U.S. Department of Energy

Energy Frontier Research Centers

One Page Overviews

Office of Science
9/11/2018; Revised 9/24/2019

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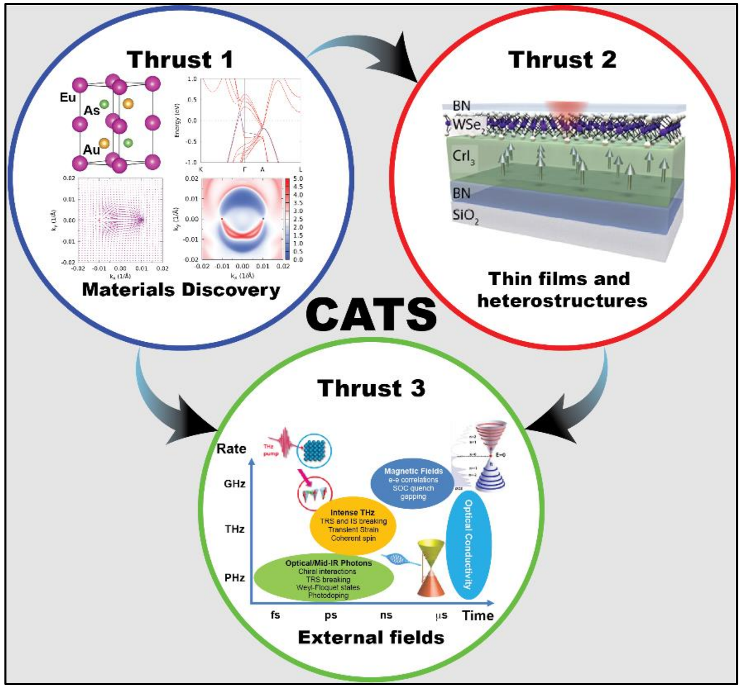
Ordered by Institution and then by Director

Center for the Advancement of Topological Semimetals (CATS)

Robert McQueeney (Ames Laboratory); Class: 2018-2022

MISSION: To understand and discover new quantum phenomena and functionality in topological materials for future applications in spin-based electronics, computing, and sensing.



https://cats.ameslab.gov

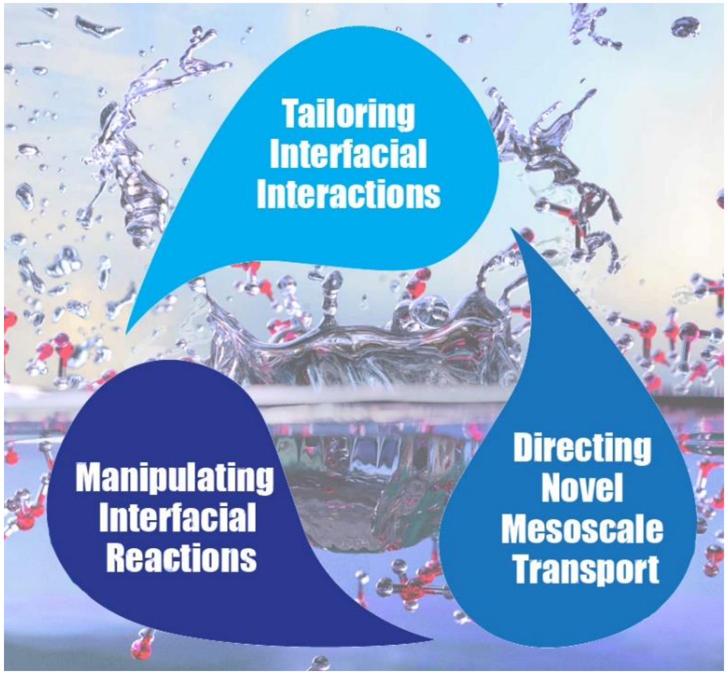
RESEARCH PLAN

CATS has crosscutting research thrusts to; (1) predict, discover, and understand new magnetic topological semimetals, (2) discover and control novel quantum states and functionality in thin films and heterostructures, and (3) investigate the manipulation of topological states with external fields.

