFSES] Matthew Kirk1, Susan Altman1, Philip Bennett5, Bayani Cardenas6, Thomas Dewers1, Mojdeh Delshad2, Eugenio Santillan2, Wen Deng1, Kuldeep Chaudhary1, and Hongku Yoon1
1Sandia National Laboratories and 2University of Texas at Austin

P1-F03 - FLEXIBLE POROUS FRAMEWORK MATERIALS FOR CARBON CAPTURE
[CGS] Daqiang Yuan1, Jinhee Park1, Weigang Lu1, Jian-Rong Li1, and Hong-Cai Zhou1
1Texas A&M University

P1-F04 - SUB-NANOMETER POROUS MEMBRANES WITH MOLECULAR LEVEL CONTROL OVER PORE CHEMISTRY FOR GAS SEPARATION
[CGS] Rami Hourani1, Nana Zhao1, Rob van der Weegen2, Beverly Zhang1, Brett A. Helms2, and Ting Xu1,2
1University of California, Berkeley and 2Lawrence Berkeley National Laboratory

P1-F05 - BIOLOGICAL AND BIOMIMETIC APPROACHES TO CONTROL CARBONATE MINERALIZATION
[NCGC] Jenny Cappuccio1, Chun-Long Chen1, Joanne Emerson2, Jillian Banfield1, Jim DeYoreo1, Ronald Zuckermann1, and Caroline Ajo-Franklin1
1Lawrence Berkeley National Laboratory and 2University of California, Berkeley

P1-G01 - SYNTHESIS AND CHARACTERIZATION OF HCP METALS WITH CONTROLLED DISLOCATION STRUCTURES
[CDP] Masafumi Tsunekane1 and Sharvan Kumar7
1Brown University

P1-G02 - ELECTROCALORIC EFFECT IN LiNbO3 AS FUNCTIONS OF PRESSURE AND TEMPERATURE
[EFree] Ronald Cohen1, Maimon Rose1, Qing Peng2, and P. Ganesh3
1Carnegie Institution of Washington; 2RPI and 3ORNL
P1-G03 - An Investigation of Radiation Damage Effects on Magnetic Structure of Iron
[CDP] Yang Wang1,2, Malcolm Stocks2, Don Nicholson2, Roger Stoller3, and Aurelian Rusanu3
1Pittsburgh Supercomputing Center, 2Carnegie Mellon University and 3Oak Ridge National Laboratory

P1-G04 - MD Simulations of Free Surface Effects on Atomic Displacement Cascades.
[CDP] Yury Oserskiy1, Andy Calder2, and 1Roger Stoller
1ORNL and 2University of Liverpool

P1-G05 - Simulation of Displacement Cascade Evolution Using Monte Carlo Methods
[CDP] Haixuan Xu1, Yury Oserskiy1, and Roger Stoller7
1Oak Ridge National Lab

P1-G06 - Large Scale Density Functional Theory Modeling of Magnetic Properties of Screw Dislocations in Alpha-Iron
[CDP] Khorgolkhuu Odbadrakh1, Aurelian Rusanu1, George Stocks1, Yang Wang2, German Samolyuk1, and Don Nicholson1
1ORNL and 2PSC

P1-G07 - Four-Dimensional Characterization of Dislocation-Defect Interactions in the TEM
[CDP] Virginia McCreary1, Grace S. Liu1, Martha Briceno1, and Ian M. Robertson7
1University of Illinois, Urbana

P1-G08 - Quantitative Tensile Testing of Mo-Alloy Nano-Fibers in a TEM
[CDP] Chisholm, Claire1,2, Bei, Hongbin2, Oh, Jason4, Syed Asif, S.A.5, Warren, Oden L.5, Shan, Zhiwei5,6, George, Easo P.4,7, and Minor, Andrew M.1,2
1University of California, Berkeley 2Lawrence Berkeley National Laboratory; 4Oak Ridge National Laboratory; 5Hysitron Incorporated; 6Xi'an Jiaotong University and 7University of Tennessee

P1-G09 - Atomistic Modeling and Laser Experiments on Shocked Cu/Nb Nanolayered Composites
[CMIME] Timothy C. Germann1, Ruifeng Zhang1, Jian Wang1, Xiang-Yang Liu1, Shengnian Luo1, Weizhong Han1, Irene Beyerlein1, and Amit Misra7
1LANL

P1-G10 - Grain Boundary Response in Shocked Copper Multicrystals: TEM Characterization and Atomistic Modeling
[CMIME] Alejandro Perez-Bergquist1, Christian Brandl1, Juan Pablo Escobedo1, Carl Trujillo1, Ellen Cerreta1, George Gray III1, and Timothy Germann1
1LANL

P1-G11 - Microstructural and Interfacial Evolutions of Cu-Nb Composites Subjected to Severe Plastic Deformation
[CMIME] E. Ekiz1, N. Q. Vo1, Y. Ashkenazy1,2, P. Bellon3, R. S. Averback1, N. Mara1, M. Pouryazdan Panah4, and H. Hahn5
1University of Illinois at Urbana-Champaign, 2Racah Institute of Physics, 3Hebrew University of Jerusalem; 4Los Alamos National Laboratory; 5Institute of Nanotechnology and Karlsruhe Institute of Technology (KIT)

P1-G12 - The Role of Grain Boundaries in Radiation Damage Evolution in SrTiO3 and TiO2
[CMIME] Aylin Karakuscu1, Blas Uberuaga1, and Chris Stanek1
1Los Alamos National Laboratory

P1-G13 - Analytical Predictions of Heterointerface Interactions with Defects
[CMIME] Kedarnath Kolluri1, Aurelien Vattre1, Abishek Kashinath1, and Michael J. Demkowicz1
1Massachusetts Institute of Technology

P1-G14 - Helium Bubble Formation at Gold Twist Boundaries
[CMIME] Michael Nastas1, Zengfeng Di1, Qiangmin Wei1, Amit Misra1, Richard Hoagland1, Yongqiang Wang1, Jonghan Won1, Xian Ming Bai1, Blas Uberuaga1, Enrique Saez1, Jeffery Hetherly3, and Alfredo Caro1
1LANL
P1-G15 - EFFECTS OF RADIATION AND ANNEALING ON MICROSTRUCTURE AND THERMAL TRANSPORT IN CeO₂
[CMSNF] Clarissa Yablinsky¹, Peng Xu¹, Anthony Schulte¹, David Hurley², Jian Gan³, and Todd Allen³
¹University of Wisconsin-Madison; ²Idaho National Laboratory and ³University of Wisconsin-Madison

P1-G16 - CHARACTERIZATION OF NUCLEAR FUEL WITH 3D ATOM PROBE
[CMSNF] Hunter Henderson¹, Billy Valderrama¹, and In-Wook Park²
¹University of Florida; ²Colorado School of Mines

P1-G17 - DEPOSITION AND POST-ANNEALING OF CERIA FILMS DEPOSITED BY PULSED UNBALANCED MAGNETRON SPUTTERING
[CMSNF] In-Wook Park¹, John Moore¹, Jianliang Lin¹, Michele Manuel², Anter El-Azab³, Todd Allen⁴, Peng Xu⁴, David Hurley⁵, Marat Khafizov⁵, and Jian Gan⁵
¹Colorado School of Mines; ²University of Florida; ³Florida State University; ⁴University of Wisconsin-Madison and ⁵Idaho National Laboratory

P1-G18 - STRUCTURE AND DYNAMICS OF IONIC LIQUID-RHODAMINE 6G SOLUTIONS: NMR, FLUORESCENCE CORRELATION SPECTROSCOPY AND MOLECULAR MODELING
[FIRST] Jianchang Guo¹, Kee Sung Han¹, Song Li², Guang Feng², P. Ganesh³, Paul R.C. Kent³, Sheng Dai³, Edward W. Hagaman³, and Robert W. Shaw³
¹Oak Ridge National Laboratory; ²Vanderbilt University and ³Oak Ridge National Laboratory

P1-G19 - ACTINIDE MATERIALS UNDER EXTREME CONDITIONS: AN EXPERIMENTAL AND COMPUTATIONAL APPROACH
[MSA] Fuxiang Zhang¹, Maik Lang¹, Jiaming Zhang¹, Jianwei Wang¹, Udo Becker¹, and R.C. Ewing¹
¹University of Michigan

P1-G20 - NANO-SCALED MATERIALS UNDER HIGH PRESSURES
[EFree] Lin Wang¹, Wenge Yang¹, Yang Ding¹, Yuyang Sun², Wendy L. Mao³, and Ko-Kwang Mao⁴
¹Carnegie Institution of Washington; ²Argonne National Laboratory; ³Stanford University and ⁴Carnegie Institution of Washington

P1-G21 - HIGH PRESSURE DISCOVERY OF RhH₂ AND AMBIENT PRESSURE RECOVERY
[EFree] Bing Li¹, Yang Ding¹, Wenge Yang¹, and Ho-Kwang (Dave) Mao⁴
¹Geophysical Lab Carnegie Institution of Washington

P1-G22 - PERSISTENCE OF JAHN-TELLER DISTORTION UP TO THE INSULATOR TO METAL TRANSITION IN LaMnO₃
[EFree] Maria Baldini¹, Viktor V. Struzhkin¹, Alex F. Goncharov¹, Paolo Postorino², and Wendy L. Mao³
¹Carnegie Institution of Washington; ²University Sapienza and ³Stanford University

P1-G23 - MELTING OF REFRACTORY MATERIALS IN EXTREME ENVIRONMENTS
[EFree] Amol¹, Liuxiang¹, and Reinhard¹
¹Carnegie Institution of Washington

P1-G24 - MAKING SUPERCONDUCTING TRANSITION TEMPERATURE HIGHER FOR ENERGY APPLICATION
[EFree] Xiao-Jia Chen¹, Viktor V. Struzhkin¹, Alexander F. Goncharov¹, Russell J. Hemley¹, and Ho-Kwang Mao¹
¹Carnegie Institution of Washington

P1-G25 - HIGH PRESSURE CHEMISTRY WITH PERIODIC MESOSTRUCTURES
[EFree] Kai Landskron¹, Paritosh Mohanty¹, Manuel Weinberger¹, Yingwei Fei², Ho-Kwang Mao², Dong Li, Tianbo Liu¹, Neil Coombs¹, Ilke Arslan¹, Nigel Browning³, and Volkan Ortalan⁴
¹Lehigh University; ²Carnegie Institution of Washington; ³University of Toronto and ⁴University of California at Davis

P1-H01 - SYNTHESIS, MODELING AND APPLICATION OF MIXED RARE EARTH OXIDES
[CALCD] Kerry Dooley¹, Michael Janik², Adam Mayernick², Rui Li¹, Matthew Krcha², Joseph Bridges¹, Sumana Adusumilli¹, and Weishi Kong¹
¹Louisiana St. Univ. and ²Pennsylvania St. Univ.
P1-H02 - A COMPUTATIONAL APPROACH TO EVALUATING CATALYST PARTICLE SIZE AND STRUCTURE EFFECTS: COMPARISONS OF HOMOGENEOUS 13-ATOM AND CORE-SHELL 38-ATOM BIMETALLIC CLUSTERS
CALCD Ming He1, James McAliley1, and David Bruce1
1Clemson University

P1-H03 - ROOM TEMPERATURE WATER SPLITTING AT THE SURFACE OF MAGNETITE
CALCD Gareth Parkinson1, Zbyněk Novotný1, Peter Jacobson1, Michael Schmid1, and Ulrike Diebold1
1TU Wien

P1-H04 - MULTI-SCALE MODELING OF CATALYSTS FOR CO2 REDUCTION TO ALCOHOLS
CALCD Aravind Asthagiri1, Susan Sinnott2, Tao Liang2, Tzu-Ray Shan2, Bryce Devine2, Donghwa Lee2, Yu-Ting Cheng2, Beverly Hinojosa2, Simon Phillipot2, Michael Janik1, and John Flake1
1The Ohio State University, 2University of Florida

