2023 EFRC-HUB-CMS-CCS PI MEETING LIGHTNING TALK CONTEST

There are more than 1,800 graduate students and postdoctoral researchers involved in the current Energy Frontier Research Centers (EFRC), BES energy storage and fuels from sunlight Energy Innovation Hubs, BES Computational Materials Sciences awards (CMS), and BES Computational Chemical Sciences awards (CCS).

In 2023, the students and postdoctoral researchers involved in the current Energy Frontier Research Centers (EFRC), BES energy storage and fuels from sunlight Energy Innovation Hubs (Hubs), BES Computational Materials Sciences awards (CMS), and BES Computational Chemical Sciences awards (CCS) were challenged to present their center's research or idea within a **100-second "Lightning Talk"** as part of the 2023 Virtual EFRC-Hub-CMS-CCS PI Meeting held on October 18-20, and October 26, 2023. Each center was invited to nominate a student or postdoctoral researcher to showcase the center's learnings or key highlights of research outcomes.

The lightning talks were separated into three meeting days and organized by research topical areas.

DOE's EFRC management team selected **3 lightning talk winners** from each of the meeting days. Winners and nominees are shown below in no particular order.

The lightning talks abstracts can be found on pages 6-74 of the 2023 EFRC-Hub-CMS-CCS PI Meeting Program Book.

Winners on September 19, 2023
(Advanced Manufacturing; Hydrogen; Separations; Solar)

Characterization Of Bacterial Microcompartment Shell Formation Through Denaturant-Induced Sheet Dismantling And Subsequent Shell Self-Assembly

[EFRC - CCBC]

Kyleigh Range[1], Joshua MacCready[2], Markus Sutter[1,2], Sam Snyder[3], Arinita Pramanik[1], Nina Ponomarenko[3], Daniel Ducat[2,4], Paul Ashby[1], Michaela TerAvest[4], Corie Ralston[1]

[1]Lawrence Berkeley National Laboratory; [2]Michigan State University; [3]Argonne National Laboratory

Kyleigh Range, an undergraduate at Cal State East Bay

Xylan Plays a Critical Role in Patterned Secondary Cell Wall Formation

[EFRC – CLSF]

Sarah A. Pfaff, Edward R. Wagner, Ying Gu, Daniel J. Cosgrove

The Pennsylvania State University

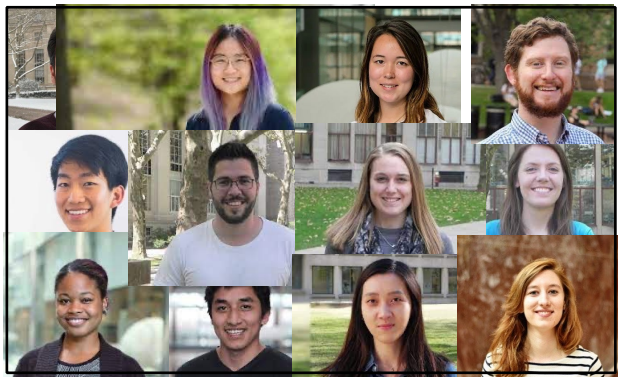
Sarah A. Pfaff

Photocatalysis in a New Light: A Biohybrid Approach for Improved Reactivity with Tunable Low-Energy Light Excitation

[EFRC – BioLEC]

Paul T. Cesana[1], Beryl X. Li[2], Claire G. Page[2,3], Samuel G. Shepard[4], Stephen I. Ting[2,5], Dvir Harris[1], Stephanie M. Hart[1], Courtney M. Olson[1], Megan A. Emmanuel[2], Jesus I. Martinez Alvarado[2], Minjung Son[1], Talia J. Steiman[2], Felix N. Castellano[4], Abigail G. Doyle[2,5], Todd K. Hyster[2,3], David W. C. MacMillan[2], Gabriela S. Schlau-Cohen[1]

[1]Massachusetts Institute of Technology; [2]Princeton University; [3]Cornell University; [4]North Carolina State University; [5]University of California, Los Angeles



Student and post-doc authors of this work, left to right, as listed in author list.

Winners on September 20, 2023
(Energy Storage; Environmental Management; Nuclear; Subsurface; Water)

The Duality in Damage: Multi-Scale Investigations Into Corrosion and Irradiation Effects in Salt-Facing Nuclear Reactor Materials

[EFRC – FUTURE]

Sean H. Mills[1,2], Ryan D. Hayes[1], Ho Lun Chan[3], Nathan Bieberdorf[1], Minsung Hong[1], Elena Romanovskaia[3], Alexandra M. Kennedy[1], Laurent Capolungo[4], Mark Asta[1], John R. Scully[3], Peter Hosemann[1], Raluca O. Scarlat[1], Andrew M. Minor[1,2]

[1]University of California Berkeley, [2]Lawrence Berkeley National Laboratory, [3]University of Virginia, [4] Los Alamos National Laboratory

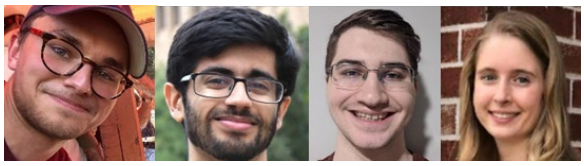
Sean Mills

Mechanisms underlying mixed salt partitioning in uncharged poly(ethylene oxide)-based membranes

[EFRC – M-WET]

Everett S. Zofchak, Aubrey E. Quigley, Jordyn G. Yoh, Kevin K. Reimund, Nathaniel A. Lynd, Benny D. Freeman, Venkat Ganesan

University of Texas at Austin



(from left) Everett Zofchak, Rahul Sujanani, Nico Marioni, and Aubrey Quigley

Mechanochemical Phenomena at the Alkali Metal/Solid Electrolyte Interface

[EFRC – MUSIC]

Catherine Haslam[1], S. Sandoval[2], B. Vishnugopi[3], J. Sakamoto[1], D. Mitlin[4], P. Mukherjee[3], M. McDowell[2]

[1]University of Michigan; [2]Georgia Institute of Technology; [3]Purdue University; [4]University of Texas, Austin

Catherine Haslam

Winners on September 26, 2023
(Microelectronics; QIS)

Leveraging the resilience of diamond with its unique material properties towards Next Generation Grid innovation

[EFRC – ULTRA]

Kelly Woo[1], Mohamadali Malakoutian[1], Matthias Muehle[2], Franz Koeck[4], Timothy Grotjohn[3], Stephen Goodnick[4], Robert Nemanich[4], Srabanti Chowdhury[1]

[1]Stanford University, [2]Fraunhofer USA Center, [3]Michigan State University, [4]Arizona State University

(from left) Kelly Woo and Mohamadali Malakoutian

Layered semiconductors are changing the game in quantum information

[EFRC – Pro-QM]

Chiara Trovatello[1]