Advanced Materials for Energy-Water Systems (AMEWS)

Seth Darling (Argonne National Laboratory); Class: 2018-2022

MISSION: To understand and design water-solid interfaces to enable future advances in materials for efficient water treatment.



http://www.anl.gov/amews

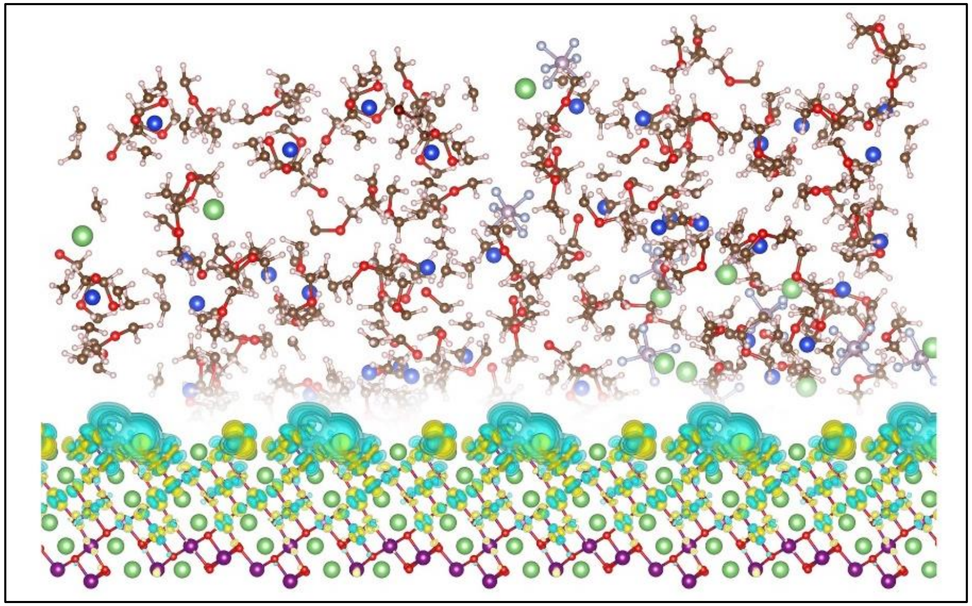
RESEARCH PLAN

AMEWS combines experiments and theory/modeling/simulation to explore interfaces between solids and aqueous fluids to gain predictive understanding of adsorption, reactivity, and transport in energy-water systems.

Center for Electrochemical Energy Science (CEES)

Paul Fenter (Argonne National Laboratory); Class: 2009-2020

MISSION: To create a robust fundamental understanding of the phenomena that control the reactivity of electrified oxide interfaces, films and materials relevant to lithium-ion battery chemistries.



http://www.cees.anl.gov

RESEARCH PLAN

CEES will probe the molecular-scale structure at electrified oxide-electrolyte interfaces, leverage advanced materials synthesis to create interfacial systems with well-defined properties (composition, structure, etc.), and develop novel approaches and chemistries to control and direct electrochemical reactivity.

