

2017 EFRC-HUB-CMS PI MEETING – GRAPHIC AGENDA FOR MONDAY, JULY 24, 2017

| | | A. Biosciences/ C. Catalysis | D. Energy Storage | H. Solar Energy Conversion | J. Materials and Chemistry by Design | B. Carbon Sequest/ G. Separation Science | E. Nuclear Energy & Waste | F. Quantum Materials |
|--------------|--------------------|---|--|---|---|--|---|---|
| Room | | <i>Thurgood North</i> | <i>Thurgood East</i> | <i>Thurgood South</i> | <i>Thurgood West</i> | <i>Lincoln 2</i> | <i>Lincoln 5</i> | <i>Lincoln 6</i> |
| Chair | | <i>Robert Stack</i> | <i>Craig Henderson</i> | <i>Chris Fecko</i> | <i>Matthias Graf</i> | <i>P. Thyagrajan</i> | <i>Philip Wilk</i> | <i>Mick Pechan</i> |
| O-1 | 1:00 PM | [CCEI] <u>Dionisios Vlachos</u> <i>U. Delaware</i> Catalysis Center for Energy Innovation | [CEES] <u>Paul Fenter</u> <i>ANL</i> Center For Electro- chemical Energy Science | [JCAP] <u>Harry Atwater</u> <i>Caltech</i> Joint Center for Artificial Photosynthesis | [CCDM] <u>John Perdew</u> <i>Temple</i> Computational Design of Functional Layered Materials | [NCGC] <u>Donald DePaolo</u> <i>LBNL</i> Center for Nanoscale Controls on Geologic CO ₂ | [EDE] <u>Yanwen Zhang</u> <i>ORNL</i> Energy Dissipation to Defect Evolution | [S3TEC] <u>Gang Chen</u> <i>MIT</i> Solid-State Solar Thermal Energy Conversion Center |
| O-2 | 1:13 PM | [CLSF] <u>Daniel Cosgrove</u> <i>Penn State</i> Center for Ligno- cellulose Structure and Formation | [FIRST] <u>D. J. Wesolowski</u> <i>ORNL</i> Fluid Interface Reactions, Structures and Transport | [UNC] <u>Thomas Meyer</u> <i>UNC Chapel Hill</i> Center for Solar Fuels | [CNGMD] <u>W. Tumas</u> <i>NREL</i> Center for Next Generation of Materials by Design | [CFSES] <u>Larry Lake</u> <i>UT Austin</i> Center for Frontiers of Subsurface Energy Security | [WastePD] <u>G. Frankel</u> <i>Ohio State</i> Performance & Design of Nuclear Waste Forms & Containers | [CPSFM] <u>Paul Kent</u> <i>ORNL</i> Center for Predictive Simulation of Functional Materials |
| O-3 | 1:26 PM | [C3Bio] <u>M. C. McCann</u> <i>Purdue</i> Center for Direct Catalytic Conversion of Biomass to Biofuels | [JCESR] <u>George Crabtree</u> <i>ANL, U. Illinois Chicago</i> Joint Center for Energy Storage Research | [ANSER] <u>M. Wasielewski</u> <i>Northwestern, ANL</i> Argonne-Northwestern Solar Energy Research Center | [MAGICS] <u>P. Vashishta</u> <i>U. Southern California</i> MATERIALS Genome Innovation for Computational Software | [GSCO2] <u>Scott Frailey</u> <i>UIUC</i> Center for Geologic Storage of CO ₂ | [CHWM] <u>H. zur Loye</u> <i>U. South Carolina</i> Center for Hierarchical Wasteform Materials | [Free] <u>Russell Hemley</u> <i>Carnegie Institution, George Washington</i> Energy Frontier Research in Extreme Environments |
| O-4 | 1:39 PM | [PARC] <u>R. Blankenship</u> <i>Wash U. St. Louis</i> Photosynthetic Antenna Research Center | [NECCES] <u>Whittingham</u> <i>Binghamton</i> NorthEast Center for Chemical Energy Storage | [CASP] <u>Victor Klimov</u> <i>LANL</i> Center for Advanced Solar Photophysics | [ICDC] <u>Laura Gagliardi</u> <i>U. Minnesota</i> Inorganometallic Catalyst Design Center | [Invited Talk] <u>James Glowina</u> <i>DOE Office of Science</i> Office of Science Sponsored Undergraduate and Graduate Student Placement Opportunities at DOE Laboratories | [CDMFTS] <u>G. Kotliar</u> <i>Rutgers</i> Computational Design of Functional Strongly Correlated Materials & Theoretical Spectro- scopy | [CES] <u>Peter Johnson</u> <i>BNL</i> Center for Emergent Superconductivity |
| O-5 | 1:52 PM | [CBES] <u>Samuel Stupp</u> <i>Northwestern</i> Center for Bio-Inspired Energy Science | [m2M] <u>Esther Takeuchi</u> <i>Stony Brook</i> Center for Mesoscale Transport Properties | [C2SEPEM] <u>Steven Louie</u> <i>LBNL, UC Berkeley</i> Computational Study of Excited-State Phenom- ena in Energy Materials | [IMASC] <u>Cynthia Friend</u> <i>Harvard</i> Integrated Mesoscale Architectures for Sustainable Catalysis | | [IDREAM] <u>Sue Clark</u> <i>PNNL</i> Interfacial Dynamics in Radiation Environments and Materials | [SHINES] <u>Jing Shi</u> <i>UC Riverside</i> Spins and Heat in Nanoscale Electronic Systems |
| O-6 | 2:05 PM | [BETCy] <u>John Peters</u> <i>Montana State, Washington State</i> Biological Electron Transfer and Catalysis EFRC | [NEES] <u>Gary Rubloff</u> <i>U. Maryland</i> Nanostructures for Electrical Energy Storage | [CE] <u>Marc Baldo</u> <i>MIT</i> Center for Excitonics | [MICCoM] <u>Giulia Galli</u> <i>U. Chicago, ANL</i> Midwest Integrated Center for Computational Materials | [UNCAGE-ME] <u>K. Walton</u> <i>Georgia Tech</i> Understanding & Control of Acid Gas- Induced Evolution of Materials for Energy | [MSA] <u>Peter Burns</u> <i>Notre Dame</i> Materials Science of Actinides | [Invited Talk] <u>Roger Falcone</u> <i>Advanced Light Source, LBNL</i> DOE Light Sources: Capabilities, Opportunities, and Access |
| O-7 | 2:18 PM | [CME] <u>R. Morris Bullock</u> <i>PNNL</i> Center for Molecular Electrocatalysis | | [LMI] <u>Ralph Nuzzo</u> <i>UIUC</i> Light-Material Interactions in Energy Conversion | | [CGS] <u>Jeffrey Long</u> <i>UC Berkeley</i> Center for Gas Separations Relevant to Clean Energy Technologies | [CAST] <u>T. Albrecht- Schmitt</u> <i>Florida State</i> Center for Actinide Science and Technology | |