P1-H05 - A DENSITY FUNCTIONAL THEORY STUDY OF SYNGAS CLEANUP WITH CERIA-BASED RARE EARTH OXIDES
CALCD Matthew Krcha1, Adam Mayernick1, Rui Li3, Kerry Dooley2, and Michael Janik1
1Pennsylvania State University and 2Louisiana State University

P1-H06 - AB INITIO CALCULATION OF REDOX POTENTIALS IN TRANSITION METAL COMPLEXES
CETM Steven J. Konezny1, Mark D. Doherty2, C. Moyses Araujo3, Oana R. Luca4, Robert H. Crabtree3, Grigorii L. Soloveichik5, and Victor S. Batista3
1Yale University, 2GE Global Research and 3Yale University

P1-H07 - INVERSE BAND STRUCTURE OF NANOSTRUCTURES: FINDING ATOMIC CONFIGURATIONS OF Si AND Ge THAT PRODUCE DIRECT GAP SUPERSTRUCTURES
CID Mayeul d'Avezac1, Jun-Wei Luo1, Alex Zunger1, and Stephan Lany1
1NREL

P1-H08 - COMPUTATIONAL DISCOVERY AND HIGH THROUGHPUT SYNTHESIS OF NEW A2BX4 AND ABX SEMICONDUCTORS FOR SOLAR ENERGY
CID Vladan Stevanovic1, Xiwen Zhang1, Andriy Zakutayev1, David Ginley1, and Alex Zunger1
1NREL

P1-H09 - WILL A DOPED WIDE GAP MATERIAL CONDUCT? POLARON VS. BANDS IN SOLAR OXIDES
CID Arjun Nagaraja1, Nicola Perry1, Thomas Mason1, Yang Tang1, Matthew Grayson1, Tula Paudel2, Stephan Lany2, and Alex Zunger2
1Northwestern University and 2NREL

P1-H10 - DESIGN AND DISCOVERY OF A NEW CLASS OF A2B04 P-TYPE CONDUCTORS
CID Giancarlo Trimarchi1, Stephan Lany2, and Kenneth Poeppelmeier1
1Northwestern University and 2NREL

P1-H11 - PHONON LIFETIMES AND THERMAL CONDUCTIVITY IN UO2: AN INTEGRATED SIMULATION AND EXPERIMENTAL APPROACH
CMSNF Aleksandr Chernatynskiy1, Charles Flint1, Judy Pang2, William Buyer3, Bennett Larson2, Mark Lumsden3, Douglas Abernathy2, and Simon Phillipot1
1University of Florida, 2Oak Ridge National Laboratory and 3National Research Council, Chalk River Laboratory

P1-H12 - ORDER-DISORDER TRANSITIONS OF FILLER SPECIES IN SKUTTERUDITES
CSTEK Hyoungchul Kim1, Massoud Kaviany1, John C. Thomas1, Anton Van der Ven1, Ctilad Uher1, and Baoling Huang2
1The University of Michigan and 2Hong Kong University of Science and Technology

P1-H13 - THEORETICAL DEVELOPMENTS AND COMPUTATIONAL MATERIALS SCIENCE FOR ENERGY SYSTEMS
EMC2 Robert Berger1, Kendra Weaver1, Ravishankar Sundararaman2, Tomas Arias2, Craig Fennie2, and Jeff Neaton1
1Lawrence Berkeley Lab and 2Cornell University
P1-H14 - DYNAMICS OF CONFINED WATER AND ELECTROLYTES
[FIRST] Suresh M. Chathoth¹, Eugene Mamontov¹, Alexander I. Kolesnikov¹, Gernot Rother¹, Michael Rouha², Peter T. Cummings³, Pasquale Fulvio¹, X. Wang¹, Sheng Dai¹, Jake McDonough², Volker Presser³, and Yury Gogotsi³
¹Oak Ridge National Laboratory; ²Vanderbilt University and ³Drexel University

P1-H15 - STRUCTURE OF ELECTROLYTES AT CARBON ELECTRODE SURFACES: COUPLING X-RAY AND NEUTRON SCATTERING WITH MOLECULAR MODELING
[FIRST] Hua Zhou¹, Paul Fenter¹, Volker Presser², Jake McDonough², Yury Gogotsi², Matthew Wander², Kevin Shuford², P. Ganesh³, Paul R.C. Kent¹, De-en Jiang³, Gernot Rother³, Ariel Chialvo³, Pasquale Fulvio¹, Sheng Dai¹, Michael Rouha⁴, Guang Feng⁴, and Peter T. Cummings⁴
¹Argonne National Laboratory; ²Drexel University; ³Oak Ridge National Laboratory and ⁴Vanderbilt University

P1-H16 - A QUANTUM CHEMICAL STUDY OF URANYL-PEROXIDE NANOCLUSTER GROWTH MECHANISMS
[MSA] Bess Vlaisavljevich¹, Pere Miro¹, Christopher Cramer¹, Peter C. Burns¹, and Laura Gagliardi
¹University of Minnesota and ²University of Notre Dame

P1-H17 - NANOSCALE CONTROL OF ACTINIDE MATERIALS
[MSA] Peter C. Burns¹, Ginger E. Sigmon¹, Daniel K. Unruh¹, Jie Ling¹, Jie Qiu¹, Christine Wallace⁴, and Jennifer E.S. Szymanski⁵
¹University of Notre Dame

P1-H18 - OXYGEN-EXCHANGE STUDIES OF URANYL COMPLEXES BY NMR
[MSA] Rene L. Johnson¹, Stephen J. Harley¹, C. Andre Ohlin¹, Adele F. Panasci¹, and William H. Casey¹
¹University of California, Davis

P1-H19 - TEMPLATING EFFECTS ON ASSEMBLY OF ACTINIDE NANO-CAPSULES
[MSA] May Nyman¹
¹Sandia National Laboratory

P1-H20 - IRRADIATION-INDUCED GRAIN GROWTH IN NANOCRystalline CERIA
[MSA] Yanwen Zhang¹,², Philip Edmondson¹, Tamás Varga³, Sandra Moll³, Fereydoon Namavar⁴, and William J. Weber¹,²
¹Oak Ridge National Laboratory and ²University of Tennessee, Knoxville; ³Pacific Northwest National Laboratory and ⁴University of Nebraska Medical Center

P1-H21 - USING ATOMIC LAYER DEPOSITION TO HINDER SOLVENT DECOMPOSITION IN LITHIUM ION BATTERIES: FIRST PRINCIPLES MODELING AND EXPERIMENTAL STUDIES
[NEES] Kevin Leung¹, Yue Qi¹, Kevin Zavadii¹, Yoon Seok Jung³, Ann Dillon³, and Andrew Cavanaugh⁴
¹Sandia National Laboratories; ²General Motors; ³National Renewable Energy Laboratory and ⁴University of Colorado

P1-H22 - ELECTRONIC STRUCTURE AND TRANSPORT IN HEUSLER ALLOYS WITH PSEUDO-GAPS
[RMSEC] S. D. (Bhanu) Mahanti¹
¹Michigan State University

P1-H23 - COMBINED COMPUTATIONAL AND EXPERIMENTAL STUDY OF METAL-MEDIATED C-O BOND FORMATION
[CCHF] Joanna R. Webb¹, Travis M. Figg², Mark J. Pouy¹, Bruce M. Prince², T. Brent Gunnoe³, Thomas R. Cundari², and John T. Groves¹
¹University of Virginia; ²University of North Texas and ³Princeton University

P1-H24 - LIGHT INDUCED SELF ASSEMBLY OF SWITCHABLE COLLOIDS
[NERC] Prateek Jha¹, Vladimir Kuzovkov², Bartosz Grzybowski¹, and Monica Olvera de la Cruz¹
¹Northwestern University and ²University of Latvia

P1-H25 - SELF-ASSEMBLY OF SWITCHABLE COLLOIDS
[NERC] Antonio Osorio¹, Igal Szleifer¹, and Sharon Glotzer¹
¹University of Michigan and ²Northwestern University
P1-I01 - MULTIMODAL IMAGING AND MODELLING OF LIGNOCELLULOSIC BIOMASS
[C3Bio] Lee Makowski, Mike Crowley, Michael Himmel, Shi-You Ding, Bryon Donohoe, Jeremy Madden, Garth Simpson, Joytsana Lal, and Ross Harder
1Northeastern University; 2NREL; 3Purdue University and 4Argonne National Laboratory

P1-I02 - HIGH-RESOLUTION X-RAY IMAGING OF DISLOCATIONS AND THEIR INTERACTIONS
[CDP] Eliot Specht, Jon Tischler, Ben Larson, Matt Brandes, Jonghan Kwon, Michael Mills, Wenjun Liu, and Gene Ice
1Oak Ridge National Laboratory; 2Ohio State University and 3Advanced Photon Source

P1-I03 - A NEW APPROACH TO MODELING PORE-SCALE REACTIVE TRANSPORT PROCESSES
[NCGC] Sergi Molins-Rafa, David Trebotich, Chaopeng Shen, and Carl Steefel
1Lawrence Berkeley National Laboratory

P1-I04 - PROBING AND MAPPING ELECTRODE PROPERTIES USING RAMAN SPECTROSCOPY
[HeteroFoaM] Kevin Blinn, Xiaxi Li, Samson Lai, Mostafa El-Sayed, Andreas Heyden, and Meilin Liu
1Georgia Institute of Technology and 2University of South Carolina

P1-I05 - EXPLORING CELLULOSE STRUCTURE BY SFG SPECTROSCOPY
[CLSF] Seong H. Kim, Christopher Lee, Daniel J. Cosgrove, Yong Bum Park, Jeffrey M. Catchmark, Jin Gu, Anna Barnette, and Laura Bradley
1The Pennsylvania State University

P1-I06 - REVEALING SOLAR FUEL GENERATION PATHWAYS USING X-RAYS
[ANSER] Lin X. Chen, David M. Tiede, Michael Mara, Jier Huang, and Oleksandr Kokhan
1Argonne National Laboratory and 2Northwestern University

P1-I07 - DESIGN AND CONTROLLED SYNTHESIS OF SINTERING-RESISTANT Cu/ZnO METHANOL SYNTHESIS CATALYSTS
NANOCONFINED IN MESOPOROUS HOSTS
[CALCD] Dr. Gonzalo Prieto, Jovana Zecevic, Dr. Heiner Friedrich, Prof. Krijn P. de Jong, and Dr. Petra E. de Jongh
1Utrecht University (The Netherlands)

P1-I08 - CROSS-CUTTING RESEARCH THRUSTS IN THE CATALYSIS CENTER FOR ENERGY INNOVATION
[CCEI] Jingguang Chen
1University of Delaware

P1-I09 - FULLY PHASE-COHERENT MULTIDIMENSIONAL SPECTROSCOPY: NOVEL METHODS FOR EXPLORING EXCITON DYNAMICS
[CE] Patrick Wen, Dylan H. Arias, Katherine W. Stone, and Keith A. Nelson
1Massachusetts Institute of Technology

P1-I10 - ADVANCED TOOLS FOR THE DEVELOPMENT OF NOVEL PHOTOVOLTAIC MATERIALS: COMBINATORIAL DEPOSITION AND ANOMALOUS X-RAY DIFFRACTION
[CID] Joanna Bettinger, Yezhou Shi, Andriy Zakutayev, Paul Ndione, Philip Parilla, John Perkins, David Ginley, and Michael Toney
1SLAC National Accelerator Laboratory and 2NREL

P1-I11 - THE TOOLS OF INTERFACE CHARACTERIZATION: THE CENTER FOR INTERFACE SCIENCE: SOLAR ELECTRIC MATERIALS
[CISSEM] Neal Armstrong, Mariola Macech, Gordon MacDonald, Samuel Graham, Yongjin Kim, Jeanne Pemberton, Oliver Monti, Anne Simon, Brooke Beam, Scott Saavedra, Bradley Macleod, and David Ginger
1University of Arizona; 2Georgia Institute of Technology and 3University of Washington