U.S. DEPARTMENT OF ENERGY | Office of Science

Argonne NATIONAL LABORATORY

ILLINOIS UNIVERSITY OF ILLINOIS AT URBANA-CHAMPAIGN

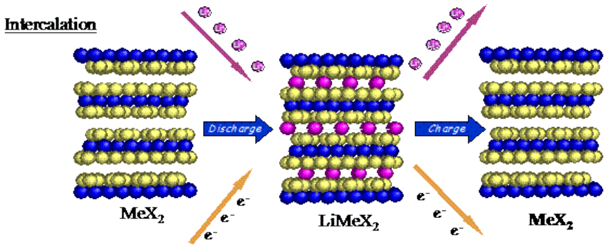
NORTHWESTERN UNIVERSITY

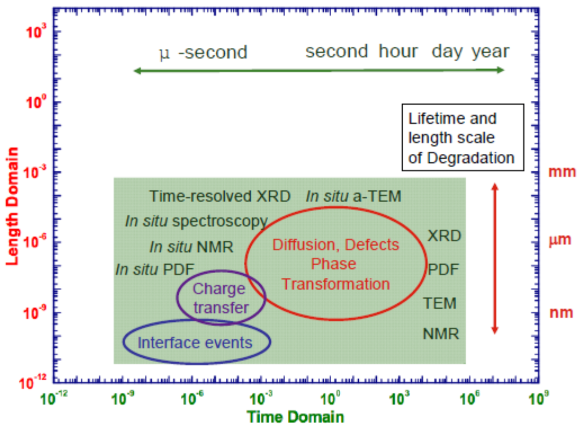
PURDUE UNIVERSITY

Northeast Center for Chemical Energy Storage (NECCES)

M. Stanley Whittingham (Binghamton University); Class: 2009-2020

MISSION: To develop an understanding of how key electrode reactions occur, and how they can be controlled to improve electrochemical performance, from the atomistic level to the macroscopic level throughout the life-time of the operating battery.





http://necces.binghamton.edu

RESEARCH PLAN

The processes that occur in batteries are complex, spanning a wide range of time and length scales. The team of experimentalists and theorists will develop and use new methodologies to determine how model compound electrodes function in real time, as batteries are cycled.

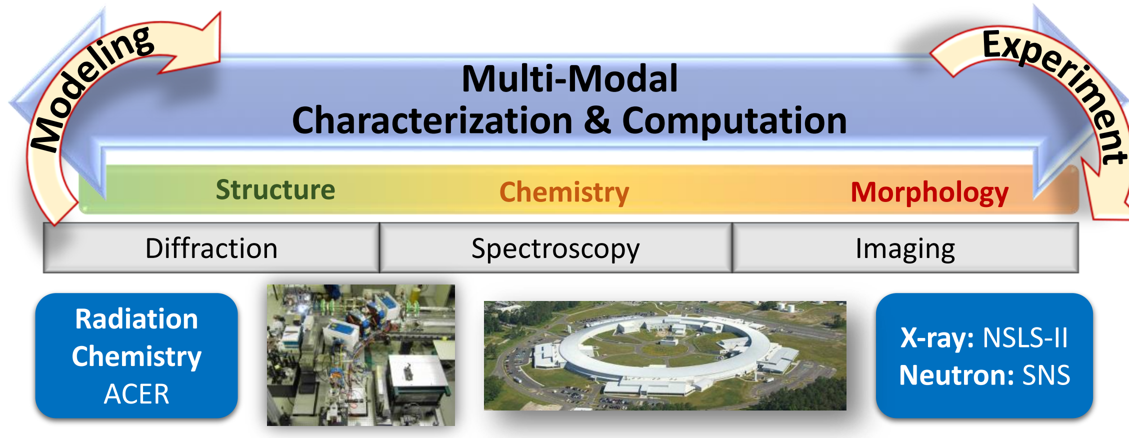
Revised 9/24/2019

U.S. DEPARTMENT OF ENERGY | Office of Science | NECCES | BINGHAMTON UNIVERSITY STATE UNIVERSITY OF NEW YORK | RUTGERS | UNIVERSITY OF CAMBRIDGE | UC San Diego | UCSB | UNIVERSITY OF MICHIGAN | Stony Brook University | Massachusetts Institute of Technology

Molten Salts in Extreme Environments (MSEE)

James Wishart (Brookhaven National Laboratory); Class: 2018-2022

MISSION: To provide a fundamental under-standing of the bulk and interfacial chemistry of molten salts that will underpin molten salt reactor technology.



https://www.bnl.gov/moltensalts/

RESEARCH PLAN

Coordinated experimental and theoretical efforts using cutting-edge capabilities at DOE-SC User Facilities and at partner institutions as well as high-performance computing will examine the atomic basis of molten salt behavior under the coupled extremes of high temperature and ionizing radiation to provide a predictive description of molten salt chemistry.