2017 EFRC-HUB-CMS PI MEETING – GRAPHIC AGENDA FOR MONDAY, JULY 24, 2017

2:30 – 3:00 PM

Break

| | | C. Catalysis | D. Energy Storage | H. Solar Energy Conversion | J. Materials and Chemistry by Design | I. Synthesis Science | E. Nuclear Energy & Waste | F. Quantum Materials |
|-------|---------|---|---|---|---|--|---|---|
| Room | | <i>Thurgood North</i> | <i>Thurgood East</i> | <i>Thurgood South</i> | <i>Thurgood West</i> | <i>Lincoln 2</i> | <i>Lincoln 5</i> | <i>Lincoln 6</i> |
| Chair | | <i>Viviane Schwartz</i> | <i>Greg Fiechtner</i> | <i>Mark Spitler</i> | <i>Matthias Graf</i> | <i>Mike Markowitz</i> | <i>Tim Fitzsimmons</i> | <i>Jim Davenport</i> |
| I-1 | 3:00 PM | [CCEI] <u>O. Abdelrahman</u> <i>U. Minnesota</i> Biomass-Derived Butadiene by Dehydration of Tetrahydrofuran | [m2M] <u>Amy Marschilok, Guihua Yu</u> <i>Stony Brook, UT Austin</i> Exploiting "Passive Materials" in Electrochemical Energy Storage Systems: The Significant Impacts of Hard Material – Soft Material ... | [UNC] <u>Kirk S. Schanze</u> <i>UT San Antonio</i> Molecular and Polymer Chromophore-Catalyst Assemblies for Solar Fuels Production | [JCAP] <u>J. T. Feaster; D. A. Torelli; Z. W. Ulissi*</u> <i>Stanford/SLAC; Caltech</i> Materials Discovery, Theory, & Characterization of Intermetallics for Electrochemical CO ₂ Reduction | [EFree] <u>Xiang Li</u> <i>Penn State</i> Novel Carbon Materials Synthesis in Extreme Environments | [CAST] <u>Kenneth Hanson</u> <i>Florida State</i> Wavelength selective photochemical transformations using electroactive ligands | [C2SEPEM] <u>D. Qiu; F. da Jornada; M. Utama*</u> <i>LBNL, UC Berkeley</i> Environmental Screening Effects in 2D Materials: Renormalization of the Bandgap, Electronic Structure, and Optical Spectra |
| I-2 | 3:20 PM | [IMASC] <u>Robert J Madix</u> <i>Harvard</i> Moving from Model Studies on Single Crystal Gold to Higher Pressure Conditions: Kinetic and Mechanistic Understanding from TAP Studies on npAu Catalysts | [NECCES] <u>Y.-M. Chiang</u> <i>MIT</i> Integrated Experimental-Computational Investigation of a Polycrystalline Battery-Electrode Particle | [PARC] <u>M. Maiuri</u> <i>Princeton</i> Coherent Wavepackets in the FMO Complex are Robust to Spectral Perturbations by Mutagenesis | [JCESR] <u>K. A. Persson</u> <i>LBNL</i> Materials Genomics Design and Electrochemical Realization of Improved Electrodes and Electrolytes for Future Multivalent Energy Storage | [CBES] <u>G. Whitesides</u> <i>Harvard</i> Soft Robotics | [CDMFTS] <u>Yongxin Yao</u> <i>Ames Lab</i> The recent development of the DFT/GW + Gutzwiller slave-boson method and package | [CCDM] <u>Arun Bansil</u> <i>Northeastern</i> The SCAN Density Functional: Success Stories for 2D, Layered and 3D Materials |
| I-3 | 3:40 PM | [ICDC] <u>M. A. Ortuño; Z. Li; A. E. Platero-Prats*</u> <i>U. Minnesota; Northwestern; ANL</i> Post-functionalized Metal–Organic Frameworks for Catalysis | [FIRST] <u>N. Osti; M. W. Thompson; K. Van Aken*</u> <i>ORNL; Vanderbilt; Drexel</i> Understanding Room Temperature Ionic Liquids & their Performance in Supercapacitors | [CE] <u>G. Schlau-Cohen</u> <i>MIT</i> Controlling energy transfer in DNA-based excitonic circuits | [CES] <u>Wai-Kwong Kwok</u> <i>ANL</i> Critical-Current-by-Design | [CLSF] <u>Jochen Zimmer</u> <i>U. Virginia</i> In vitro Reconstitution of Plant Cellulose Biosynthesis | [CHWM] <u>N. B. Shustova</u> <i>U. South Carolina</i> Well-Defined Actinide-Based Frameworks | [CPSFM] <u>Olle Heinonen</u> <i>ANL</i> Towards experimentally validated, predictive quantum simulations of vanadium and nickel oxides |
| I-4 | 4:00 PM | [BETCy] <u>C. E. Lubner</u> <i>NREL</i> Electron Bifurcation – Mechanistic First Principles | [JCESR] <u>Brett A. Helms</u> <i>LBNL</i> Tailoring Polymers of Intrinsic Microporosity to Meet the Growing Demands for Fast Ion Transport in Electrochemical Energy Storage Devices | [UNC] <u>J. M. Papanikolas</u> <i>UNC Chapel Hill</i> Ultrafast Injection and Recombination Dynamics at SnO ₂ /TiO ₂ Core/Shell and NiO Interfaces for Solar Fuels Production | [ICDC] <u>Donald G. Truhlar</u> <i>U. Minnesota</i> Modeling Structure and Activity for Catalysts Supported on Metal–Organic Frameworks | [CBES] <u>Sharon Glotzer</u> <i>U. Michigan</i> Clathrate Colloidal Crystals | [WastePD] <u>Jie Lian</u> <i>RPI</i> Design and Performance of Ceramic Waste Forms for Iodine and Chlorine Sequestration with High Waste Loadings | [MAGICS] <u>David Fritz</u> <i>SLAC/Stanford</i> Ultrafast experiments and quantum dynamics of layered materials |