[1]Columbia University

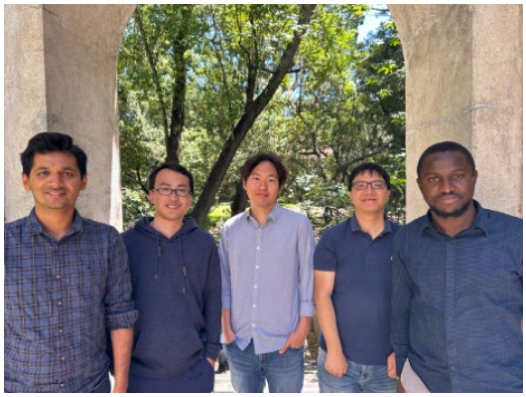
Chaira Trovatello

Diverse Nature of Excitonic States in Transition Metal Dichalcogenide Moiré Superlattices

[CMS – C2SEPEM]

Mit H. Naik[1,2], Hongyuan Li[1,2], Chen Hu[1,2], Woochang Kim[1,2], Yusuf Shaidu[1,2], Ziyu Xiang[1,2], Jeffrey B. Neaton[1,2], Felipe H. da Jornada[3], Feng Wang[1,2], and Steven G. Louie[1,2]

[1]University of California at Berkeley; [2]Lawrence Berkeley National Lab; [3]Stanford University



(from left) Mit H. Naik, Hongyuan Li, Woochang Kim, Chen Hu and Yusuf Shaidu

Lightning Talk Challenge Finalists

Speeding Up Materials Synthesis By Manipulating Transport

[EFRC – GENESIS]

Gabrielle E. Kamm[1], John J. Ferrari[1], Guanglong Huang[2], Eymana Maria[2], Danrui Hu[1], Simon M. Vornholt[2], Rebecca D. McAuliffe[3], Gabriel M. Veith[3], Katsuyo S. Thornton[2], Wenhao Sun[2], Karena W. Chapman[1]

[1]Stony Brook University, [2]University of Michigan, [3]Oak Ridge National Laboratory.

(from left) Gabrielle Kamm, John Ferrari and Eymana Maria

Accelerating Energy-Efficient Advanced Materials Discovery: Degradable pDCPD Thermosets

[EFRC – REMAT]

Yasmeen S. AlFaraj[1], Anna A. Cramblitt[2], Somesh Mohapatra[1], Yuyan Wang[1], Avni Singhal[1], Benjamin Suslick[2], Jeff Moore[2], Nancy Sottos[2], Rafael Gomez-Bombarelli[1], Jeremiah A. Johnson[1]

[1]Massachusetts Institute of Technology, [2]University of Illinois Urbana-Champaign

Yasmeen AlFaraj

A Tandem Photoelectrochemical/Photothermal System for CO_2 Reduction to Liquid Fuels

[Hub – LiSA]

Aisulu Aitbekova,[1,2] Kyra Yap,[1,3] Matthew Salazar,[1,2] Magel Su,[1,2] Tobias A. Kistler,[1,4] Peter Agbo,[1,4] Theodor Agapie,[1,2] Jonas C. Peters,[1,2] Thomas F. Jaramillo,[1,3] Alexis T. Bell,[1,4] Harry A. Atwater[1,2]

[1]Liquid Sunlight Alliance, [2]California Institute of Technology, [3]SLAC National Accelerator Laboratory, [4]Lawrence Berkeley National Laboratory

Aisulu Aitbekova

Circular Polyolefins: Design Principles For Sustainable Plastics

[EFRC – CPI]

Sam Marsden[1], María Ley-Flores[1], Riccardo Alessandri[1], Isabella Vettese[1], Zubin Kumar[1], Archit Chabbi[2], Juan J. de Pablo[1], Stuart J. Rowan[1]

[1]University of Chicago; [2]Rice University

(from upper left) Sam Marsden, Isabella Vettese, and Zubin Kumar (from lower left) María Ley-Flores, Riccardo Alessandri, and Archit Chabbi

Automating model space selection in fragment-based multireference methods

[CCS – ExaPUC]]

Matthew R. Hermes[1], Valay Agarawal[1], Laura Gagliardi[1], Cong Liu[2], Christopher Knight[2], Rishu Khurana[2]

[1]University of Chicago; [2]Argonne National Laboratory

Matthew R. Hermes

Efficient and Scalable, High-Fidety Green's function theory of Electronic Structure and Response functions

[CCS – QuestC]

Peyton Cline[1], Mushir Thodika[1], Casey Eichstaedt , Dimitar Pashov[2], Brian Cunningham[3], Myrta Gruening[3], Mark van Schilfgaarde[1]

[1]National Renewable Energy Laboratory, [2]King's College London, [3]Queen's University Belfast

Mark van Schilfgaarde

Stable solid molecular hydrogen above 900K from a machine-learned potential trained with diffusion Quantum Monte Carlo

[CMS – QMC-HAMM]

Hongwei Niu,[1] Yubo Yang,[2,3] Scott Jensen,[3] Markus Holzmann,[4] Carlo Pierleoni,[5] and David M. Ceperley[3]

[1]Harbin Institute of Technology; [2]Flatiron Institute; [3]University of Illinois Urbana-Champaign; [4]University Grenoble Alpes; [5]University of L'Aquila

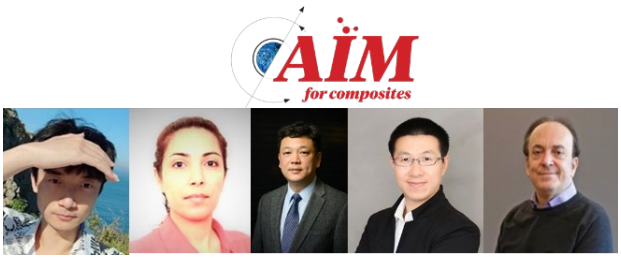
Scott Jensen

Predicting Transient Response of Composites Subject to Dynamic Loading Using Deep Neural Operator Learning

[EFRC – AIM for Composites]

Minglei Lu[1], Elham Kiyani[2], Gang Li[1], Zhen Li[1], George Karniadakis[2].

[1]Clemson University; [2]Brown University



AIM Team

Electrocatalytic Properties of Pulsed Laser-Deposited Titanium Dioxide And Titanium Oxynitride Thin Films Grown on Photo-Adsorbing Single Crystal Substrates with Different Orientations

[EFRC – CEDARS]

Sheila Cherono[1], Ikenna Chris-Okoro[1], Swapnil Shankar Nalawade[1], Austin Reese[2], Brady Bruno[2], Jacob Som[2], R. Soyoung Kim[3], Johannes Mahl[3], Junko Yano[3], Ethan Crumlin[3], Jin Suntivich[2], Tanja Cuk[4], Bishnu Bastakoti[1], Y.Yun[1], Shyam Aravamudhan[1], Dhananjay Kumar[1]

[1]North Carolina Agricultural and Technical State University; [2]Cornell University; [3]Lawrence Berkeley National Laboratory; [4]University of Colorado at Boulder

Sheilah Cherono

Mechanistic Insights of RuO_2-Mediated Butene Electrosynthesis

[EFRC– CD4DC]