P1-I12 - SPATIALLY RESOLVED THERMAL TRANSPORT IN SURROGATE NUCLEAR FUEL MATERIALS WITH ENGINEERED MICROSTRUCTURES
[CMSNF] Marat Khafizov, David Hurley, In-Wook Park, John Moore, Jianliang Lin, Ryan Deskins, and Anter El-Azab
1Idaho National Laboratory; 2Colorado School of Mines; 3Florida State University and 4Florida State University
P1-I13 - PHASE FIELD MODELING OF VOIDS NUCLEATION AND GROWTH IN IRRADIATED MATERIALS  
[CNSMNF] Srujan Rakkam¹, Thomas Hochrainer¹, Todd Allen², and Anter El-Azab³  
¹Florida State University; ²University of Wisconsin-Madison and ³Florida State University

P1-I14 - CONTROLLED NANOSTRUCTURE FABRICATION FOR PHOTOVOLTAICS AND STORAGE USING STM-ALD  
[CNEEC] Philip Van Stockum¹, James Mack¹, and Fritz Prinz¹  
¹Stanford University

P1-I15 - STRUCTURE OF Li[LiM]O₂ ELECTRODES FOR LITHIUM-ION BATTERIES  
[CST] Karalee Jarvis¹, Zengquiang Deng¹, Eun Sung Lee¹, Penghao Xiao¹, Graeme Henkelman¹, Arumugam Manthiram¹, and Paulo Ferreira¹  
¹University of Texas at Austin

P1-I16 - INSTRUMENTATION FOR NANOSCALE THERMOMETRY AND PICOWATT CALORIMETRY  
[CSTEC] Pramod Reddy¹, Seid Sadat¹, Yi-Jie Chau¹, and Aaron Tan¹  
¹University of Michigan

P1-I17 - BEAM-ASSISTED NANOSTRUCTURING IN THIN FILMS FOR THERMOELECTRICS  
[CSTEC] Michael Warren¹, Yuwei Li¹, Vladimir Stoica¹, Lynn Endicott¹, Guoyu Wang¹, Adam Wood¹, Justin Canniff¹, Roy Clarke¹, Cirad Uher¹, and Rachel Goldman¹  
¹University of Michigan

P1-I18 - UNIQUE CAPABILITIES AND TECHNIQUES: REAL-TIME HIGH-ENERGY X-RAY DIFFRACTION AND REAL-TIME STEM  
[EMC2] Jun Young Ko¹, Yingchao Yu¹, Manuel Plaza¹, Xin Huang¹, Alexander Kazimirov¹, Huolin Xin¹, Robert Hovden¹, Megan Holtz¹, Julia Mundy¹, David Muller¹, Joel Brock¹, and Hector Abruna¹  
¹Cornell University

P1-I19 - IN-SITU S/TEM CHARACTERIZATION OF ELECTRODE/ELECTROLYTE INTERACTIONS FOR ENERGY STORAGE APPLICATIONS  
[FIRST] Raymond R. Unocic³, Leslie A. Adamczyk³, Nancy J. Dudney³, P. Ganesh³, Paul R.C. Kent³, De-en Jiang³, and Karren L. More³  
³Oak Ridge National Laboratory

P1-I20 - SYNTHESIS OF OXIDE ‘NANOBOWLS’ AND ‘ARMOR-COATED’ ACTIVE SITES BY TEMPLATED ALD: A NEW PARADIGM IN HETEROGENEOUS CATALYST SYNTHESIS  
[IACT] Canlas Christian P.¹, Lu, Junling², Ray, Natalie¹, Lee, Sungsik², Winans, Randall², Elam, Jeffrey², Stair, Peter¹, and Notestein, Justin¹  
¹Northwestern University; ²Argonne National Laboratory

P1-I21 - STABILIZATION OF SUPPORTED METAL NANOPARTICLE CATALYSTS USING ATOMIC LAYER DEPOSITION  
[IACT] Junling Lu¹, Hao Feng¹, Peter C. Stair², and Jeffrey W. Elam  
¹Argonne National Laboratory; ²Northwestern University

P1-I22 - DIRECT-WRITE ASSEMBLY OF TRANSPARENT CONDUCTING ELECTRODES FOR FLEXIBLE PHOTOVOLTAICS  
[LMI] Bok Y. Ahn¹, David Lorang¹, Ralph G. Nuzzo¹, and Jennifer A. Lewis¹  
¹University of Illinois

P1-I23 - LIGHT-INDUCED PATTERN FORMATION DURING THE GROWTH OF CHALCOGENIDE FILMS  
[LMI] Bryce Sadtler¹, Joseph Beardslee¹, and Nathan Lewis¹  
¹California Institute of Technology

P1-I24 - THERMOCHEMICAL STUDIES OF ACTINIDE MATERIALS  
[MSA] T. Shvareva¹, C. Armstrong¹, T.J. Park¹, B. Hanken¹, and A. Navrotsky¹  
¹University of California, Davis
P1-I25 - Charge-Storage Processes in Model MnO$_2$-Li-HOPG Systems: Electrochemical SPM and UHV-STM Investigations

[NEES] Satyaveda C. Bharath$^1$, Wentao Song$^1$, Janice E. Reutt-Robey$^1$, and Kevin R. Zavadil$^2$

$^1$University of Maryland and $^2$Sandia National Laboratories

P1-I26 - Laser Enhanced Atom Probe (LEAP) Tomography

[RMSSEC] Ivan D. Blum$^1$, Jiaqing He$^1$, John Androulakis$^1$, David N. Seidman$^1$, Vinayak P. Dravid$^1$, and Mercouri G. Kanatzidis$^1$

$^1$Northwestern University

P1-I27 - Structure of Interfaces for Organic Photovoltaic Materials

[RPEMSC] Theanne Schiros$^1$

$^1$Columbia University

P1-I28 - Studying the Fundamentals of Heat Transport at Short Distances

[S3TEC] Jeremy Johnson$^1$, Kara Manke$^1$, Jeffrey Eliason$^1$, Alexei Maznev$^1$, Keith Nelson$^1$, Austin Minnich$^1$, Maria Luckyanova$^1$, Kimberlee Collins$^1$, Gang Chen$^1$, Adam Jandl$^1$, Mayank Bulsara$^1$, Eugene Fitzgerald$^1$, and Mildred Dresselhaus$^1$

$^1$MIT

P1-I29 - World-Class Instrumentation for Discovering the Fundamentals of Photovoltaic and Solar Fuels Devices

[UNC] Kyle Brennaman$^1$, John Papanikolas$^1$, Thomas Meyer$^1$, Andrew Moran$^1$, Christopher Fecko$^1$, and Malcolm Forbes$^1$

$^1$UNC Chapel Hill

P1-I30 - Facile Pt-to-Pt Methyl Group Transfer in O$_2$(DPMS)PtII(Me(X))-Systems in Water (X = OH$^-$, I$^-$)

[CCHF] Anna V. Sberegaeva$^1$ and Andrei N. Vedernikov$^1$

$^1$University of Maryland

P1-I31 - MSN Supported Pt Complexes for Olefin Hydroarylation

[CCHF] Jeremy R. Andreatta$^1$, Hung-Ting Chen$^1$, T. Brent Gunnoe$^1$, Victor S.-Y. Lin$^3$, and Brian G. Trewyn$^3$

$^1$University of Virginia; $^2$Iowa State University and $^3$Iowa State University

P1-I32 - Hydrocarbon Oxidation in Aqueous and Nonaqueous Medium by Metal Oxo Catalysts

[CCHF] Amit Paul$^1$, Aaron K. Vannucci$^1$, Jonathan F. Hull$^1$, Zuofeng Chen$^1$, Daniel H. Ess$^2$, Michael R. Norris$^1$, Javier J. Concepcion$^1$, and Thomas J. Meyer$^1$

$^1$UNC Chapel Hill and $^2$Brigham Young University

P1-I33 - A BV Type Oxidation for Re-Aryl Oxy-Functionnalization

[CCHF] Steven M. Bischof$^1$, Mu-Jeng Cheng$^1$, Robert J. Nielsen$^1$, T. Brent Gunnoe$^3$, William A. Goddard III$^2$, and Roy A. Periana$^1$

$^1$The Scripps Research Institute; $^2$California Institute of Technology and $^3$University of Virginia

P1-I34 - Thinking Like Nature: Making and Breaking Strong Bonds with Synthetic Metalloporphyrins

[CCHF] Thomas P. Umile$^1$, Wei Liu$^1$, Erika M. Milczek$^1$, Rodney D. Swartz, II$^1$, Dawn Wallace$^1$, and John T. Groves$^1$

$^1$Princeton University

P1-I35 - Dianionic Pyridine Ligands for CH and O$_2$ Activation at a Single Palladium Center

[CCHF] Dao-Yong Wang$^1$ and Andrei N. Vedernikov$^1$

$^1$University of Maryland

P1-I36 - In-Situ Nanoelectrochemistry

[NECCES] Dongli Zeng$^1$, Feng Wang$^1$, Yimei Zhu$^1$, Jason Graetz$^1$, Y. Shirley Meng$^2$, Thomas McGilvray$^2$, Ming-Che Yang$^2$, and Danijel Gostovic$^2$

$^1$Brookhaven National Laboratory and $^2$University of California, San Diego
P1-I37 - Nanomaterials Synthesis with DNA-Programmed Nanoparticle Assembly
[NERC] Macfarlane, Robert\textsuperscript{1}, Jones, Matthew\textsuperscript{1}, and Mirkin, Chad\textsuperscript{1}
\textsuperscript{1}Northwestern University

P1-I38 - High-Pressure Synchrotron X-ray Spectroscopic Methods for Studying 3d and 4f Electronic Transitions
[EFree] Yang Ding\textsuperscript{1}, Daniel Haskel\textsuperscript{2}, Jungho Kim\textsuperscript{2}, Michel Van Veenendaal\textsuperscript{2}, Paul Chow\textsuperscript{1}, Yuming Xiao\textsuperscript{1}, and Ho-kwang Mao\textsuperscript{1}
\textsuperscript{1}Carnegie Institution of Washington; \textsuperscript{2}Argonne National Laboratory

P1-I39 - First Vibrational Sum Frequency Spectroscopic Studies of Energy-Relevant Organic Species on Highly Ordered Pyrolytic Graphite
[FIRST] Jennifer L. Achtyl\textsuperscript{1}, Daniela M. Anjos\textsuperscript{2}, Avram M. Buchbinder\textsuperscript{1}, Yu Cai\textsuperscript{3}, Matthew Neurock\textsuperscript{3}, Steven H. Overbury\textsuperscript{2}, and Franz M. Geiger\textsuperscript{1}
\textsuperscript{1}Northwestern University; \textsuperscript{2}Oak Ridge National Laboratory and \textsuperscript{3}University of Virginia
Poster Session #2  
Friday May 27, 2011, 10:00 – 11:30 am

P2-A01 - UPDATING THE ROAD TO A 10% EFFICIENT ORGANIC PHOTOVOLTAIC: DEVELOPING A MODEL OF EXCITON DISSOCIATION APPROPRIATE TO THE ORGANIC HETEROJUNCTION  
[ANSER]  Brett Savoie¹, Jon Servaites¹, Mark Ratner¹, and Tobin Marks⁷  
¹Northwestern University

P2-A02 - TOWARDS THE RECONSTRUCTION OF EXCITON DYNAMICS VIA FLUORESCENCE AND TRANSMISSION MULTIDIMENSIONAL ELECTRONIC SPECTROSCOPY  
[CE]  Alejandro Perdomo-Ortiz¹, Joel Yuen-Zhou⁷, Sangwoo Shim⁷, Geoffrey A. Lott², Andrew H. Marcus², Jacob J. Krich¹, Jacob Sanders¹, Patrick Rebentrost¹, Stephanie Vallee¹, and Alan Aspuru-Guzik⁷  
¹Harvard University and ²University of Oregon