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| I-5 | 4:20 PM | [ANSER] J. T. Hupp <i>Northwestern</i> A new family of catalysts for solar fuels: Cofactor-like catalysts on mesoporous MOF supports | [m2M] Y.Zhu,K.Takeuchi <i>BNL, Stony Brook</i> Contributions to Inter- and Intra-Rod Ion Transport in Tunnel Structured Materials: Implications for Electro-chemical Energy Storage | [JCAP] Chengxiang Xiang <i>Caltech</i> Modeling, Simulation and Prototyping of Solar-Fuel Devices | [CGS] Berend Smit <i>UC Berkeley</i> Computational Screening of Nanoporous Materials for Gas Separations | [EFree] Tianshu Li <i>George Washington</i> Silicon Clathrates as New Energy Materials | [CAST] Eric Schelter <i>U. Pennsylvania</i> Synthesis of actinide hydroxylamine complexes and characterization of their electronic structures | [CPSFM] L.Shulenburg <i>SNL</i> Advances in many-body simulations of materials |
| I-6 | 4:40 PM | [CME] Simone Raugei <i>PNNL</i> Reversible Enzymatic H ₂ production/oxidation Uses Different Pathways for the Forward and reverse Reaction | [FIRST] Jianzhong Wu <i>UC Riverside</i> Electrical Double Layer in Porous Electrodes - Capacitance, Capacitive Mixing, and Electro-Osmosis | [ANSER] B. Rudshteyn; K. Materna; N. La Porte* <i>Yale; Northwestern</i> The Pyridine Alkoxide Ligand Works for Water Oxidation Catalysts Both in Theory & in Practice | [ICDC] Omar Farha <i>Northwestern</i> Tuning the Catalytic Activity of Few-atom Clusters Deposited in Metal–Organic Frameworks | [LMI] Jennifer A. Lewis <i>Harvard</i> Patterning Polarized Photonic Nanocomposites via Direct Ink Writing | [MSA] May Nyman <i>Oregon State</i> Actinide Polynuclear Speciation and Implications in Nuclear Energy | [CCDM] John P. Perdew <i>Temple</i> Band Gaps from Hybrid Density Functionals for 1D, 2D, and 3D Solids: The Right Answer for the Right Reason |

5:00 – 6:30 PM

Poster Session, Exhibition Hall C

7:00 – late

ECN Event: Board Games with Dinner at The Board Room DC (all welcome)