Joseph Hupp,[1] Chibueze V Amanchukwu,[2] Anna Wuttig,[2] Ksenija D Glusac[3], Laura Gagliardi[2], Gautam Stroscio,[2] Arturo Sauza de la Vega,[2] Hannah Fejzic,[2] Reginaldo J. Gomes,[2] Špela Kunstelj,[2] Biki Behera[3]

[1]Northwestern University; [2]The University of Chicago; [3]Unviersity of Illinois at Chicago

Špela Kunstelj

Interactive Dynamic Energy Analysis (IDEA): A New Tool for Predicting Catalytic Reaction Pathways through Joint Density-Functional Theory

[EFRC – CABES]

Colin R. Bundschu, Mahdi Ahmadi, Juan Felipe Méndez-Valderrama, Héctor D. Abruña, Tomás A. Arias

Cornell University

Enhanced Methanol Production from Photoelectrochemical CO_2 Reduction via Interface and Microenvironment Tailoring

[Hub – CHASE]

Bo Shang[1], Fengyi Zhao[2], Yuanzuo Gao[1], Jing Li[1], Conor L. Rooney[1], Colton Sheehan[3], Oliver Leitner[1], Langqiu Xiao[3], Thomas E. Mallouk[3], Tianquan Lian[2], Hailiang Wang[1]

[1]Yale University; [2]Emory University; [3]University of Pennsylvania

Hailiang Wang

High-Throughput Potential-Dependent Modeling of the Electrochemical Nitrogen Reduction Reaction

[CCS – BEAST]

Cooper Tezak,[1] Nicholas Singstock,[1] Abdulaziz Alherz,[1] Derek Vigil-Fowler,[2] Christopher Sutton,[3] Ravishankar Sundararaman,[4] Charles Musgrave.[1]

[1]Univeristy of Colorado Boulder, [2]National Renewable Energy Laboratory, [3]University of South Carolina, [4]Rensselaer Polytechnic Institute.

Cooper Tezak

Automated Generation of Microkinetics for Heterogeneously Catalyzed Reactions Considering Correlated Uncertainties

[CCS – ECC]

Bjarne Kreitz, C. Franklin Goldsmith

Brown University

Bjarne Kreitz

Functionalized Ionic liquid electrolyte controls CO_2 electroreduction product selectivities and overpotentials over transition metals

[EFRC – 4C]

Saudagar Dongare[1], Oguz K. Coskun[1], Louise Berben[2], Manu Gautam[3], Bijandra Kumar[4], Joshua Spurgeon[3], Robert Sacci[5], Anastassia N. Alexandrova[6], and Burcu Gurkan[1]

[1]Case Western Reserve University; [2]University of California, Davis; [3]University of Louisville; [4]Elizabeth City State University; [5]Oak Ridge National Laboratory; [6] University of California, Los Angeles

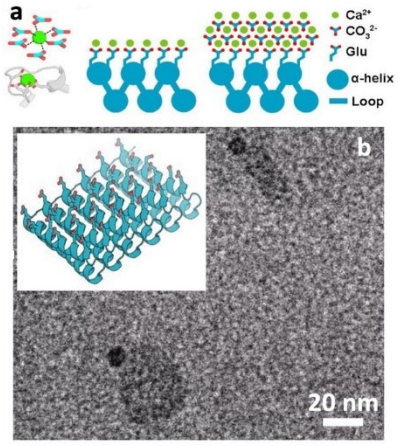
(From upper left) Saudagar Dongare, Oguz K. Coskun, Manu Gautam; (From middle left) Louise Berben, Bijandra Kumar, Joshua Spurgeon; (From lower left), Robert Sacci, Anastassia N. Alexandrova, and Burcu Gurkan

Directing Polymorph Specific Calcium Carbonate Formation With De Novo Designed Protein Templates

[EFRC – CSSAS]

Fatima Davila-Hernandez[1]

[1]University of Washington



a - Schematic illustrating concept for a flat helical repeat protein designed de novo to template the organization of Ca^{2+} and CO_3^{2-} ions into a crystalline motif in order to drive crystal nucleation, b - Frame from an in situ TEM movie showing the nucleation of calcite (dark gray) adjacent to supramolecular assemblies (light gray) of Ca^{2+} ions and designed proteins having the structure shown in the inset.

Combining X-Ray Scattering and Optical Spectroscopy to Characterize Ion and Solvent Intercalation in π-conjugated Polymers and Their Impact on Optoelectronic Function

[EFRC – SPECS]

Spencer Yeager[1]

[1]University of Arizona

A Multiscale Computational Framework for Biomolecular Energy Transduction: From Electrons to the Mesoscale

[CCS – CMSET]

[1]Scott Kaiser, [1]Sahithya Sridharan Iyer, [1]Daniel Beckett, [1]Siva K. Dasetty, [3]Tomasz Skora, [2]Garnet K. L. Chan, [3]Tamara Bidone, [1]Andrew Ferguson, [1]Gregory A. Voth

[1]University of Chicago, [2]California Institute of Technology, [3]University of Utah

(from left) Scott Kaiser, Sahithya Sridharan Iyer

Catalytic Chemical Recycling of Post-Consumer Polyethylene

[EFRC – iCOUP]

Shilin Cui[1], Alejandra Arroyave[2], Andrew L. Kocen[1], Jaqueline C. Lopez[1], Anne M. LaPointe[1], Massimiliano Delferro[2], Geoffrey W. Coates[1]

[1]Cornell University; [2]Argonne National Laboratory

Shilin Cui

Exploring Symmetry Breaking and Structural Dimensionality Engineering in HOIPs: Unraveling Emergent Spin, Electronic, and Optical Properties

[EFRC – CHOISE]

Yi Xie,[1] Jack Morgenstein,[1] Gabrielle Koknat,[1] Nicholas J. Weadock,[2] Junxiang Zhang,[2] Heshan Samuditha Weerasinghe Hewa Walpitage,[3] Peter C. Sercel,[4] Alan Phillips,[5] Naidel A. M. S. Caturello,[6] John Colton,[7] Xiaoping Wang,[8] Ruyi Song,[1] Benjamin G. Bobay,[1] Jeffrey Blackburn,[5] Matthew C. Beard,[5] Zeev Valy Vardeny,[3] Seth Marder,[2] Michael F Toney,[2] Volker Blum,[1] and David B. Mitzi[1]

[1]Duke University; [2]University of Colorado Boulder; [3]University of Utah; [4]Center for Hybrid Organic Inorganic Semiconductors for Energy; [5]National Renewable Energy Laboratory; [6]Federal University of ABC; [7]Brigham Young University; [8]Oak Ridge National Laboratory

Mechanisms That Govern Long-Term Stability of ZIF-8-Based Porous Liquids

[EFRC – UNCAGE-ME]

Matthew J. Hurlock,[1] Matthew S. Christian,[1] Jessica M. Rimsza,[1] and Tina M. Nenoff[1]