P2-A03 - ULTRAFAST EXCITONIC PROPERTIES IN SOLAR ENERGY MATERIALS REVEALED BY MULTIDIMENSIONAL SPECTROSCOPY  
[CE]  Dylan Arias¹, Patrick Wen¹, Kathy Stone¹, Brian Walker¹, Sebastiaan Vlaming¹, Mouni Bawendi¹, Robert Silbey¹, Vladimir Bulovic⁷, Jeremy Baumberg², and Keith Nelson⁷  
¹MIT and ²University of Cambridge

P2-A04 - SOLAR POWERED LASERS  
[CE]  Carmel Rotschild¹, Phil Reusswig¹, Matt Tomes², Hiroshi Mendoza¹, Trisha Andrews¹, Tim Swager¹, Tal Carmon², and Marc Baldo¹  
¹MIT and ²University of Michigan, Ann Arbor

P2-A05 - SINGLE FISSION IN ORGANIC SEMICONDUCTOR SOLAR CELLS  
[CE]  Priya Jadhav¹, Aseema Mohanty¹, Jason Sussman¹, Jiye Lee¹, and Marc Baldo⁷  
¹Massachusetts Institute of Technology

P2-A06 - SINGLE INFRARED-EMITTING NANOCRYSTAL FLUORESCENCE DYNAMICS USING SUPERCONDUCTING NANOWIRE DETECTORS  
[CE]  Raoul E. Correa¹, Eric A. Dauler¹, Gautham Nair¹, Si A. Pan¹, Danna Rosenberg¹, Andrew J. Kerman¹, Francesco Marsili¹, Xiaolong Hu¹, Karl K. Berggren¹, and Moungi G. Bawendi⁷  
¹Massachusetts Institute of Technology

P2-A07 - DEVELOPMENT OF TRANSITION METAL OXIDE CONTACTS FOR HIGH PERFORMANCE ORGANIC PHOTOVOLTAICS  
[CEEM]  Andres Garcia¹, Thomas Vanderpool², Gregory C. Welch², Sergio Paniagua-Barrantes³, Seth Marder³, Guillermo C. Bazan², David S. Ginley¹, Joseph J. Berry¹, and Dana Olson³  
¹National Renewable Energy Laboratory; ²University of California, Santa Barbara, California and ³Georgia Institute of Technology

P2-A08 - A MODULAR MOLECULAR FRAMEWORK FOR UTILITY IN SMALL-MOLECULE SOLUTION-PROCESSED ORGANIC PHOTOVOLTAIC DEVICES  
[CEEM]  Gregory Welch¹, Yangming Sun¹, Wei Lin Leong¹, Alan Heeger¹, and Gui Bazan¹  
¹UCSB

P2-A09 - SEMI-RANDOM MULTICHROMOPHORIC RR-P3HT ANALOGUES FOR SOLAR PHOTON HARVESTING  
[CE]  Beate Burkhart¹, Petr P. Khilyabich¹, and Barry C. Thompson¹  
¹University of Southern California

P2-A10 - IMPORTANCE OF THE ORGANIC/INORGANIC INTERFACE IN HYBRID SOLAR CELLS  
[CE]  Matthew J. Greaney¹, David H. Webber¹, Petr Khilyabich¹, Barry C. Thompson¹, and Richard L. Brutchey¹  
¹University of Southern California

P2-A11 - UNDERSTANDING THE INTERPLAY OF SINGLET AND TRIPLET EXCITONS IN SENSITIZED SINGLET FISSION MATERIALS  
[CE]  Sean T. Roberts¹, R. Eric McAnally¹, Cody W. Schlenker¹, Vincent Barlier¹, Joseph N. Mastron¹, Yuyuan Zhang¹, Mark E. Thompson¹, and Stephen E. Bradforth¹  
¹University of Southern California
P2-A12 - WAVEGUIDE SPECTROSCOPIES TO CHARACTERIZE ORGANIC THIN FILM/TRANSPARENT CONDUCTING OXIDE INTERFACES
[CISSEM] Anne Simon1, Zeynep Ozkan Araci1, Hsiao-Chu Lin1, Neal Armstrong1, Scott Saavedra1, Nate Polasek1, Dominic McGrath1, Ajaya Sigdel1, Joseph Berry2, O’ Neil Smith3, Yanrong Shi3, and Seth Marder3
1University of Arizona; 2National Renewable Energy Laboratory and 3Georgia Institute of Technology

P2-A13 - TOWARDS UNDERSTANDING STRUCTURE OF DONOR/ACCEPTOR ORGANIC INTERFACES IN ORGANIC PHOTOVOLTAIC SYSTEMS
[CISSEM] Benjamin Wunsch1, Mariacristina Rumi1, David Bucknall1, Seth Marder1, Jeremy Gantz2, Xerxes Steirer2, and Neal Armstrong2
1Georgia Institute of Technology and 2University of Arizona

P2-A14 - NEW PHthaLOCyANINE MATERIALS FOR ORGANIC PHOTOVOLTAICS AND INTERFACE MODIFICATION
[CISSEM] Edgardo Hernandez1, Mayank Mayukh1, Clarissa Sema1, Jessica Roberts1, Nate Polasek1, Dominic McGrath1, Diogenes Placencia1, Neal Armstrong1, Hsiao-Chu Lin1, Scott Saavedra1, and Erin Ratcliff1
1University of Arizona

P2-A15 - ENERGETICS OF OXIDE SELECTIVE INTERLAYERS AND TRANSPARENT CONDUCTING OXIDES
[CISSEM] Jens Meyer1, Erin Ratcliff2, Ajaya Sigdel3, Xerxes Steirer3, Andres Garcia3, Joseph Berry3, David Ginle3, Dana Olson3, Paul Ndione4, Edwin Widjonarko1, Neal Armstrong1, and Antoine Kahn1
1Princeton University; 2University of Arizona and 3National Renewable Energy Laboratory

P2-A16 - INVESTIGATING TRANSPARENT CONDUCTING OXIDES, AND THE SURFACE INITIATED GROWTH AND CHARACTERIZATION OF POLYMER BRUSHES ON METAL OXIDES
[CISSEM] Judith Jenkins1, Joseph Berry2, Natalia Doubina3, Sergio Paniagua4, Neal Armstrong1, Antoine Kahn5, Jens Meyer1, Seth Marder1, Christine Luscombe1, Ajaya Sigdel5, Paul Ndione6, and Erin Ratcliff1
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P2-A17 - MICROSCOPIC THEORY OF EXCITON DISSOCIATION
[CST] Adam P. Willard1, Loren Kaake1, Jonathan Moussa1, Xiaoyang Zhu1, James R. Chelikowsky1, and Peter J. Rossky1
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P2-A18 - PROBING THE ORIGINS OF CONJUGATED POLYMER MORPHOLOGY: SINGLE MOLECULE STUDIES OF CHAIN INTERACTION IN A P3HT DERIVATIVE TRIBLOCK COPOLYMER
[CST] Johanna Brazard1, Robert J. Ono1, Takuji Adachi1, Songsu Kang1, Joshua C. Bolinger1, Christopher W. Bielawski1, Paul F. Barbara1, and David A. Vanden Bout1
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P2-A19 - NEW SYNTHETIC METHODOLOGIES FOR THE PREPARATION OF DONOR-ACCEPTOR BLOCK COPOLYMERS
[CST] Robert J. Ono1, Jonathan D. Radcliffe1, Songsu Kang1, Young-Gi Lee1, Zong-Quan Wu1, Zicheng Li1, and Christopher W. Bielawski1
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P2-A20 - HIGH EFFICIENCY ORGANIC NANOCRYSTALLINE SOLAR CELLS BASED ON SQUARaine MATERIALS
[CSTEC] Guodan Wei1, Siyi Wang2, Xin Xiao1, C. Kyle Renshaw1, Mark E. Thompson2, and Stephen R. Forrest2
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P2-A21 - PLASMON-ENHANCED EXCITON GENERATION IN ORGANIC PHOTOVOLTAICS
[CSTEC] Matt Sykes1, Kwang Hyup An1, Brian Roberts1, Pei-Cheng Ku1, and Max Shtein1
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P2-A22 - TITANIA BOUND FULLERENES AS CHARGE-TRANSFER MEDIATORS IN ORGANIC PHOTOVOLTAICS
[MEEM] Jordan C. Aguirre1, Bertrand Tremolet de Villers1, Krastina Petrova1, Robert Thompson1, Benjamin J. Schwartz1, Yves Rubin1, and Sarah H. Tolbert1
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P2-A23 - ENHANCING EFFICIENCIES IN DYE SENSITIZED SOLAR CELLS USING NOVEL MOLECULAR ADDITIVES
[PHaSE] Jayant Kumar1, Akshay Kokil1, J. Matthew Chudomel2, Paul Homnick2, and Paul M. Lahti2
1UMass Lowell and 2UMass Amherst
P2-A24 - NANOCOMPOSITES FOR SOLAR CELL APPLICATIONS
[PHaSE] Emily Pentzer\(^1\) and Todd Emrick\(^1\)
\(^1\)University of Massachusetts Amherst

P2-A25 - OPTICAL PROBES OF EXCITON DYNAMICS AND CORRELATION WITH INTERNAL STRUCTURE IN ORGANIC/INORGANIC SEMICONDUCTING NANO PARTICLES
[PHaSE] Joelle Labastide\(^1\), Mina Baghgar\(^1\), Austin Cyphersmith\(^1\), Harihara Venkatraman\(^1\), D. Venkataraman\(^1\), and Michael D. Barnes\(^1\)
\(^1\)UMass Amherst

P2-A26 - THERMODYNAMIC STABILITY AND SELF-ASSEMBLY OF HETEROGENEOUS SEMICONDUCTOR QUANTUM DOTS FOR PHOTOVOLTAIC APPLICATIONS
[PHaSE] Sumeet C. Pandey\(^1\), Jun Wang\(^1\), T. J. Mountzjaris\(^1\), and Dimitrios Maroudas\(^1\)
\(^1\)University of Massachusetts Amherst

P2-A27 - NANOSTRUCTURED ORGANIC PHOTOVOLTAICS FROM CONTORTED CORONENES
[RPEMSC] Alon Gorodetsky\(^1\)
\(^1\)Columbia University

P2-A28 - RE-DEFINING PHOTOVOLTAIC EFFICIENCY THROUGH MOLECULE SCALE CONTROL
[RPEMSC] James Yardley\(^1\), Louis Brus\(^1\), and Tony Heinz\(^1\)
\(^1\)Columbia University

P2-A29 - MEASUREMENTS OF EXCITON DYNAMICS AND SYMMETRIES IN NANOMATERIALS
[RPEMSC] Jonathan Schuller\(^1\)
\(^1\)Columbia University

P2-A30 - NEW CONDUCTING MATERIALS FOR PHOTOVOLTAICS
[RPEMSC] Marshall Cox\(^1\)
\(^1\)Columbia University

P2-B01 - SPECTRAL PHONON TRANSPORT PROPERTIES OF THERMOELECTRIC MATERIALS FROM FIRST-PRINCIPLES CALCULATIONS
[S3TEC] Keivan Esfarjani\(^1\), Zhiting Tian\(^1\), Takuma Shiga\(^1\), Tengfei Luo\(^1\), Junichiro Shiomi\(^2\), Jivtesh Garg\(^1\), Olivier Delaire\(^3\), and Gang Chen\(^1\)
\(^1\)MIT; \(^2\)U Tokyo and \(^3\)ORNL

P2-B02 - PLANAR DYE-SENSITIZED PHOTOVOLTAICS: CAVITY MODE ENHANCEMENT TO 1.0 V
[ANSER] Alex Martinson\(^1\), Noel Giebink\(^1\), Gary Wiederrecht\(^1\), Daniel Rosenmann\(^1\), Michael Pellin\(^1\), and Michael Wasielewski\(^1\)
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P2-B03 - PLASMONIC NANOARCHITECTURES IN PHOTOVOLTAIC AND PHOTOELECTROCHEMICAL DEVICES: ENHANCING LIGHT ABSORPTION THROUGH LOCALIZED SURFACE PLASMON RESONANCE
[ANSER] Erica DeMarco\(^1\), Patrick Shively\(^1\), Michael DeVries\(^1\), Hanning Chen\(^1\), George Schatz\(^1\), Michael Pellin\(^1\), and Joseph Hupp\(^1\)
\(^1\)Northwestern University and \(^2\)Argonne National Laboratory