2017 EFRC-HUB-CMS PI MEETING – GRAPHIC AGENDA FOR TUESDAY, JULY 25, 2017

| | | C. Catalysis | D. Energy Storage | H. Solar Energy Conversion | G. Separation Science | I. Synthesis Science | E. Nuclear Energy & Waste | A. Biosciences |
|-------|---------|--|--|--|--|--|--|--|
| Room | | <i>Thurgood North</i> | <i>Thurgood East</i> | <i>Thurgood South</i> | <i>Thurgood West</i> | <i>Lincoln 2</i> | <i>Lincoln 5</i> | <i>Lincoln 6</i> |
| Chair | | <i>Chris Bradley</i> | <i>Michael Sennett</i> | <i>Refik Kortan</i> | <i>P. Thiyagrajan</i> | <i>Bonnie Gersten</i> | <i>John Vetrano</i> | <i>Bob Stack</i> |
| II-1 | 8:30 AM | [IMASC] <u>M. Stamatakis</u> <i>University College London</i> First-Principles Kinetic Monte Carlo Simulations of C1 Chemistries on Pure Metals and Single Atom Alloys | [NECCES] <u>Y.-C. Lin; M. V. Hidalgo; S. Sallis*</u> <i>UCSD; Binghamton</i> Thermodynamic Stability, Voltage and Diffusion Kinetics of Li_xVOPO_4 ($x=0,1,2$) Vanadyl Phosphate ... | [ANSER] <u>M. Kanatzidis</u> <i>Northwestern</i> Lead-free Perovskite Films for Heterojunction Depleted Perovskite Solar Cells | [UNCAGE-ME] <u>R. Lively</u> <i>Georgia Tech</i> Engineering Nanoporous Materials with Increased Acid Gas Resistance | [CNGMD] <u>Gerbrand Ceder, Andriy Zakutayev</u> <i>LBNL, NREL</i> Discovery and Synthesis of Novel Nitrides with Targeted Functionality | [IDREAM] <u>Kevin Rosso</u> <i>PNNL</i> Interfacial Dynamics of Boehmite & Gibbsite in Extreme Environments: Connecting Across Spatial Scales | [CLSF] <u>A. Singh; J. N. Burris; X. Xin*</u> <i>North Carolina State; Penn State</i> The Nanomachine that Synthesizes Cellulose in Plants |
| II-2 | 8:50 AM | [UNCAGE-ME] <u>Zili Wu</u> <i>ORNL</i> Role of Surface Structure and Dopants on the Interaction Between Acid Gases and Metal Oxide Catalysts | [m2M] <u>Alan West, Amy Marschilok</u> <i>Columbia, Stony Brook</i> Electrochemically Induced Phase evolution of High Capacity Layered Materials: Complementary Insights ... | [CE] <u>William Tisdale</u> <i>MIT</i> Luminescent 2D Metal Halide Perovskite Nanoplatelets | [CGS] <u>Walter S. Drisdell</u> <i>LBNL</i> Determining Mechanisms of Gas Adsorption in MOFs by Combining X-ray Spectroscopy & Theory | [MAGICS] <u>P. Vashishta</u> <i>U. Southern California</i> Computational synthesis of layered materials using CVD & exfoliation | [EDDE] <u>Eva Zarkadoula</u> <i>ORNL</i> Molecular Dynamics Simulations of Cascades: Effects of Ion-Electron Interactions in Irradiated Alloys | [C3Bio] <u>N. C. Carpita</u> <i>Purdue</i> Redesigning the structure of biomass for carbon- and energy-efficient catalytic & pyrolytic transformations |