[1]Sandia National Laboratories

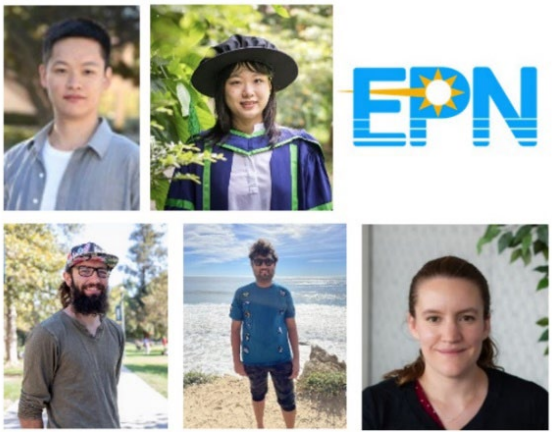
(from left) Matthew J. Hurlock, Matthew Christian

Temporal Evolution of Nanomaterials Structure and Function during Hydrogen Evolution Induction Period for State-of-the-Art Pt-Loaded Rh-Doped $SrTiO_3$ Nanoparticles

[EFRC – EPN]

Zejie Chen[1], Wenjie Zang[1], Justin T. Mulvey[1], Pushp Raj Prasad[1], Jocienne N. Nelson[2], Akihiko Kudo[3], Xiaoqing Pan[1], Joseph P. Patterson[1], A. Alec Talin[2], Shane Ardo[1]

[1]University of California Irvine; [2]Sandia National Laboratories; [3]Tokyo University of Science



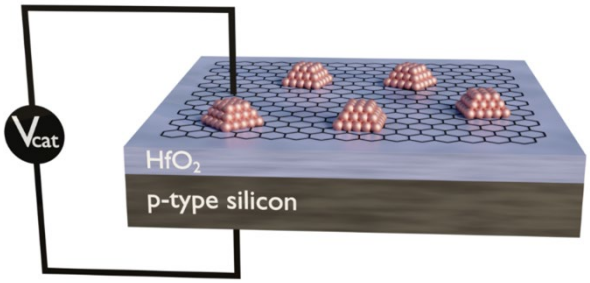
(from upper left) Zejie Chen, Wenjie Zang; (from lower left) Justin T. Mulvey, Pushp Raj Prasad, Jocienne N. Nelson

Center for Programmable Energy Catalysis

[EFRC – CPEC]

Paul J. Dauenhauer[1]

[1]University of Minnesota



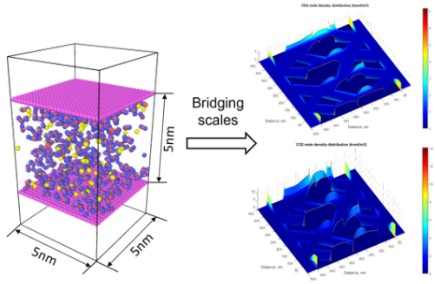
A catalytic condenser modulates the charge density of metal nanoclusters to alter surface reactions.

Coupled Phase Behavior and Transport in Complex Confined Nanoporous Networks

[EFRC – CMC-UF]

Lingfu Liu[1], Nijat Rustamov[1], Saman Aryana[1]

[1]University of Wyoming



(left) A Schematic of a nano-slit containing a CH_4-CO_2 mixture, (right) Mole density distribution of the mixture in a confined pore network.

Why does dissolving salt in water decrease its dielectric permittivity

[CCS – CSI]

Chunyi Zhang[1,2], Shuwen Yue[1], Athanassios Z. Panagiotopoulos[1], Michael L. Klein[2], Xifan Wu[2]

[1]Temple University; [2]Princeton University

Probing Higher Order Phonon Anharmonicity in Ceramic Nuclear Fuels under Temperature and Pressure Extremes

[EFRC – TETI]

Saqeeb Adnan[1], Amey Khanolkar[2], Marat Khafizov[1], Chris Marianetti[3], Michael Manley[4], David H. Hurley[2]

[1]The Ohio State University; [2]Idaho National Laboratory; [3]Columbia University; [4]Oak Ridge National Laboratory

Experimental Observations of Chemo-mechanical coupling during Carbon Mineralization in Fractures

[EFRC – GMCS]

Chelsea Wren Neil[1], Haylea Nisbet[1], Uwaila Iyare[1], Yun Yang[1], Bill Carey[1], Hari Viswanathan[1], Peter Kang[2]

[1]Los Alamos National Laboratory; [2]University of Minnesota

Chelsea Wren Neil

Advances in the Effects of Ionizing Radiation on the Stability and Reactivity of Molten Salts

[EFRC – MSEE]

Alejandro Ramos-Ballesteros[1,2], Kazuhiro Iwamatsu[3], Santanu Roy[4], Ruchi Gakhar[1], Phillip Halstenberg[5], Michael E. Woods[1], Bobby Layne[3], Jay A. LaVerne[2] , Simon M. Pimblott,[1] James F. Wishart[3], and Gregory P. Holmbeck[1]

[1]Idaho National Laboratory, [2]University of Notre Dame, [3]Brookhaven National Laboratory, [4]Oak Ridge National Laboratory, [5]University of Tennessee, Knoxville

(left) Alejandro Ramos-Ballesteros, (right) Radiation-induced defects in solid chloride salts.

Structure and Solvation Dynamics of Deep Eutectic Solvents

[EFRC – BEES2]

Desiree Mae Prado[1], Rathiesh Pandian[1], Ibrahim Alfurayj[1], Xiaochen Shen[1], Carla Fraenza[2], Stephanie Spittle[3], William Brackett[3], Bryce Hansen[4], Kaylie Glynn[4], Yong Zhang[5], Brian Doherty[6], Robert Savinell[1], Steve Greenbaum[2], Joshua Sangoro[4], Edward Maginn[5], Mark Tuckerman[6], and Clemens Burda[1]

[1]Case Western Reserve University; [2]Hunter College of CUNY; [3]University of Tennessee, Knoxville; [4]The Ohio State University; [5]University of Notre Dame; [6]New York University

Desiree Mae Prado

Experimentally-Informed State Dependent Atomic Forces in Real Fluid Ensembles

[EFRC – MUSE]

Brennon L. Shanks, Michael P Hoepfner

University of Utah

Reducing the energy barrier for proton transport in polymers under anhydrous conditions

[EFRC – FaCT]

Zitan Huang[1], Michelle Lehmann[3], Michael Hickner[2], Tomonori Saito[3], Ralph Colby[1]

[1]Penn State University; [2]Michigan State University; [3]Oak Ridge National Laboratory

Zitan Huang

New reactive force fields explore molecular reactivity in concentrated electrolytes

[EFRC – IDREAM]

Maxime Pouvreau[1], Qing Guo[2], Hsiu-Wen Wang[3], Gregory K. Schenter[1], Carolyn I. Pearce[1,4], Aurora E. Clark[2,1], Kevin M. Rosso[1]

[1]Pacific Northwest National Laboratory; [2]University of Utah; [3]Oak Ridge National Laboratory; [4]Washington State University

Maxime Pouvreau

Modeling Ion Exchange in Faujasites: A Methods Study using Density Functional Theory

[EFRC – CHWM]

An T. Ta[1], Ayoub Daouli[2], R. Seaton Ullberg[1], Vanessa Proust[3], Agnès Grandjean[3], Michael Badawi[2], Simon R. Phillpot[1]