P2-B04 - SYNTHESIS AND CHARACTERIZATION OF SILICON QUANTUM DOTS AS NOVEL MATERIALS FOR GENERATION III SOLAR CELLS
[CASP] Brian J. Simonds\(^1\), Jeremy D. Fields\(^1\), and P. Craig Taylor\(^1\)
\(^1\)Colorado School of Mines

P2-B05 - SIZE- AND COMPOSITION-DEPENDENT CARRIER MULTIPLICATION STUDIES ON PbSe, PbS AND PbSSE QDS
[CASP] Jayson T. Stewart\(^1\), Aaron G. Midgett\(^1\), Lazaro A. Padilha\(^1\), Danielle K. Smith\(^1\), Jeffrey M. Pietyga\(^2\), Joseph M. Luther\(^1\), Matthew C. Beard\(^3\), Arthur J. Nozik\(^2\), and Victor I. Klimov\(^2\)
\(^1\)Los Alamos National Laboratory; \(^2\)National Renewable Energy Laboratory and \(^3\)University of Colorado
P2-B06 - CHARGE TRANSPORT STUDIES IN PbSe AND PbS NANOCRYSTAL FILMS
[CASP] Matt Law¹, Yao Liu¹, Markelle Gibbs¹, Jason Tolentino¹, and Rachelle Ihly¹
¹University of California, Irvine

P2-B07 - GERMANIUM AND SILICON NANOCRYSTAL THIN-FILM FIELD EFFECT TRANSISTORS PROCESSED FROM SOLUTIONS
[CASP] Zachary Holman¹, Chin-Yi Liu¹, and Uwe Kortshagen¹
¹University of Minnesota

P2-B08 - NANOPATTERNING FOR ADVANCED NANOWIRE PHOTOVOLTAIC DEVICES
[CEN] Anuj R. Madaria¹, Maoqing Yao¹, ChunYung Chi¹, Ruijuan Li¹, Chenxi Lin¹, Ningfeng Hunag¹, P. Daniel Dapkus¹, Michelle Povinelli¹, and Chongwu Zhou¹
¹University of Southern California

P2-B09 - UNDERSTANDING AND EXPLOITING STOICHIOMETRY ASYMMETRY TO CREATE ENHANCED P-TYPE OXIDE SPINELS
[CID] Andriy Zakutayev¹, Tula Paudel¹, John Perkins¹, Nicola Perry², Thomas Mason², Joanna Bettinger³, Yezhou Shi³, Michael Toney³, Stephan Lany¹, David Ginley¹, and Alex Zunger¹
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P2-B10 - CONFORMAL COATING OF SIZE-CONTROLLED LEAD SULFIDE QUANTUM DOTS BY ATOMIC LAYER DEPOSITION AND IRRADIATION
[CNEEC] Hee Joon Jung¹, Neil P. Dasgupta¹, Orlando Trejo¹, Matthew T. McDowell¹, Aaron Hryciw¹, Robert Sinclair¹, and Fritz B. Prinz¹
¹Stanford University

P2-B11 - QUANTUM DOTS: FROM INTERFACES TO INTERMEDIATE BAND ABSORPTION
[CSTEC] Simon Huang¹, Divine P. Kumah¹, Jia-Hung Wu¹, Naj S. Husseini¹, Andrey V. Semichaevsky², Harley T. Johnson¹, Roy Clarke², and Rachel S. Goldman¹
¹University of Michigan and ²University of Illinois

P2-B12 - TRANSFORMATION OPTICS FOR PHOTOVOLTAICS
[LMI] Christopher Gladden¹, Majid Gharghi¹, Ze’ev Abrams¹, and Avi Niv¹
¹UC Berkeley

P2-B13 - NOVEL LIGHT TRAPPING SCHEMES FOR SOLAR CELL APPLICATIONS
[LMI] Emily Kosten¹, Emily Warren¹, and Harry Atwater¹
¹California Institute of Technology

P2-B14 - LIGHT-MATTER INTERACTIONS IN PERIODIC 3D PHOTONIC STRUCTURES
[LMI] Hailong Ning¹, Augustin Mihi¹, Erik Nelson¹, John Rogers¹, and Paul Braun¹
¹UIUC

P2-B15 - SI NANOPHOTONICS: EXTREME LIGHT LOCALIZATION FOR THERMAL AND SOLAR ENERGY CONVERSION
[LMI] Jeffrey T Hill¹, Alexander G Krause¹, Amir Safavi-Naeini¹, and Oskar Painter¹
¹California Institute of Technology

P2-B16 - MECHANISMS OF NANOSTRUCTURE FORMATION AND INSTABILITY IN Bi2Te3
[S3TEC] Chuang Deng¹, Samuel Humphry-Baker¹, Weishu Liu¹, and Christopher Schuh¹
¹MIT

P2-B17 - SOLAR THERMOELECTRIC POWER CONVERSION
[S3TEC] Daniel Kraemer¹, Kenneth McEnaney¹, Bed Poudel², Hsien-Ping Feng¹, J. Christopher Caylor², Bo Yu³, Xiao Yan³, Yi Ma³, Xiaowei Wang³, Dezhi Wang³, Andrew Muto¹, Matteo Chiesa¹, Zhifeng Ren³, and Gang Chen¹
¹MIT; ²GMZ Energy; ³Boston College and ⁴Masdar Institute of Science and Technology

P2-B18 - DESIGN AND GLOBAL OPTIMIZATION OF HIGH-PERFORMANCE SOLAR THERMOPHOTOVOLTAIC SYSTEMS
[S3TEC] Peter Bermel¹, Michael Ghebrebrhan¹, Yi Xiang Yeng¹, Youngsuk Nam¹, Evelyn Wang¹, John Joannopoulos¹, Ivan Celanovic¹, and Marin Soljacic¹
¹MIT
P2-B19 - 2D METALLIC PHOTONIC CRYSTALS AS SELECTIVE EMITTERS FOR SOLAR THERMOPHOTOVOLTAIC ENERGY CONVERSION
[S3TEC] Yi Xiang Yeng, Michael Ghebrebrhan, Peter Bermel, Walker Chan, John Joannopoulos, Marin Soljačić, and Ivan Celanovic
MIT

P2-B20 - NANO STRUCTURED THERMOELECTRIC MATERIALS (Bi,Sb)2(Se,Te,S)3
[S3TEC] Weishu Liu, Qian Zhang, Qing Jie, Yucheng Lan, Kevin Lucas, Cyril Opeil, Zhifeng Ren, Shuo Chen, Chris Carlton, Yang Shao Horn, Mildred Dresselhaus, and Gang Chen
Boston College and MIT

P2-B21 - TOWARDS LIGHT HARVESTING POLYMERS PREPARED BY LIVING POLYMERIZATION FEATURING PENDANT IONIC TRANSITION METAL COMPLEXES (iTMCS)
[UNC] Yali Sun, Egle Puodziukynaite, John R. Reynolds, and Kirk S. Schanze
University of Florida

P2-B22 - ENERGY TRANSFER IN RUTHENIUM AND OSMIUM FUNCTIONALIZED COILED-COIL PePTIDES
[UNC] Stephanie Bettis, Dale Wilger, Christopher Materese, Maria Minakova, Garegin Papoian, John M. Papanikolas, and Marcey L. Waters
University of North Carolina at Chapel Hill

P2-C01 - GROUP 6 DINITROGEN COMPLEXES SUPPORTED BY DIPHOSPHINE LIGANDS CONTAINING PROTON RELAYS: TOWARD THE REDUCTION OF DINITROGEN TO AMMONIA
Pacific Northwest National Laboratory

P2-C02 - MULTI-FUNCTIONAL, BIOMIMETIC POROUS CHALCOGENIDE FRAMEWORKS: ELECTRO- AND PHOTOCATALYSTS FOR SOLAR FUELS
Northwestern University

P2-C03 - CATALYTIC TRANSFORMATION OF BIOMASS POLYSACCHARIDES
[C3Bio] Nate Mosier, Eurick Kim, Joshua Abbott, Craig Barnes, and Mahdi Abu-Omar
Purdue University and University of Tennessee

P2-C04 - METABOLIC FLUX ANALYSIS OF OIL PRODUCTION IN DEVELOPING SEEDS OF CAMELINA
[CABS] Lisa Carey
Michigan State University

P2-C06 - BIOMIMETIC CATALYSTS FOR HYDROGEN EVOLUTION
University of Illinois and Northwestern University

P2-C07 - STRUCTURAL CHARACTERIZATION OF WATER OXIDATION CATALYSTS COVALENTLY BOUND TO TiO2 SURFACES
Yale University

P2-C08 - METAL CATALYZED OXIDATION OF BIOREFINERY LIGNIN
[C3Bio] Diana Cedeno and Joseph J. Bozell
University of Tennessee
P2-C09 - Transition Metal Based Catalyst Development and Catalytic Deconstruction of Native and Engineered Biomass
[C3Bio] Hui Wei¹, Haibing Yang², Joe Cox², Bryon S. Donohoe¹, Peter N. Ciesielski¹, Michael E. Himmel¹, Angus Murphy², Wendy Peer², Maureen McCann², Melvin P. Tucker¹, and Mahdi M. Abu-Omar²
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P2-C10 - Biochemical Mechanisms of Cellulose Biosynthesis
[C3Bio] Anna T. Olek¹, Lake Paul¹, Catherine Rayon¹, Subhangi Ghosh¹, and Nicholas C. Carpita¹
¹Purdue University

P2-C11 - Catalytic Transformations of Lignin Studied by Using a Novel Mass Spectrometric Approach
[C3Bio] Trenton H. Parsell¹, Laura J. Haupert¹, Lucas M. Amundson¹, Benjamin C. Owen¹, Christopher L. Marcum¹, Tiffany M. Jarrell¹, Christopher J. Pulliam¹, Padrmaja Narra¹, Mohammad Sabir Aqueel¹, Nelson R. Vinueza¹, Joseph J. Bozell¹, Hilkka I. Kenttamaa¹, and Mahdi M. Abu-Omar¹
¹Purdue University

P2-C12 - Direct Production of Molecules in the Fuel Range by Selective Tailoring of Biomass Fast-Pyrolysis
[C3Bio] Piotr Gawecki¹, Andrew D. Smeltz¹, Matthew R. Hurl¹, David J. Horton II¹, Nelson R. Vinueza¹, Nicholas J. Nugent¹, Rakesh Agrawal¹, W. Nicholas Delgass¹, Hilkka I. Kenttamaa¹, William E. Anderson¹, and Fabio H. Ribeiro¹
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P2-C13 - Capturing Genetic Diversity for Advanced Biofuels in Camelina
[CABS] Jillian Collins-Silva¹, Rebecca Cahoon¹, and Edgar Cahoon¹
¹University of Nebraska

P2-C14 - Enhancing Photosynthetic Efficiency of Chlamydomonas Reinhardtii
[CABS] Shayani Pieris¹
¹Donald Danforth Plant Science Center

P2-C15 - Analyzing the Induction of Oil Production in Chlamydomonas
[CABS] Rahul Deshpande¹ and Yair Shachar-Hill¹
¹Michigan State University

P2-C16 - Production of Hydrocarbons in Oilseed and Algae
[CABS] Yasuhiro Higashi¹, Xiaohong Feng¹, and Toni M Kutchan¹
¹Danforth Plant Science Center

P2-C17 - Artificial Hydrogenases: Properties of [Ni-Ru(arene)] Complexes in a Peptide Framework
[BISfuel] Arnab Dutta¹ and Anne K. Jones¹
¹Arizona State University