| II-3 | 9:10 AM | [ICDC] <u>Bruce Gates</u> <i>UC Davis</i> Zr6 Nodes of Metal Organic Frameworks as Platforms for Single-Site Metal Catalysts | [CEES] <u>Jeffrey P. Greeley</u> <i>Purdue</i> Atomistic Studies of Nucleation and Growth in Conversion Reactions for Lithium-Ion Batteries | [S3TEC] <u>J. Shuai, D. Singh</u> <i>U. Houston, U. Missouri</i> Novel High Performance P- and N-Type Zintl Thermoelectrics | [UNCAGE-ME] <u>Bobby G. Sumpter</u> <i>ORNL</i> Linking Morphology and Interfacial Interactions to Acid Gas Uptake | [EDDE] <u>Shijun Zhao; Taini Yang; Shi Shi*</u> <i>ORNL; U. Michigan; U. Wisconsin</i> Effects of Alloy Complexity on Defect Production & Microstructural Evolution in Concentrated Alloys | [CHWM] <u>Hui Wang</u> <i>U. South Carolina</i> Multimetallic Nanoparticles: Alloys, Intermetallics, and Heterostructures | [CLSF] <u>D. J. Cosgrove</u> <i>Penn State</i> Cellulose structure, Organization and Interactions with Matrix Polysaccharides and Proteins |
| II-4 | 9:30 AM | [IMASC] <u>M. Salmeron</u> <i>LBNL</i> Structure And Reactivity of Noble Metal & Alloy Catalysts Characterized By In Situ Microscopy and Spectroscopy | [NECCES] <u>I. D. Seymour</u> <i>U. Cambridge</i> Advances in NMR Methodology of Paramagnetic Li-ion Battery Cathode Materials | [LMI] <u>A. Paul Alivisatos</u> <i>LBNL</i> Luminescent Concentrators as Light Compressors | [CGS] <u>R. L. Siegelman; A. C. Forse*</u> <i>UC Berkeley</i> Rational Design of New Materials for Carbon Dioxide Capture | [CNGMD] <u>David Ginley, Kristin Persson</u> <i>NREL, LBNL</i> Synthesis of Functional Polymorphic Materials | [WastePD] <u>Seong Kim</u> <i>Penn State</i> Understanding the formation, structure, and stability of the passivating layer formed on nuclear waste glass during aqueous corrosion | [CBES] <u>Kyle Bishop</u> <i>Columbia</i> Programming the Dynamics of Colloidal Machines |
| II-5 | 9:50 AM | [JCAP] <u>Guiji Liu</u> <i>LBNL</i> Integrated Photoelectrodes for CO_2 RR | [FIRST] <u>Nina Balke</u> <i>ORNL</i> Heterogeneity of Charge Storage Processes in Electrochemical Capacitors | [CE] <u>Mircea Dinca</u> <i>MIT</i> Transport in 2D Metal-Organic Frameworks | [UNCAGE-ME] <u>R. M. Marti; J. D. Howe*</u> <i>Wash. U.; Georgia Tech</i> Understanding Structure and Dynamics of CO_2 Adsorbed in Open-Site MOFs | [CGS] <u>Brett A. Helms</u> <i>LBNL</i> Diamine-Appended $\text{Mg}_2(\text{dobpdc})$ Nanorods as Fillers in Mixed-Matrix Membranes for Efficient CO_2/N_2 Separat. | [IDREAM] <u>Jay LaVerne</u> <i>Notre Dame</i> Radiation Driven Modification of Boehmite and Gibbsite | [CLSF] <u>Yaroslava Yingling</u> <i>North Carolina State</i> All-Atom Structural Model of Plant Cellulose Synthase and Cellulose Synthase Complex |