[1]University of Florida, Gainesville, [2]University of Lorraine, [3]CEA, DES, ISEC, DMRC, Univ Montpellier

(from left): An T. Ta, Ayoub Daouli, R. Seaton Ullberg, Vanessa Proust

Ion Transport in MoS_2 Nanochannels

[EFRC – AMEWS]

Eli Hoenig

University of Chicago

New Routes to Hydrogen Incorporation in $SrTiO_3$

[EFRC – HEISs]

Megan Burrill[1], Yea-Shine Lee[1], Roberto dos Reis[1], Zhi Li[1], Erica Truong[1], Guennnadi Evmenenko[1], James R. Rondinelli[1], Vinayak P. Dravid[1], Chris Wolverton[1], Yan-Yan Hu[2], Michael J. Bedzyk[1], Sossina M. Haile[1]

[1]Northwestern University; [2]Florida State University

Megan Burrill

Refractory Transition Metal Oxides as Electrodes in Lithium-Ion Batteries

[EFRC – SCALAR]

Ashlea Patterson,[1] Yunkai Luo,[2] Yucheng Zhou,[2] Laurent Pilon,[2] Bruce Dunn,[2] Ram Seshadri[1]

[1]University of California, Santa Barbara, [2]University of California, Los Angeles

Nanofluidic Platforms for Addressing Knowledge Gaps at the Water-Energy Nexus

[EFRC – CENT2]

Yu-Ming Tu[1], Rahul Prasanna Misra[1], Matthias Kuehne[2], Hananeh Oliaei[3], Cody L. Ritt[1], Samuel Faucher[1], Kyle Sendgikoski[4], Xintong Xu[5], John Cumings[4], Arun Majumdar[5], Narayana Aluru[3], Daniel Blankschtein[1], and Michael S. Strano[1*]

[1]Massachusetts Institute of Technology; [2]Brown University; [3]University of Illinois Urbana-Champaign; [4]University of Maryland; [5]Stanford University

(from left) Yu-Ming Tu, Rahul Prasanna Misra, Matthias Kuehne, and Cody L. Ritt

Multiscale Nuclear-Electronic Orbital Quantum Dynamics in Complex Environments

[CCS – NEOQD]

Eleftherios Lambros[1], Aodong Liu[1], Mathew Chow[2], Sharon Hammes-Schiffer[2], Xiaosong Li[1]

[1]University of Washington; [2]Yale University

Studying the Impact of Interactions on Nonlinear Optical Processes Using Real-Time Ab-Initio Based Simulations

[CMS – NPNEQ]

Sangeeta Rajpurohit[1], Xavier Andrade[1]

[1]Lawrence Berkeley National Laboratory

FLOSIC for Complex Anion-Solvent Solutions

[CCS – FLOSIC]

Kushantha P. K. Withanage[1], Alexander I. Johnson[1], Mark R. Pederson[1] and Koblar A Jackson[2]

[1]The University of Texas at El Paso, [2]Central Michigan University

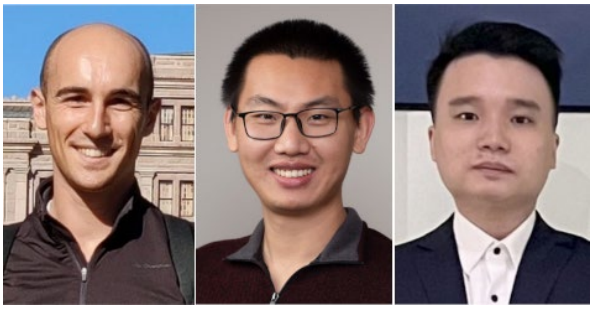
Kushantha Withanage

Ab Initio Many-Body Theory of Polarons

[CMS – EPW]

Jon Lafuente-Bartolome[1,2], Chao Lian[1], Weng Hong Sio[1,2], Idoia G. Gurtubay[2], Asier Eiguren[2], Feliciano Giustino[1]

[1]The University of Texas at Austin, [2]University of the Basque Country at Bilbao, [3]University of Macau



(from left): Jon Lafuente-Bartolome, Chao Lian, Weng Hong Sio

Superfluid density through a Van Hove singularity: Sr_2RuO_4 under uniaxial strain

[EFRC – QSQM]

Eli Mueller[1,2], Yusuke Iguchi[1], Fabian Jerzembeck[3], Marisa L. Romanelli[4], Jorge O. Rodriguez[4], Clifford W. Hicks[5], Yoshiteru Maeno[6], Vidya Madhaven[4], Kathryn A. Moler[1,2]

[1]SLAC National Accelerator Laboratory; [2]Stanford University; [3]Max Planck Institute; [4]University of Illinois, Urbana-Champaign; [5]University of Birmingham; [6]Kyoto University

(from left) Eli Mueller, Marisa Romanelli, Jorge Rodriguez, Fabian Jerzembeck

Predictive Inverse Design of Neuronal Components

[EFRC – REMIND]

Timothy D. Brown,[1,2] Suhas Kumar,[1] Adelaide Bradicich,[2] R. Stanley Williams,[2] Patrick J. Shamberger[2]

[1]Sandia National Laboratories—Livermore; [2]Texas A&M University

Timothy D. Brown

Towards accurate polaritonic potential energy surfaces with cavity quantum electrodynamics complete active space configuration interaction theory

[CCS – MAPOL]

Nam Vu[1], Niranjan Govind[2], Jonathan Foley[1]

[1]University of North Carolina-Charlotte; [2]Pacific Northwest National Laboratory

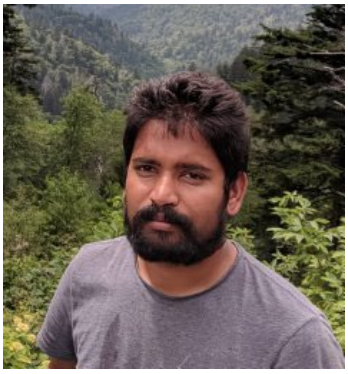
Dr. Nam Vu

Theoretical RIXS investigation of the infinite layers nickelates

[CMS – Comscope]

Umesh Kumar[1], Corey Melnick[2], Gabriel Kotliar[1,2]

[1]Rutgers University; [2]Brookhaven National Lab



Umesh Kumar

Fragile superconductivity in a Dirac metal

[EFRC – IQM]

Chris J. Lygouras[1], Junyi Zhang[1], Jonah Gautreau[2], Mathew Pula[2], Sudarshan Sharma[2], Shiyuan Gao[1,3], Tanya Berry[1], Thomas Halloran[1], Peter Orban[1], Gael Grissonnanche[3], Juan R. Chamorro[1], Kagetora Mikuri[3], Dilip K. Bhoi[4], Maxime A. Siegler[1], Kenneth J.T. Livi[1], Yoshiya Uwatoko[4], Satoru Nakatsuji[1,4,5,6], B. J. Ramshaw[3,6], Yi Li[1], Graeme M. Luke[2,7], Collin L. Broholm[1,8], and Tyrel M. McQueen[1].