P2-C18 - Preparation of Highly Porous Transparent Antimony-Doped Tin Oxide (ATO) Electrodes for Solar Fuel Production
[BISfuel] Alex M. Volosin¹, Dominik S. Schmitt², and Dong-Kyun Seo¹
¹Arizona State University and ²Johannes Gutenberg University

P2-C19 - Proton-Coupled Electron Transfer in Artificial Photosynthetic Models for Light-Driven Water Oxidation
[BISfuel] Jackson D. Megiatto, Jr. ¹, Benjamin D. Sherman¹, Antaeres' Antoniuk-Pablant¹, Gerdenis Kodis¹, Ana L. Moore¹, Thomas A. Moore¹, and Devens Gust¹
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P2-C20 - Design and Assembly of an Artificial Oxygen-Evolving Complex in DNA Nanostructures
[BISfuel] Kimberly Rendek¹, Chad Simmons¹, Justin Flory¹, Sudipta Biswas¹, Xixi Wei¹, Chenxiang Lin¹, Sandip Shinde¹, Ingo Grojohann¹, Raimund Fromme¹, Giovanna Ghirlanda¹, Hao Yan¹, Yan Liu¹, and Petra Fromme¹
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P2-C21 - MOLTEN METAL ANODES FOR DIRECT CARBON FUEL CELLS
[CCEI] Abhimanyu Jayakumar1, John Vohs1, and Raymond Gorte1
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P2-C22 - CATALYSIS FOR BIOMASS REFORMING
[CCEI] Michael Salciccioli1, Weiting Yu1, Mark Barteau1, Jingguang Chen1, and Dion Vlachos1
University of Delaware

P2-C23 - CATALYTIC STUDIES OF REFORMING OF OXYGENATES
[CCEI] Sarah Tupy1, Tushar Vispute2, George Huber2, Jingguang Chen1, and Dionisios Vlachos1
University of Delaware and UMass-Amherst

P2-C24 - CORRELATING SURFACE SCIENCE WITH FIRST-PRINCIPLES STUDIES OF BIOMASS DERIVATIVES
[CCEI] Weiting Yu1, Mark Barteau1, and Jingguang Chen1
University of Delaware

P2-C25 - RENEWABLE GASOLINE RANGE AROMATICS FROM CATALYTIC FAST PYROLYSIS OF WOODY BIOMASS
[CCEI] Yu-Ting Cheng1 and George W. Huber1
UMass-Amherst

P2-C26 - SOOT FORMATION IN FUEL COMBUSTION - THE ROLE OF AROMATIC DIRADICALS
[CEFRC] Enoch Dames1 and Hai Wang1
University of Southern California

P2-C27 - COMBUSTION KINETICS STUDY OF T-BUTANOL AND ITS PRINCIPAL INTERMEDIATES, I-BUTENE, ACETONE, AND METHANE
[CEFRC] Joseph Lefkowitz1, Joshua Heyne1, Sang Hee Won1, Stephen Dooley1, Hwanho Kim1, Francis Haas1, Saeed Jahangirian1, Frederick Dryer1, and Yiguang Ju1
Princeton

P2-C28 - TURBULENT COMBUSTION OF FUTURE TRANSPORTATION FUELS
[CEFRC] Stephen Pope1, Jacqueline Chen2, Haifeng Wang1, Chun Sang Yoo2, and Gaurav Bansal2
Cornell University and Sandia National Lab

P2-C29 - BIOCHEMICAL CHARACTERIZATION OF GLUCONACETOBACTER HANSENII CELLULOSE SYNTHESIS
[CLSF] Prashanti R. Iyer1, Jeffrey M. Catchmark1, Nicole R. Brown1, and Ming Tien1
The Pennsylvania State University

P2-C30 - DOES XYLOGLUCAN REALLY TETHER CELLULOSE IN PRIMARY CELL WALLS? EVIDENCE FOR A MINOR, STRUCTURAL FORM OF XYLOGLUCAN
[CLSF] Yong Bum Park1 and Daniel J. Cosgrove1
The Pennsylvania State University

P2-C31 - SIZE EFFECT OF CELLULOSE MICROFIBRIL AND ITS INTERACTION WITH HEMICELLULOSE
[CLSF] Zhen Zhao1, Linghao Zhong1, and James D. Kubicki1
The Pennsylvania State University

P2-C32 - HEMICELLULOSE AND PECTIN INTERACTIONS WITH CELLULOSE
[CLSF] Joshua D. Kittle1, Xiaosong Du1, Xiao Zhang1, Chen Qian1, Maeve Budi1, Alan R. Esker1, Feng Jiang1, Maren Roman1, Jing Gu2, and Jeffrey M. Catchmark2
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P2-C33 - AB-INITIO STRUCTURE PREDICTION OF A CELLULOSE SYNTHASE PROTEIN
[CLSF] Latsavongsakda Sethaphong1, Abhishek Singh1, and Yaroslava G. Yingling1
North Carolina State University

P2-C34 - THE USE OF INTERDIGITATED ARRAY (IDA) ELECTRODES TO INVESTIGATE ELECTROCATALYTIC REACTIONS
[CME] Fei Liu1, Yongxin Li1, John A. Roberts1, Dan Dubois2, Morris Bullock2, and Bruce A. Parkinson1
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P2-C35 - NMR STUDIES ON THE ROLE OF PROTON RELAYS IN NICKEL CATALYSTS FOR OXIDATION OR PRODUCTION OF HYDROGEN
[CME] O’Hagan, Molly¹, Shaw, Wendy¹, Yang, Jenny Y.¹, Appel, Aaron M.¹, Rakowski DuBois, M.¹, DuBois, Daniel L.¹, and Bullock, R. Morris¹
¹Pacific Northwest National Laboratory

P2-C36 - MOLECULAR TRANSITION METAL COMPLEXES FOR DIOXYGEN ACTIVATION AND REDUCTION
[CME] Tristan Tronic¹, Colin Carver¹, Johanna Blacquiere¹, Benjamin Matson¹, Werner Kaminsky¹, Tianbiao Lu², Mary Rakowski-DuBois², and James Mayer¹
¹University of Washington and ²Pacific Northwest National Lab

P2-C37 - PLASMONS AND RUST FOR SOLAR ENERGY CONVERSION
[CNEEC] Isabell Thomann¹, Blaise Pinaud¹, Zhebo Chen¹, Bruce M. Clemens¹, Thomas F. Jaramillo¹, and Mark. L. Brongersma¹
¹Stanford

P2-C38 - A STUDY OF OER ON TRANSITION METAL OXIDES
[CNEEC] Monica Garcia Mota¹, Aleksandra Vojvodic², Horia Metiu³, Isabela C. Man⁴, Jan Rossmeisl⁴, and Jens K. Norskov⁵
¹Stanford University, ²SUNCAT Center for Interface Science and Catalysis SLAC National Accelerator Laboratory; ³University of California, Santa Barbara and ⁴Technical University of Denmark

P2-C39 - HYDROGEN PRODUCTION ON NANOSTRUCTURED MoS₂ BY ELECTROCATALYSIS AND SOLAR PHOTOELECTROCHEMISTRY
[CNEEC] Zhebo Chen¹, Hee Joon Jung¹, Robert Sinclair¹, and Thomas F. Jaramillo¹
¹Stanford University

P2-C40 - PROTON-COUPLED ELECTRON TRANSFER AT FLUID-SOLID INTERFACES: MECHANISTIC PATHWAYS FOR ELECTROCATALYTIC AND PHOTOCATALYTIC REACTIONS
[FIRST] Daniela M. Anjos¹, Glen Alliger¹, Alexander I. Kolesnikov¹, Yu Cai², Matthew Neurock², Zili Wu¹, John McDonough³, Yury Gogotsi³, Gilbert M. Brown¹, and Steven H. Overbury¹
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P2-C41 - THE DECOMPOSITION OF FORMIC ACID AND BUTYL FORMATE FOR THE CONVERSION OF BIOMASS TO BIOFUELS
[IACT] Brandon O'Neill¹, Elif Gurbuz¹, and James Dumesic¹
¹University of Wisconsin-Madison

P2-C42 - AN NMR STUDY OF THE MECHANISM OF THE DEHYDRATION OF D-FRUCTOSE USING ¹³C LABELING
[IACT] Jing Zhang¹ and Eric Weitz¹
¹Northwestern University

P2-C43 - HYDROGEN PRODUCTION FROM GLYCEROL: REACTION MECHANISM ANALYSIS VIA KINETICS AND OPERANDO SPECTROSCOPY
[IACT] Paul Dietrich¹, Rodrigo Lobo², Neng Guo², Tianpin Wu², Bradley Fingland², Fabio Ribeiro¹, Nicholas Delgass¹, Jeffrey Miller¹, and James Dumesic³
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P2-C44 - CATALYSTS PREPARED BY ATOMIC LAYER DEPOSITION FOR CONVERSION OF BIOMASS TO CHEMICALS
[IACT] Yomaira J. Pagan-Torres¹, Jean Marcel R. Gallo¹, Dong Wang¹, Hien N. Pham¹, Joseph A. Libera¹, Christopher L. Marshall¹, Jeffrey W. Elam², Abhaya K. Dayte³, and James A. Dumesic¹
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P2-C45 - LIGHT-HARVESTING PIGMENT DISTRIBUTION IN ALGAE AND CYANOBACTERIA DETERMINED BY HYPERSPECTRAL CONFOCAL FLUORESCENCE MICROSCOPY
[PARC] Aaron M. Collins¹, Michelle Liberton², Sangeeta Negi³, Howland D.T. Jones¹, Omar F. Garcia¹, Michael B. Sinclair¹, Himadri B. Pakrasi², Richard T. Sayre³, and Jerilyn A. Timlin¹
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P2-C46 - PARC COMMUNICATION STRATEGIES: STREAMING, ONLINE, AND VIRTUAL
[PARC] Elizabeth Dorland
Washington University in St. Louis

P2-C47 - WINNING THE FUTURE: ENERGY EDUCATION FOR THE NEXT GENERATION
[PARC] Rachel Ruggirello
Washington University in St. Louis

P2-C48 - ENERGY TRANSFER IN PHOTSYNTHETIC LIGHT-HARVESTING COMPLEXES FOR BIO-HYBRID SOLAR UTILIZATION
[PARC] William Bricker and Cynthia Lo
Washington University in St. Louis

P2-C49 - CHROMOPHORE-CATALYST SELF-ASSEMBLED BILAYERS FOR LIGHT DRIVEN CATALYSIS
The University of North Carolina at Chapel Hill

P2-C50 - THE DEVELOPMENT OF CATALYSTS FOR ELECTROCHEMICAL AND PHOTOCHEMICAL CO₂ REDUCTION
The University of North Carolina at Chapel Hill

P2-C51 - CATALYTIC MECHANISM FOR SINGLE-SITE WATER OXIDATION PROCESS: A THEORETICAL STUDY
[UNC] Xiangqian Hu
Duke University

P2-D01 - HIGH POWER NANOSTRUCTURED ANODES, CATHODES AND THERMAL PROTECTANT FOR LI-ION BATTERIES: FABRICATION BY NOVEL BIO-INSPIRED, KINETICALLY CONTROLLED, LOW-TEMPERATURE CATALYSIS
[CEEM] Daniel E. Morse and Hong-Li Zhang
University of California, Santa Barbara

P2-D02 - CHARACTERIZATION OF ENGINEERED GRAPHENES FOR HIGH CAPACITY ELECTRODES
[CEES] Cary M. Hayner and Sudeshna Chattopadhyay
Northwestern University

P2-D03 - THEORETICAL STUDIES OF SURFACES, INTERFACES AND NOVEL MATERIALS IN ELECTRICAL ENERGY STORAGE SYSTEMS
[CEES] Maria Chan, Scott Kirklin, Hakim Iddir, Kah Chun Lau, Jishnu Bhattacharya, David Snydacker, Jeff Greeley, Chris Wolverton, and Larry Curtiss
Argonne National Laboratory and Northwestern University