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10:10 – 10:40AM Break

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| Chair | | <i>Wade Sisk</i> | <i>Lane Wilson</i> | <i>Tom Settersten</i> | <i>Matthias Graf</i> | <i>Tom Russell</i> | <i>Bob Stack</i> | <i>Jim Rhyne</i> |
| III-1 | 10:40 AM | [C3Bio] <u>M. Abu-Omar</u> <i>UC Santa Barbara</i> Catalytic conversion of lignin first to chemical synthons for making materials and fuels | [CEES] <u>R. Warburton</u> ; <u>B. Nicolau</u> ; <u>K. Letchworth-Weaver*</u> <i>Purdue; UIUC; ANL</i> Understanding and Controlling the Reactivity of LiMn ₂ O ₄ -Electrolyte Interfaces | [S3TEC] <u>Marin Soljacic</u> <i>MIT</i> Nanophotonics for tailoring emission and absorption of light | [CPSFM] <u>Paul Kent</u> <i>ORNL</i> Effectively developing and distributing open source code and data: experiences from QMCPACK | [NCGC] <u>Sally Benson</u> <i>Stanford</i> Towards Resolution of Conflicting Information about the Influence of CO ₂ Exposure on Wetting Properties and Residual Gas Trapping | [BETCy] <u>Diep Nguyen</u> ; <u>Jonathan Yuly*</u> <i>U. Georgia; Duke</i> Mechanistic insights into energy conservation by flavin-based electron bifurcation | [SHINES] <u>C.-L. Chien</u> <i>Johns Hopkins</i> Exploiting spin-chiral topological surface states in Kondo insulator SmB ₆ thin films |
| III-2 | 11:00 AM | [CCEI] <u>M. J. Gilkey</u> <i>U. Delaware</i> Metal-free cleavage of C-O bonds to form adipic acid from biomass derivatives | [NEES] <u>K. Gregorczyk</u> <i>U. Maryland</i> Vapor Phase Chemistry for Protection Layers and Solid-state 3D Batteries | [CASP] <u>J. M. Luther</u> <i>NREL</i> Quantum Dot Device Structures for High Efficiency Photoconversion | [MICCoM] <u>F. Gygi</u> <i>UC Davis</i> Development and Interoperability of the Qbox First-Principles Molecular Dynamics Code | [GSCO2] <u>J. Druhan</u> <i>UIUC</i> Linking Chemical Transformations to Physical Integrity Through Direct Imaging of Fluid Transport Properties in Mt. Simon Core During CO ₂ Injection | [PARC] <u>Rafael Saer</u> <i>Wash U. St. Louis</i> Energy Transfer Fundamentals in Nature's Molecular Wires: Lessons from Native & Genetically-Modified FMO Pigment-Protein Complexes | [CES] <u>Mark P.M. Dean</u> <i>BNL</i> Nature of the charge density waves in cuprate superconductors |
| III-3 | 11:20 AM | [C3Bio] <u>H. I. Kenttamaa</u> <i>Purdue</i> Fast hydroxyprolysis, catalytic conversion & in situ hydrodeoxygenation produce drop-in hydrocarbon fuels from biomass | [JCESR] <u>Kevin R. Zavadil</u> <i>SNL</i> Polysulfide Solubility Suppression Through Electrolyte Redesign as a Path Toward Practical Lithium-Sulfur Batteries | [LMI] <u>Paul V. Braun</u> <i>UIUC</i> 3D Gradient Refractive Index Micro-Optics for Enhanced Control of Light | [C2SEPEM] <u>J. DeSlippe</u> <i>LBNL</i> Large-Scale GW Calculations on Pre-Exascale HPC Systems | [CFSES] <u>Tip Meckel</u> <i>UT Austin</i> Advances in Understanding Buoyancy-Dominated Flow in Heterogeneous Geologic Systems | [BETCy] <u>Anne K. Jones</u> ; <u>Paul W. King</u> <i>Arizona State; NREL</i> Oxidative Inactivation of [FeFe]-Hydrogenase as a Model for Redox Tuning of Enzyme Active Site Reactivity | [SHINES] <u>C.-N. Lau</u> <i>UC Riverside/OSU</i> Long-Distance Spin Transport Through a Graphene Quantum Hall Antiferromagnet |
| III-4 | 11:40 AM | [CCEI] <u>K. E. Joseph</u> <i>U. Minnesota</i> Tunable synthesis of Oleo-Furan Surfactants via Acylation of Biomass-Derived Furans | [CEES] <u>Kan-Sheng Chen</u> <i>Northwestern</i> Interfacial Properties of Graphene/Lithium Manganese Oxide Spinel Cathodes for Lithium-Ion Batteries | [S3TEC] <u>David Bierman</u> ; <u>Veronika Stelmakh*</u> <i>MIT</i> Tailoring Thermal Emission for High Performance Solar Thermophotovoltaic Devices | [MAGICS] <u>A. Nakano</u> <i>U. Southern California</i> Scalable simulation software and data analytics for Layered materials | [NCGC] <u>Ian Bourg</u> <i>Princeton</i> Solubility of Gases (CO ₂ , CH ₄ , H ₂ , Noble Gases) in Clay Interlayer Nanopore Water | [PARC] <u>Matt Cuneo</u> <i>ORNL</i> Probing Photosynthetic Antenna Complexes with Neutrons: from Individual Hydrogen Atoms to Hierarchical Assemblies | [EFree] <u>M. Somayazulu</u> <i>Carnegie Institution</i> Potential New Superhydride Superconductors |