[1]Johns Hopkins University; [2]McMaster University; [3]Cornell University; [4]University of Tokyo; [5]CREST, Japan Science and Technology Agency; [6]Canadian Institute for Advanced Research; [7]TRIUMF, Vancouver, Canada; [8]NIST Center for Neutron Research.

Chris Lygouras

Harnessing Quantum Geometry for the Detection and Manipulation of Antiferromagnetism

[EFRC – CATS]

Jianxiang Qiu[1], Zumeng Huang[2], Junyeong Ahn[1], Zhe Sun[2], Anyuan Gao[1], Jian Tang[2], Houchen Li[1], Ashvin Vishwanath[1], Qiong Ma[2], Suyang Xu

[1]Harvard University; [2]Boston College

Manipulating Molecular Entanglement Via Inelastic Scattering Of Itinerant Electrons

[EFRC – M²QM]

Christian Bunker, Silas Hoffman[1], Xuanyan Jiang[1], Eric Swizter[3], Shuang-Long Liu[1], Garnet Chan[6], Hai-Ping Cheng[1,8], George Christou[1], Arthur Hebard[1], Richard Hennig[1], Steve Hill[2,7], Mark Pederson[4], Talat Rahman[3], Michael Shatruk[2], John Stanton[1], Neil Sullivan[1], Samuel Trickey[1], Vivien Zapf[5], Xiaoguang Zhang[1], and Xiao-Xiao Zhang[1]

[1]University of Florida; [2]Florida State University; [3]University of Central Florida; [4]University of Texas El Paso, [5]Los Alamos National Laboratory; [6]California Technology Institute; [7]National Laboratory of High Magnetic Field, [8]Northeastern University

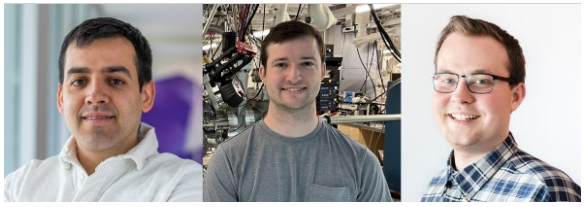
Christian Bunker

Atomic Scale Polarization Switching in Novel Ferroelectrics

[EFRC – 3DFeM]

Sebastian Calderon V,[1] John Hayden,[2] Steven M. Baksa,[2] William Tzou,[1] Susan Trolier-McKinstry,[2] Ismaila Dabo,[2] Jon-Paul Maria,[2] Elizabeth C. Dickey[1]

[1]Carnegie Mellon University, [2]Pennsylvania State University



(from left) Sebastian Calderon, John Hayden, Steven M. Baksa

Long-range, Non-local Switching of Spin Textures in a Frustrated Antiferromagnet

[EFRC – NPQC]

Shannon C. Haley[1,2], Valeria Rosa Rocha[1,2], Eran Maniv[3], Tessa Cookmeyer[1,2], Susana Torres-Londono[1], Meera Aravinth[1], Joel Moore[1,2], Robert J. Birgeneau[1], James G. Analytis[1,2]

[1]University of California, Berkeley; [2]Lawrence Berkeley National Laboratory; [3]Ben-Gurion University of the Negev

Valeria Rosa Rocha

Thermodynamics of Non-linear Optical Responses of Ferroelectrics

[CMS – COMMS]

Aiden Ross[1], Rui Zu[1], Anna Morozovska[2], Venkatraman Gopalan[1], Long-Qing Chen[1]

[1]Penn State University, [2]Ukraine Academy of Sciences.

(from left) Aiden Ross, Rui Zhu

Non-local Interactions in Hydrogenated Perovskite Nickelate Synaptic Networks

[EFRC – Q-MEEN-C]

Ravindra S. Bisht[1], Jaeseoung Park[2], Haoming Yu[3], Chen Wu[4], Nikhil Tilak[1], Sylvie Rangan[1], Tae J. Park[3], Yifan Yuan[1], Sarmistha Das[4], Uday Goteti[4], Hee Taek Yi[1], Hussein Hijazi[1], Abdullah Al-Mahboob[5], Jerzy T. Sadowski[5], Hua Zhou[6], Seongshik Oh[1], Eva Y. Andrei[1], Monica T. Allen[4], Duygu Kuzum[2], Alex Frañó[4], Robert C. Dynes[4], and Shriram Ramanathan[1]

[1]Rutgers University; [2]Purdue University; [4]University of California San Diego; [5]Brookhaven National Laboratory; [6]Argonne National Laboratory

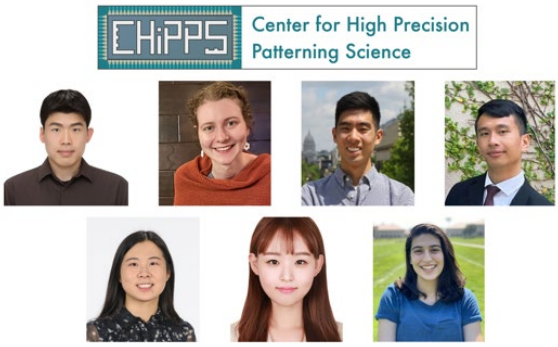
Ravindra S. Bisht

Pushing the Precision Limits in EUV Lithography: Overcoming Stochastics with Directed Self-Assembly and Area-Selective Atomic Layer Deposition

[EFRC – CHiPPS]

Kyunghyeon Lee[1,2], Emma Vargo[3], Christopher J. Eom[1,2], Areza Sumitro[3], Beihang Yu[3], Yujin Lee[4], Maggy Harake[4], Rachel Segalman[5], Stacey Bent[4], Ricardo Ruiz[3], Paul F. Nealey[1,2]

[1]Argonne National Laboratory; [2]University of Chicago; [3]Lawrence Berkeley National Laboratory; [4]Stanford University; [5]University of California, Santa Barbara



(from upper left) Kyunghyeon Lee, Emma Vargo, Christopher J. Eom, Areza Sumitro (from lower left) Beihang Yu, Yujin Lee, Maggy Harake

Circular Dichroism of Crystals from First Principles

[CCS – ADEPTS]

Christian Multunas[1], Andrew Grieder[2], Junqing Xu2, Yuan Ping[2,3], and Ravishankar Sundararaman[1], Rafi Ullah

[1]Rensselaer Polytechnic Institute; [2]University of Wisconsin-Madison; [3]University of California, Santa Cruz

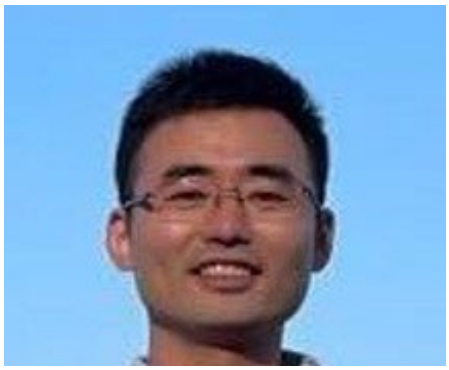
Christian Multunas

Engineering the Formation of Spin-Defects from First Principles

[CMS – MICCoM]

Cunzhi Zhang[1], Francois Gygi [2], Giulia Galli [3, 1]