P2-D04 - FUNDAMENTAL STUDIES OF SILICON LITHIATION FOR BATTERY ANODES
[CEES] Tim Fister, Maria Chan, Paul Fenter, Jeff Greeley, Jason Goldman, Brandon Long, Michael Cason, Ralph Nuzzo, and Andy Gewirth
Argonne National Laboratory and University of Illinois Urbana Champaign

P2-D05 - MICRO/NANO-PHASE CARBON ANODES FOR LITHIUM-ION BATTERIES
[CEES] Vilas G. Pol, Laila Jaber-Ansari, Mark C. Hersam, and Michael M. Thackeray
Argonne National Laboratory and Northwestern University

P2-D06 - DESIGN OF ELECTROLYTES AND MEMBRANES FOR DEHYDROGENATION FUEL CELL SYSTEMS
[CETM] Kyle Clark, Zulima Martin, Tobias Brecht, Peter Driscoll, Xiaobing Zhu, Ravi Potrekar, John B. Kerr, and Gary Yeager
LBNL and GE Global Research
P2-D07 - HOMOGENEOUS REDOX CATALYSIS OF DEHYDROGENATION REACTIONS
[CETM] Leah Rubin1, John Arnold1, John B. Kerr1, Peter Driscoll1, Dan Kellenberger1, Oana R. Luca2, Robert H. Crabtree3, and Guillermo Zappi3
1LBNL; 2Yale University and 3GE Global Research

P2-D08 - APPLICATIONS OF HIGH POTENTIAL QUINONES AND PINCER COMPLEXES FOR VIRTUAL HYDROGEN STORAGE
[CETM] Oana R. Luca1, Steven J. Konezny1, Jeremy M. Praetorius1, Kurt M. Luthy1, Ting Wang1, Grigoriei L. Soloveichik2, Mark D. Doherty1, Davide L. Simone2, Victor S. Batista3 and Robert H. Crabtree3
1Yale University; 2GE Global Research and 3Yale University

P2-D09 - USE OF LIQUID FUEL CELL FOR EVALUATION OF SYSTEM COMPONENTS
[CETM] Tracy Huang1, Lakshmi Krishnan1, Davide Simone1, Mark D. Doherty1, Grigoriei L. Soloveichik1, Guillermo D. Zappi1, Matthew Rainka1, Oltea Siclovan1, Thomas Miebach1, John Kerr2, and Judith Stein1
1GE Global Research and 2LBNL

P2-D10 - INVESTIGATING THE HYSTERESIS OF THE FeF3/Li NANOSCALE ELECTRODE REACTION
[CNEEC] John Vajo1, Jun Liu1, Wen Li1, John Wang1, and Ping liu1
1HRL

P2-D11 - KINETICS OF Li+ DIFFUSION IN OLIVINE PHOSPHATES
[CST] Gopi Krishna Phani Dathar1, Daniel Sheppard1, Nicholas Delone1, Jing Wu1, Keith J. Stevenson1, and Graeme Henkelman1
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P2-D12 - PdCo@Pd/C CORE-SHHELL NANOPARTICLES AND PT-DECORATED PdCo@Pd/C FOR OXYGEN REDUCTION
[EMC2] Deli Wang1, Huolin Xin1, David Muller1, Francis DiSalvo1, and Hector Abruna1
1Cornell University

P2-D13 - FUEL CELL ELECTROCATALYST DEVELOPMENT AND CHARACTERIZATION
[EMC2] Eric Rus1, Hongsen Wang1, Anna Legard1, Michele Tague1, Bruce van Dover1, and Hector Abruna1
1Cornell University

P2-D14 - SOLVENT PROCESSABLE TETRAALKYLAMMONIUM-FUNCTIONALIZED POLYETHYLENE FOR USE AS AN ALKALINE ANION EXCHANGE MEMBRANE
[EMC2] Henry Kostalik, IV1, Timothy Clark1, Nocholas Robertson1, and Geoffrey Coates1
1Cornell University

P2-D15 - BATTERY MATERIALS AND ARCHITECTURES
[EMC2] Michael Lowe1, Zichao Yang1, Jayaprakash Navaneedhakrishnan1, Jennifer Nugent1, Jie Gao1, Hector Abruna1, Lynden Archer1, and Stephen Burkhardt1
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P2-D16 - HIGH THROUGHPUT METHODS FOR ELECTROCATALYST DISCOVERY
[EMC2] Eva Smith1, Michele Tague1, John Gregoire1, Darren Dale1, Anna Legard1, Bruce van Dover1, Frank DiSalvo1, Richard Hennig1, and Hector Abruna1
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P2-D17 - CARBON ONIONS FOR IMPROVED ELECTRICAL ENERGY STORAGE
[FIRST] J. McDonough1, P. Ganesh2, P. Fulvio2, V. Mochalin1, V. Presser1, S. Dai2, P.R.C. Kent2, and Y. Gogotsi1
1Drexel University and 2Oak Ridge National Laboratory

P2-D18 - NANOSTRUCTURED MnO, FOR SUPERCAPACITORS
[HeteroFoam] Min-Kyu Song1, Shuang Cheng1, Feng Liu1, and Meilin Liu1
1Georgia Institute of Technology and 2University of Utah
P2-D19 - THE ROLE OF MATERIAL STRUCTURE AND COMPOSITION IN NANOSTRUCTURED TRANSITION METAL OXIDE ELECTROCHEMICAL CAPACITORS
[MEEM] Veronica Augustyn, Zheng Chen, Jong Youn Kim, Thomas Quickel, Sarah Tolbert, Yunfeng Lu, and Bruce Dunn
1University of California, Los Angeles

P2-D20 - CONTINUUM-LEVEL SIMULATION OF CONVERSION REACTIONS: FROM A Li-CU-TiS2 SYSTEM TO A Li-Fe-F SYSTEM
[NECCES] Hui-Chia Yu, Tapiwa Mushove, Jishnu Bhattacharya, Chen Ling, Anton Van der Ven, Katsuyo Thornton, Glenn G. Amatucci, and Nathalie Pereira
1 University of Michigan and 2 Rutgers University

P2-D21 - CHARACTERIZATION OF LI-ION BATTERY MATERIALS AND PROCESSES USING MAGNETIC STUDIES
1 Binghamton University; 2 Brookhaven National Laboratory; 3 Rutgers University; 4 and University of California, San Diego

P2-D22 - AMORPHOUS SnCo-CARBON ANODE: UNDERSTANDING THE REACTION MECHANISM
1 Binghamton University; 2 Brookhaven National Laboratory; 3 Stony Brook University; 4 Lawrence Berkeley Laboratory; 5 Georgia Institute of Technology

P2-D23 - USING SYNCHROTRON BASED X-RAY DIFFRACTION AND ABSORPTION TO UNDERSTAND LiFePO4 AND FeF2 AS CATHODE MATERIALS FOR LITHIUM BATTERIES
[NECCES] Xiao-Jian Wang, Kyung-Wan Nam, Xiao-Qing Yang, Nathalie Pereira, and Glenn G. Amatucci
1 Brookhaven National Laboratory and 2 Rutgers University

P2-D24 - FUNDAMENTAL INSIGHTS INTO PERFORMANCE LIMITATIONS OF OXOANION CATHODE MATERIALS
[NECCES] Yuri Janssen, Shouhang Bo, Lin-Shu Du, Derek Middlemiss, Peter Khalifah, and Clare P. Grey
1 Stony Brook University

P2-D25 - NANOELECTRODE NETWORKS: CHEMISTRY AND MECHANICS AT NANOSTRUCTURED INTERFACES
[NEES] Hongwei Liao, Alexandra H. Brozena, Khim Karki, Yin Zhang, John Cumings, and YuHuang Wang
1 The University of Maryland, College Park

P2-D26 - NANOSCALE ENGINEERING FOR Si-BASED HIGH PERFORMANCE Li ION BATTERIES
[NEES] Jeong-Hyun Cho, Xianglong Li, Xiao Hua Liu, Jian Yu Huang, and S. Thomas Picraux
1 Los Alamos National Laboratory and 2 Sandia National Laboratories

P2-D27 - HETEROGENEOUS NANOTUBES AND NANOWIRES: FABRICATION, MECHANISM, AND ELECTROCHEMICAL CHARACTERIZATION FOR SUPERCAPCITORS
[NEES] Jonathon Duay, Stefanie A Sherrill, Sung Kyoung Kim, and Sang Bok Lee
1 University of Maryland

P2-D28 - NANOARCHITECTURED 3D ELECTRODES FOR Li-ION MICROBATTERIES
[NEES] Ekaterina Pomerantsseva, Konstantinos Gerasopoulos, Xinyi Chen, Gary Rubloff, James Culver, Chunsheng Wang, and Reza Ghodssi
1 University of Maryland, College Park

P2-D29 - ELECTRON TRANSPORT IN CHARGE-SEPARATED NANOPARTICLE FILMS DRIVEN BY EXTERNAL FIELDS: A NON-EQUILIBRIUM APPROACH
[NERC] Anthony Costa, Jason Green, and Igal Szleifer
1 Northwestern University
P2-D30 - ACCESSING TETRATHIAFULVALENE RADICAL DIMERS AND NON-EQUILIBRIUM STATES IN MECHANICALLY INTERLOCKED MOLECULES
[NERC] Gokhan Barin1, Ali Coskun1, Jason M. Spruell1, and J. Fraser Stoddart1
1Northwestern University

P2-E01 - DEVELOPMENT OF SOLID OXIDE CELLS FOR ENERGY CONVERSION AND STORAGE
[HeteroFoaM] Chenghao Yang1, Chao Jin1, and Fanglin (Frank) Chen1
1University of South Carolina

P2-E02 - APPLICATION OF PULSED ELECTRIC CURRENT SINTERING ON NEW THERMOELECTRIC OXIDES
[RMSSEC] Chang Liu1 and Donald T. Morelli1
1Michigan State University

P2-E03 - WAVELENGTH DOWNCONVERSION MATERIALS FOR SOLID-STATE LIGHTING
[SSLS] James E. Martin1, Lauren Rohwer1, and May Nyman1
1Sandia National Laboratories

P2-E04 - NANOWIRE AND NANOPARTICLE COMPOSITES FOR EFFICIENT THERMOELECTRICS
[CEEM] Benjamin Curtin1, Hong Lu1, Jacqueline Hall1, Chris Palmstrøm1, Arthur Gossard1, and John Bowers1
1University of California - Santa Barbara

P2-E05 - COMBUSTION AT HIGH PRESSURE
[CEFRC] Jeffrey S. Santner1, Michael P. Burke1, Frederick L. Dryer1, and Yiguang Ju1, Swetaprovo Chaudhuri1, Peng Zhang1, Fujia Wu1, and Chung K. Law1, David F. Davidson2 and Ronald K. Hanson2, Bryan W. Weber3, Muthunja Uddi1, Apurba Das4, and Chih-Jen Sung3, Fokion N. Egelopoulos5, and Stephen J. Klippenstein5
1Princeton University; 2Stanford University; 3University of Connecticut; 4University of Southern California and 5Argonne National Laboratory

P2-E06 - MATERIALS AND SYNTHESIS OF KNOWN SUPERCONDUCTORS
[CES] Jian-Min Zuo1, Hefei Hu1, Ivan Bozovic2, Cedomir Petrovic2, Genda Gu2, Lei Fang3, Wai-Kwon Kwok3, Mercouri Kanatizidis3, and Jim Eckstein1
1University of Illinois; 2Brookhaven National Lab and 3Argonne National Lab

P2-E07 - SUPERCONDUCTORS AS AN ENERGY CARRIER
[CES] Qiang Li1, Peter Johnson1, Vyacheslav Solovyov1, Wai-K Wong Kwok2, George Crabtree2, Ulrich Welp2, Vitalii Vlasko-Vlaskov2, Alexei Koshelev2, Venkat Selvamanackam3, and Alexis Malozemoff3
1Brookhaven National Lab; 2Argonne National Lab; 3SuperPower Inc. and 4American Superconductor Corp