12:00 – 1:30 PM Lunch

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| Room | | <i>Thurgood North</i> | <i>Thurgood East</i> | <i>Thurgood South</i> | <i>Thurgood West</i> | <i>Lincoln 2</i> | <i>Lincoln 5</i> | <i>Lincoln 6</i> |
| Chair | | <i>Chris Fecko</i> | <i>Craig Henderson</i> | <i>Jane Zhu</i> | <i>Jim Davenport</i> | <i>Jim Rustad</i> | <i>Philip Wilk</i> | <i>Mick Pechan</i> |
| IV-1 | 1:30 PM | [CME] James M. Mayer <i>Yale</i> Advancing Molecular Electrocatalysis using Linear Free Energy Relationships | [JCESR] Joaquin Rodriguez-Lopez <i>UIUC</i> Versatile Macromolecular Design for Emerging Size-Selective Non-Aqueous Redox Flow Batteries | [UNC] Taylor H. Moot; Lesheng Li* <i>UNC Chapel Hill</i> Identification and Passivation of the Defect States in NiO for Photovoltaic and Solar Fuel Applications | [MICCoM] J. de Pablo <i>U. Chicago, ANL</i> SSAGES and COPSS - Modern Software for Advanced Materials Modeling | [GSCO2] R. Makhnenko <i>UIUC</i> Hydro-Mechanical Aspects of Deep CO ₂ Storage | [MSA] Maik Lang <i>U. Tennessee</i> Actinide Materials Under Extreme Condition: Local Defect Structure and Disorder | [SHINES] G. Yin; X. Ma* <i>UCLA; UT Austin</i> Magnetic skyrmions in ferromagnetic/heavy-metal multi-layers |
| IV-2 | 1:50 PM | [BETCy] Lance Seefeldt, Caroline Harwood <i>Utah State; U. Washington</i> Light Driven N-H and C-H Bond Formation by Nitrogenase | [FIRST] Yury Gogotsi <i>Drexel</i> High-Rate Electrical Energy Storage Enabled by Metallic Conductivity of MXenes | [ANSER] T. J. Marks <i>Northwestern</i> Soft Matter and Hybrid Solar Cell Interfacial Science | [C2SEPEM] Chao Yang <i>LBNL</i> Low-Rank Approximation for Solving the Bethe-Salpeter Equation | [CFSES] Pania Newell <i>SNL</i> Performance Assessment of Jointed/Faulted Caprock During CO ₂ Sequestration | [EDDE] Karren L. More <i>ORNL</i> Defect Generation, Evolution, and Dynamics in Irradiated Concentrated Solid Solution Alloys | [CES] James Eckstein <i>UIUC</i> Superconductivity in the Topological Insulator Bi ₂ Se ₃ |
| IV-3 | 2:10 PM | [UNC] Gerald J. Meyer <i>UNC Chapel Hill</i> A General Approach for Generation of Catalytic High Valent Metal Oxo Species Reveals Photoinduced One Electron, Two Proton Transfer Reactivity | [NEES] A. Alec Talin <i>SNL</i> Solid State Li-ion Batteries: Advancing Performance Through Fundamental Understanding | [JCAP] Jeff B. Neaton <i>LBNL</i> Discovery of new solarfuels photoanode materials with a combination of high-throughput theory and experiment | [MICCoM] M. Govoni <i>ANL, U. Chicago</i> Development of the WEST Code for Large Scale GW Code and of Data Infrastructure | [GSCO2] Dalton; M. G. D. Ordonez; S. Fuchs; P. Kabir; Z. Shi; M. Tkach* <i>NETL; UIUC; UT Austin; U. Southern California</i> Geochemical Reactions During Geological Carbon Sequestration Can Decrease Fracture ... | [WastePD] J. R. Scully <i>U. Virginia</i> Integrated Computational Materials Design of a Corrosion Resistant High Entropy Alloy for Harsh Environments: The Science Behind it | [SHINES] Kang L. Wang <i>UC Los Angeles</i> Topological spintronic heterostructures and their properties – examples of the collaborative research in SHINES |
| IV-4 | 2:30 PM | [CCDM] D. R. Strongin <i>Temple</i> Theory and Computation Working with Experiment to Understand and Improve Water Splitting Catalysts | [NECCES] M. D. Radin <i>UC Santa Barbara</i> The Materials Physics of Lithium (De)intercalation in Layered Oxide Cathodes | [CASP] Cherie R. Kagan <i>U. Pennsylvania</i> Mechanisms for Charge Transport and Photoconductance in Mesoscale Quantum Dot Assemblies | [CNGMD] S. Lany, J. Tate <i>NREL, OSU</i> Novel Phase Diagram Behavior and Materials Design in Heterostructural Semiconductor Alloys | [NCGC] Hang Deng <i>LBNL</i> Investigation of Fracture Alteration using a Coupled Modeling and Experimental Approach | [CHWM] T. M. Besmann <i>U. South Carolina</i> Volume Based Thermodynamics Approach Applied to Salt Inclusion Materials | [CDMFTS] C. C Homes <i>BNL</i> Optical properties of the narrow-gap semiconductor FeSb ₂ |