[1]University of Chicago; [4]University of California, Davis; [3]Argonne National Laboratory



Cunzhi Zhang

A New Generation of Rare-Earth Pseudopotentials and Applications to Quantum Materials

[CMS – CPSFM]

Gani Annaberdiyev[1], Haihan Zhou[2], Benjamin Kincaid[2], Guangming Wang[2], Subhasish Mandal[3], Jaron T. Krogel[1], Lubos Mitas[2], Panchapakesan Ganesh[1]

[1]Oak Ridge National Laboratory; [2]North Carolina State University; [3]West Virginia University

Gani Annaberdiyev

Chemomechanical Modification of Quantum Emission in Monolayer WSe_2

[EFRC – CMQT]

M. Iqbal Bakti Utama[1], Hongfei Zeng[1], Tumpa Sadhukhan[1], Anushka Dasgupta[1], S. Carin Gavin[1], Riddhi Ananth[1], Dmitry Lebedev[1], Wei Wang[2], Jia-Shiang Chen[2], Kenji Watanabe[3], Takashi Taniguchi[3], Tobin J. Marks[1], Xuedan Ma[2], Emily A. Weiss[1], George C. Schatz[1], Nathaniel P. Stern[1], Mark C. Hersam[1]

[1]Northwestern University; [2]Argonne National Laboratory; [3]National Institute for Materials Science, Japan

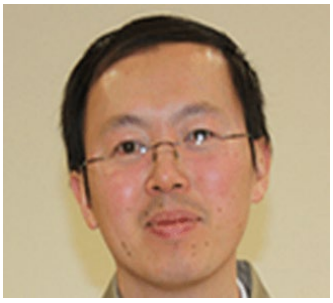
M. Iqbal Bakti Utama

Impacts of Short-range Order on Properties of Group IV Alloys

[EFRC – μ-ATOMS]

Shunda Chen[1], Shang Liu[2], Xiaochen Jin[1], Yunfan Liang[3], J. Zach Lentz[4], Lilian Vogl[5], Damien West[3], Dragica Vasileska[6], Shui-Qing Yu[7], Paul McIntyre[4], Andrew Minor[5], Shengbai Zhang[3], Jifeng Liu[2], Tianshu Li[1]

[1]George Washington University; [2]Dartmouth College; [3]Rensselaer Polytechnic Institute; [4]Stanford University; [5]University of California, Berkeley; [6]Arizona State University; [7]University of Arkansas



Dr. Shunda Chen

Controlling Light Emission from Monolayer MoS_2 With Dielectric Metasurfaces

[EFRC – PTL]

S. C. Lau[1], Y. Liu[1], W. S. Cheng[2], A. Johnson[1], Q. Li[1], E. Simmerman[1], O. Karni[1,3], J. Hu[1], F. Liu[1], M. Brongersma[1], T. F. Heinz[1,3], and J. A. Dionne[1]

[1]Stanford University. [2]National Cheng Kung University, Taiwan. [3]SLAC National Accelerator Laboratory

ACRONYMS

ENERGY FRONTIER RESEARCH CENTERS (EFRCs)

[EFRC – 3DFeM2] Center for 3D Ferroelectric Microelectronics Manufacturing
Susan Trolier-McKinstry, The Pennsylvania State University
Class: 2020 – 2028

[EFRC – 4C] Center for Closing the Carbon Cycle
Jenny Yang, University of California, Irvine
Class: 2022-2026

[EFRC – AIM] Artificially Intelligent Manufacturing Paradigm for Composites
Srikanth Pilla, Clemson University
Class: 2022-2026

[EFRC – AMEWS] Advanced Materials for Energy-Water Systems
Seth Darling, Argonne National Laboratory
Class: 2018 – 2026

[EFRC – BEES2] Breakthrough Electrolytes for Energy Storage Systems
Burcu Gurkan, Case Western Reserve University
Class: 2018 – 2026

[EFRC – BioLEC] Bioinspired Light-Escalated Chemistry
Gregory Scholes, Princeton University
Class: 2018 – 2026

[EFRC – CABES] Center for Alkaline-Based Energy Solutions
Héctor Abruña, Cornell University
Class: 2018 – 2026

[EFRC – CATS] Center for the Advancement of Topological Semimetals
Robert McQueeney, Ames National Laboratory
Class: 2018 – 2026

[EFRC – CCBC] The Center for Catalysis in Biomimetic Confinement
Cheryl Kerfeld, Michigan State University
Class: 2022-2026

[EFRC – CD4DC] Catalyst Design for Decarbonization Center
Laura Gagliardi, University of Chicago
Class: 2022-2026

[EFRC – CEDARS] Center for Electrochemical Dynamics and Reactions on Surfaces
Dhananjay Kumar, North Carolina A&T State University
Class: 2022-2026

[EFRC – CENT2] Center for Enhanced Nanofluidic Transport – Phase 2
Michael Strano, Massachusetts Institute of Technology
Class: 2018 – 2026

[EFRC – CHiPPS] Center for High Precision Patterning Science
Ricardo Ruiz, Lawrence Berkeley National Laboratory
Class: 2022-2026

[EFRC – CHOISE] Center for Hybrid Organic Inorganic Semiconductors for Energy
Matthew Beard, National Renewable Energy Laboratory
Class: 2018 – 2026

[EFRC – CHWM] Center for Hierarchical Waste Form Materials
Hanno zur Loye, University of South Carolina
Class: 2016 – 2025

[EFRC – CLSF] Center for Lignocellulose Structure and Formation
Daniel Cosgrove, Pennsylvania State University
Class: 2009 – 2024

[EFRC – CMC-UF] Center for Mechanistic Control of Unconventional Formations
Anthony Kovscek, Stanford University
Class: 2018 – 2024

[EFRC – CMQT] Center for Molecular Quantum Transduction
Michael Wasielewski, Northwestern University
Class: 2020 – 2028

[EFRC – CPEC] Center for Programmable Energy Catalysis
Paul Dauenhauer, University of Minnesota
Class: 2022-2026

[EFRC – CPI] Center for Plastics Innovation
LaShanda Korley, University of Delaware
Class: 2020 – 2028

[EFRC – CSSAS] Center for the Science of Synthesis Across Scales
François Baneyx, University of Washington
Class: 2018 – 2026

[EFRC – EPN] Ensembles of Photosynthetic Nanoreactors
Shane Ardo, University of California, Irvine
Class: 2022-2026

[EFRC – FaCT] Fast and Cooperative Ion Transport in Polymer-Based Electrolytes
Valentino Cooper, Oak Ridge National Laboratory
Class: 2022-2026

[EFRC – FUTURE] Fundamental Understanding of Transport Under Reactor Extremes
Blas Uberuaga, Los Alamos National Laboratory
Class: 2018 – 2026

[EFRC – GENESIS] A Next Generation Synthesis Center
John Parise, Stony Brook University
Class: 2018-2024

[EFRC – GMCS] Center for Interacting Geo-processes in Mineral Carbon Storage
Emmanuel Detournay, University of Minnesota
Class: 2022-2026