P2-E08 - PROBING THE HIGH TC-SUPERCONDUCTING ORDER PARAMETER WITH PHOTOOEMISSION AND POLARIZED X-RAYS.
[CES] Peter Johnson1, Peter Abbamonte2, Juan Carlos Campuzano3, John Hill1, James Lee4, and Mike Norman3
1Brookhaven National Laboratory; 2University of Illinois and 3Argonne National Laboratory

P2-E09 - THE BEHAVIOR OF IRON-BASED SUPERCONDUCTORS
[CES] George W. Crabtree1, Seamus J. C. Davis4, Russell Giannetta3, Laura Greene3, Wai-Kwong Kwok1, Cedomir Petrovic1, Ulrich Welp3, Hamood Z. Arham2, Lei Fang3, Cassi R. Hunt1, Wan Kyu Park3, and Alexei E. Koshelev1
1Argonne National Laboratory; 2Brookhaven National Laboratory and 3University of Illinois at Urbana-Champaign

P2-E10 - UNDERSTANDING PAST FAILURE OF EARTH ABUNDANT MATERIALS SUCH AS FeS2 TO BE GOOD SOLAR ABSORBERS - PROBLEMS AND CURE
[CID] Douglas Keszler1, John Wager1, Vorrunutch Jieratum1, Ram Ravichandran1, Brian Pelatt, Emmeline Altschul1, Robert Kykyneshi1, and Liping Yu1-P2
1Oregon State University and 2NREL

P2-E11 - NANOSTRUCTURED CERIA-BASED ANODES FOR LOW TEMPERATURE SOLID OXIDE FUEL CELLS
[HeteroFoaM] James Wright1, Meilin Liu2, and Anil Virkar1
1University of Utah and 2GeorgiaTech
P2-E12 - NEW ANODE MATERIALS WITH ENHANCED TOLERANCE TO SULFUR AND COKING
[HeteroFoaM] Lei Yang1, Yongman Choi2, and Meilin Liu1
1Georgia Tech and 2Brookhaven National Lab

P2-E13 - NOVEL PROTON CONDUCTORS WITH ENHANCED CHEMICAL STABILITY
[HeteroFoaM] Siwei Wang1, Fei Zhao1, Fanglin Chen1, and Kyle Brinkman2
1University of South Carolina and 2Savannah River National Laboratory

P2-E14 - SINGLE MOLECULE PHOTODRIVEN MACHINES FOR TRANSDUCING PHOTON ENERGY INTO MECHANICAL ENERGY
[NERC] Ignacio Franco1, Martin McCullagh1, Mark A. Ratner1, and George C. Schatz1
1Northwestern University

P2-E15 - NON-EQUILIBRIUM CHIRAL ASSEMBLY
[NERC] Thomas Hermans1 and Bartosz Grzybowski1
1NERC

P2-E16 - UNUSUAL THERMOELECTRIC PROPERTIES OF VANADIUM BASED ORGANIC COMPOUNDS
[RMSSEC] A. M. Chamoire1, C. M. Jaworski1, C.-Y. Kao1, A. J. Epstein1, and J. P. Heremans1
1The Ohio State University

P2-E17 - THERMOELECTRIC PROPERTIES OF SKUTTERUDITE-BASED NANOCOMPOSITES
[RMSSEC] Chen Zhou1, Jeffery Sakamoto1, and Donald Morelli1
1Michigan State University

P2-E18 - BORON SEGREGATION AT GRAIN BOUNDARIES IN COSi ALLOYS
[RMSSEC] Edgar Lara-Curzio1, Melanie J. Kirkham1, Harry M. Meyer III1, Shengyong Qin1, An-Ping Li1, Hui Sun2, and Don Morelli2
1ORNL and 2Michigan State University

P2-E19 - CONTROLLING THE LIGHT AND HEAVY HOLE BANDS OF P-TYPE PbTe WITH K AND NA CO-DOPING
[RMSSEC] John Androulakis1, Iliya Todorov2, Duck-Young Chung2, Guoyu Wang3, Ctirad Uher1,3, and Mercouri Kanatzidis1
1Northwestern University; 2Argonne National Laboratory and 3University of Michigan

P2-E20 - NANOSTRUCTURED MATERIALS BASED ON PbTe/Bl2Te3 FOR THERMOELECTRIC APPLICATIONS
[RMSSEC] Shreyashi Ganguly1, Kevin Zhou2, Donald Morelli2, Jeff Sakamoto2, Ctirad Uher2, and Stephanie L. Brock1
1Wayne State University and 2Michigan State University

P2-E21 - IMPACT OF CRYSTALLINE DEFECTS ON THE EFFICIENCY OF BLUE LIGHT EMITTING DIODES FOR SOLID-STATE LIGHTING
[SSLS] Tania A. Henry1, Andrew M. Armstrong1, Mary H. Crawford1, and Dan D. Koleske1
1Sandia National Laboratories

P2-E22 - LASERS FOR SOLID-STATE LIGHTING
[SSLS] A. Neumann1, J. J. Wierer2, W. Davis3, Y. Ohno3, S. R. J. Brueck1, and J. Y. Tsao2
1UNM; 2SNL and 3NIST

P2-E24 - LASING FROM OPTICALLY PUMPED GALLIUM NITRIDE NANORODS
[SSLS] Jeremy Wright1, Qiming Li1, Igal Brener1, Willie Luk1, George Wang1, and Luke Lester2
1Sandia National Laboratories and 2University of New Mexico

P2-F01 - STRUCTURE AND DYNAMICS OF CO2-BEARING FLUIDS AT NANOSCALE INTERFACES
[NCGC] David Cole1, Gernot Rother2, Lukas Vlcek2, Mirek Gruszkiewicz2, and Larry Anovitz2
1Ohio State University and 2Oak Ridge National Laboratory

P2-F02 - CO2 FROM BENCHTOP TO OUTCROP: MULTIPHASE REACTIVE TRANSPORT AND A NATURAL ANALOGUE FOR LEAKAGE
[CFSES] Hongkyu Yoon1, Matt Balhoff2, Steve Bryant3, Peter Eichhubl1, Tom Dewers1, Yashar Mehmani1, and Tie Sun1
1Sandia National Laboratories and 2University of Texas at Austin
P2-F03 - MULTIPHYSICS MODELS OF CAPROCK FRACTURING DURING CO2 INJECTION
[CFSES] Mario Martinez\(^1\), Joe Bishop\(^1\), Panio Newell\(^1\), Sean McKenna\(^1\), Sanjay Srinivasan\(^2\), Peter Eichhubl\(^2\), Tom Dewers\(^1\), and Alex Reinhart\(^1\)
\(^1\)Sandia National Laboratories and \(^2\)University of Texas at Austin

P2-F04 - ALTERATIONS IN MECHANICAL PROPERTIES OF ROCKS DUE TO CO2 INJECTION -- IMPLICATIONS FOR FIELD SCALE MONITORING OF SEQUESTRATION PROCESSES
[CFSES] Mrinal Sen\(^1\), Sean McKenna\(^2\), Ranjana Ghosh\(^1\), Hongkyu Yoon\(^2\), Son Phan\(^1\), Sanjay Srinivasan\(^1\), and Rui Zhang\(^1\)
\(^1\)University of Texas at Austin and \(^2\)Sandia National Laboratories

P2-F05 - INSIGHTS INTO MECHANISMS FOR CO2 SEEPAGE BASED ON FIELD OBSERVATIONS AT CRYSTAL GEYSER NATURAL ANALOG
[CFSES] Peter Eichhubl\(^1\), Matt Balhoff\(^1\), Steve Bryant\(^1\), Tom Dewers\(^2\), Larry Lake\(^1\), Sanjay Srinivasan\(^1\), Young Kim\(^1\), and Alex Urquhart\(^2\)
\(^1\)University of Texas at Austin and \(^2\)Sandia National Laboratories

P2-F06 - TAKING FUNDAMENTALLY NEW MATERIALS FOR CO2 CAPTURE TOWARD APPLICATION: AN EFRC/NETL COLLABORATION
[CGS] David Luebke\(^1\), Hunaid Nulwala\(^1\), Erik Albenze\(^2\), Damodaran Krishnan Achary\(^3\), Lang Sui\(^1\), and Wei Shi\(^2\)
\(^1\)NETL; \(^2\)URS and \(^3\)University of Pittsburgh

P2-F07 - MODEL DEVELOPMENT FOR RAPID SCREENING OF ADSORBENT MATERIALS USING IDEAL ADSORBED SOLUTION THEORY AND MOLECULAR SIMULATION
[CGS] Joseph Swisher\(^1\) and Berend Smit\(^1,2\)
\(^1\)UC Berkeley and \(^2\)LBNL

P2-F08 - FIRST-PRINCIPLES CALCULATIONS OF THE INTERACTION BETWEEN CO2 AND METAL-ORGANIC FRAMEWORKS
[CGS] Roberta Poloni\(^1,2\), Allison Dzubak\(^3\), Jeffrey B. Neaton\(^4\), Laura Gagliardi\(^5\), Giulia Galli\(^6\), and Berend Smit\(^1\)
\(^1\)University of California, Berkeley; \(^2\)LBNL; \(^3\)University of Minnesota and \(^4\)University of California, Davis

P2-F09 - METAL-ORGANIC FRAMEWORKS AS MATERIALS FOR CARBON DIOXIDE CAPTURE
[CGS] Eric Bloch\(^1\), Zoey Herm\(^1\), Kenji Sumida\(^1\), Thomas McDonald\(^1\), Jarad Mason\(^1\), Hye Jin Choi\(^1\), Joseph Swisher\(^1\), Bered Smit\(^1\), Rajamani Krishna\(^1\), and Jeffrey R. Long\(^1\)
\(^1\)UC Berkeley and \(^2\)University of Amsterdam

P2-F10 - UNDERSTANDING GAS ADSORPTION IN ZEOLITIC IMIDAZOLATE FRAMEWORKS: MOLECULAR MODELING
[MEEM] Keith Ray\(^1\), David Olmsted\(^1\), Ning He\(^2\), Jessica Burton\(^1\), Yao Houndonougbo\(^3\), Brian Laird\(^2\), and Mark Asta\(^1\)
\(^1\)UC Berkeley; \(^2\)University of Kansas and \(^3\)Eastern Washington University

P2-F11 - UNDERSTANDING GAS ADSORPTION IN ZEOLITIC IMIDAZOLATE FRAMEWORKS: EXPERIMENTAL SYNTHESIS AND CHARACTERIZATION
[MEEM] William Morris\(^1\)
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P2-F12 - UPSCALING PORE SCALE CARBONATE PRECIPITATION RATES TO THE CONTINUUM SCALE
[NCGC] Carl Steefel\(^1\), Catherine Noiriel\(^2\), Li Yang\(^1\), and Jonathan Ajo-Franklin\(^1\)
\(^1\)Lawrence Berkeley National Laboratory and \(^2\)Universite de Lille, France

P2-F13 - AGING IN DISSOLUTION AND PRECIPITATION RATES FOR MINERALS RELEVANT TO CO2 SEQUESTRATION
[NCGC] Dan Reeves\(^1\), Dan Rothman\(^1\), and Don DePaolo\(^2\)
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P2-F14 - CARBON DIOXIDE - WATER INTERFACIAL TENSION UNDER GEOLOGIC CO2 STORAGE CONDITIONS: A MOLECULAR DYNAMICS SIMULATION STUDY
[NCGC] Laura Nielsen\(^1\) and Ian Bourg\(^2\)
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P2-F15 - In Situ Kinetic Analysis of Calcium Carbonate Nanoparticle Formation Using Grazing Incidence Small Angle X-ray Scattering

[NCGC] Young-Shin Jun¹, Alex Fernandez-Martinez², Yandi Hu¹, and Glenn Waychunas²

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