2017 EFRC-HUB-CMS PI MEETING – GRAPHIC AGENDA FOR TUESDAY, JULY 25, 2017

| | | C. Catalysis | D. Energy Storage | H. Solar Energy Conversion | J. Materials and Chemistry by Design | B. Carbon Sequestration | E. Nuclear Energy & Waste | F. Quantum Materials |
|-------------|----------------|---|--|--|--|---|--|---|
| Room | | <i>Thurgood North</i> | <i>Thurgood East</i> | <i>Thurgood South</i> | <i>Thurgood West</i> | <i>Lincoln 2</i> | <i>Lincoln 5</i> | <i>Lincoln 6</i> |
| IV-5 | 2:50 PM | [CME] <u>Shannon S. Stahl</u> <i>U. Wisconsin</i> Development of Molecular Mediators for Improved Electrochemical Energy Conversion | [CEES] <u>Maria Chan</u> <i>ANL</i> Characterization and modeling of oxygen reactivity and structural evolution during electrochemical charging of Li-rich Li_5FeO_4 | [C2SEPEM] <u>J. B. Neaton</u> <i>LBNL, UC Berkeley</i> Origins of Singlet Fission in Solid Pentacene from an Ab Initio Green's-Function Approach | [EDDE] <u>Yuri N. Osetskiy</u> <i>ORNL</i> Diffusion and Mass Transport in Concentrated Solid Solution Alloys: Features and Effects to Radiation Damage | [CFSES] <u>Matt Balhoff</u> <i>UT Austin</i> Rock Mechanical Alteration Due to Flow of CO_2 -Charged Brine: Shear Strength of Crystal Geysers Outcrop Samples | [CAST] <u>Ryan Baumbach</u> <i>Florida State/NHMFL</i> Harnessing the f-electron state in novel high temperature waste forms | [S3TEC] <u>Vazrik Chiloyan, Keith Nelson</u> <i>MIT</i> Thermal transport on experimentally imposed length scales: Non-diffusive kinetics, phonon mean free paths, and first- ... |
| IV-6 | 3:10 PM | [JCAP] <u>Jens K. Nørskov</u> <i>SLAC</i> Understanding trends in CO_2 reduction electro-catalysis | [NEES] <u>Yue Qi</u> <i>Michigan State</i> Quantify the Fundamental Irreversible Structural and Chemical Changes for Nanostructure Designs in Battery Applications | [CASP] <u>Matthew Beard</u> <i>NREL</i> Carrier Multiplication in Semiconductor Quantum Dots: Current Status and Future Prospects | [IDREAM] <u>Aurora Clark</u> <i>Washington State</i> Developing a Multiscale Understanding of Aluminum Transformations with Integrated Simulation and Spectroscopy | [GSCO2] <u>A. Elbanna</u> <i>UIUC</i> Towards a Multiscale Physics Based Framework for Modeling Fluid Infiltrated Fault Zones with an Eye for Induced Seismicity in Energy Applications | [MSA] <u>Albert Migliori</u> <i>LANL</i> New Insights into the Physics and Aging of Plutonium Metal | [CDMFTS] <u>S. Choi</u> <i>BNL</i> Transport properties of correlated FeSb_2 : first principles combined with dynamical mean field theory |

3:30 – 5:00 **Poster Session II, Exhibition Hall C; 4:15 Announce winners of the *Graduate Student and Postdoctoral Team Science Competition***