[EFRC – HEISs] Hydrogen in Energy and Information Sciences
Sossina Haile, Northwestern University
Class: 2022-2026

[EFRC – iCOUP] Institute for Cooperative Upcycling of Plastics
Aaron Sadow, Ames National Laboratory
Class: 2020 – 2028

[EFRC – IDREAM] Interfacial Dynamics in Radioactive Environments and Materials
Carolyn Pearce, Pacific Northwest National Laboratory
Class: 2016 – 2028

[EFRC – IQM] Institute for Quantum Matter
Collin Broholm, Johns Hopkins University
Class: 2018 – 2024

[EFRC – M2QM] Center for Molecular Magnetic Quantum Materials
Xiaoguang Zhang, University of Florida
Class: 2018 – 2026

[EFRC – MSEE] Molten Salts in Extreme Environments
James Wishart, Brookhaven National Laboratory
Class: 2018 – 2026

[EFRC – MUSE] Multi-scale Fluid-Solid Interactions in Architected and Natural Materials
Milind Deo, University of Utah
Class: 2018-2024

[EFRC – MUSIC] Mechano-Chemical Understanding of Solid Ion Conductors
Jeff Sakamoto, University of Michigan
Class: 2022-2026

[EFRC – M-WET] Center for Materials for Water and Energy Systems
Benny Freeman, University of Texas at Austin
Class: 2018 – 2026

[EFRC – NPQC] Center for Novel Pathways to Quantum Coherence in Materials
Joel Moore, Lawrence Berkeley National Laboratory
Class: 2018 – 2024

[EFRC – PTL] Photonics at Thermodynamic Limits
Shanhui Fan, Stanford University
Class: 2018 – 2024

[EFRC – Pro-QM] Programmable Quantum Materials
Dmitri Basov, Columbia University
Class: 2018 – 2026

[EFRC – Q-MEEN-C] Quantum Materials for Energy Efficient Neuromorphic Computing
Ivan Schuller, University of California, San Diego
Class: 2018 – 2026

[EFRC – QSQM] Quantum Sensing and Quantum Materials
Peter Abbamonte, University of Illinois Urbana-Champaign
Class: 2020 – 2026

[EFRC –REMAT] Center for Regenerative Energy-Efficient Manufacturing of Thermoset Polymeric Materials
Nancy Sottos, University of Illinois Urbana-Champaign
Class: 2022-2026

[EFRC – REMIND] Reconfigurable Electronic Materials Inspired by Nonlinear Neuron Dynamics
R. Stanley Williams, Texas A&M Engineering Experiment Station
Class: 2022-2026

[EFRC – SCALAR] Center for Synthetic Control Across Length-scales for Advancing Rechargeables
Sarah Tolbert, University of California, Los Angeles
Class: 2018-2024

[EFRC – SPECS] Center for Soft PhotoElectroChemical Systems
Erin Ratcliff, University of Arizona
Class: 2022-2026

[EFRC – TETI] Center for Thermal Energy Transport under Irradiation
David Hurley, Idaho National Laboratory
Class: 2018 – 2026

[EFRC – μ-ATOMS] Manipulation of Atomic Ordering for Manufacturing Semiconductors
Shui-Qing Yu, University of Arkansas
Class: 2022-2026

[EFRC – ULTRA] Ultra Materials for a Resilient, Smart Electricity Grid
Robert Nemanich, Arizona State University
Class: 2020 – 2026

[EFRC – UNCAGE-ME] Center for Understanding and Control of Acid Gas-induced Evolution of Materials for Energy
Ryan Lively, Georgia Institute of Technology
Class: 2014 – 2026

ENERGY INNOVATION HUBS (HUB)

[Hub – CHASE] Center for Hybrid Approaches in Solar Energy to Liquid Fuels
Jerry Meyer, University of North Carolina at Chapel Hill
Started: 2020

[Hub – LiSA] Liquid Sunlight Alliance
Harry Atwater, California Institute of Technology
Started: 2020

COMPUTATIONAL MATERIALS SCIENCES (CMS)

[CMS – C2SEPEM] Center for Computational Study of Excited-State Phenomena in Energy Materials
Steven G. Louie, Lawrence Berkeley National Laboratory
Started: 2016

[CMS – COMMS] Computational Mesoscale Science and Open Software for Quantum Materials
Long-Qing Chen, The Pennsylvania State University
Started: 2019

[CMS – COMSCOPE] Center for Computational Material Spectroscopy and Design
Gabriel Kotliar, Brookhaven National Laboratory
Started: 2015

[CMS – CPSFM] Center for Predictive Simulation of Functional Materials
Paul Kent, Oak Ridge National Laboratory
Started: 2016

[CMS – EPW] Toward Exascale Computing of Electron-Phonon Couplings for Finite-Temperature Materials Design
Feliciano Giustino, University of Texas at Austin
Started: 2019

[CMS – MICCoM] Midwest Integrated Center for Computational Materials
Giulia Galli, Argonne National Laboratory
Started: 2015

[CMS – NPNEQ] Center for Non-Perturbative Studies of Functional Materials under Non-Equilibrium Conditions
Tadashi Ogitsu, Lawrence Livermore National Laboratory
Started: 2019

[CMS – QMC-HAMM] From Accurate Correlated Quantum Simulations to Mesoscopic Scales
Lucas Wagner, University of Illinois Urbana-Champaign
Started: 2019

COMPUTATIONAL CHEMICAL SCIENCES (CCS)

[CCS – ADEPTS] Ab-initio Density-matrix Exascale-Parallelized Dynamics and Transport for Selectivity
Yuan Ping, University of Wisconsin-Madison
Started: 2022

[CCS – BEAST] Beyond-DFT Electrochemistry with Accelerated and Solvated Techniques
Ravishankar Sundararaman, Rensselaer Polytechnic Institute
Started: 2021

[CCS – CMSET] Center for Multiscale Simulation of Energy Transduction
Gregory Voth, University of Chicago
Started: 2022

[CCS – CSI] Chemistry in Solution and at Interfaces
Roberto Car, Princeton University
Started: 2018

[CCS – ECC] Exascale Catalytic Chemistry Project
Judi Zádor, Sandia National Laboratories
Started: 2017

[CCS – ExaPUC] Exascale Multireference Wave Function Theory Method for Transition Metal Catalysis
Laura Gagliardi, University of Chicago
Started: 2022

[CCS – FLOSIC] Fermi-Lowdin Orbital Self-Interaction Correction Center
Koblar Alan Jackson, Central Michigan University
Started: 2017

[CCS – MAPOL] Center for MAny-Body Methods, Spectroscopies, and Dynamics for Molecular POLaritonic Systems
Niranjan Govind, Pacific Northwest National Laboratory
Started: 2022

[CCS – NEOQD] Multiscale Nuclear-Electronic Orbital Quantum Dynamics in Complex Environments
Hammes-Schiffer, Sharon, Princeton University
Started: 2022

[CCS – QuestC] Hierarchical Scalable Green's Function Modeling of Chemistry at Interfaces
Mark van Schilfgaarde, National Renewable Energy Laboratory
Started: 2021