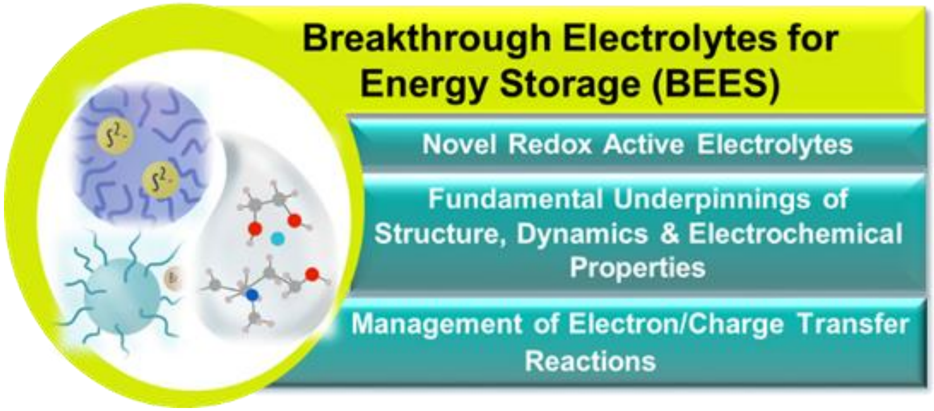
Revised 9/24/2019

U.S. DEPARTMENT OF ENERGY | Office of Science | BROOKHAVEN NATIONAL LABORATORY | INL | OAK RIDGE National Laboratory | The University of Iowa | University of Notre Dame | Stony Brook University

Breakthrough Electrolytes for Energy Storage (BEES)

Robert Savinell (Case Western Reserve University); Class: 2018-2022

MISSION: To develop a fundamental understanding of: (i) solvation and transport properties; (ii) electrode-electrolyte interfaces; and (iii) electron transfer reactions in deep eutectic solvents and soft nanoparticle electrolytes.



http://engineering.case.edu/EFRC BEES

RESEARCH PLAN

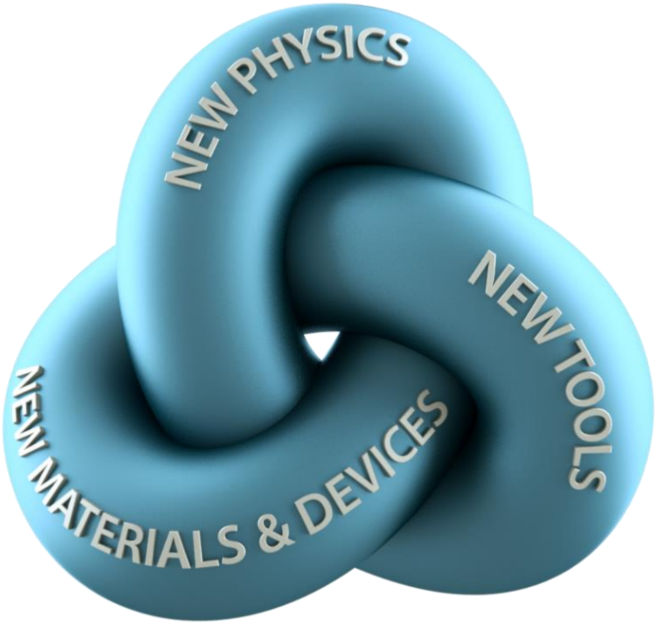
Synergizing experimental and theoretical investigations, BEES researchers employ electroanalytical techniques, spectroscopy, synchrotron based X-ray and neutron techniques, as well as advanced computational methods to probe structures, fundamental properties, and interfacial chemistry. This fundamental know-how will enable design and synthesis of new electrolytes that will transform energy storage.

Revised 9/24/2019

Programmable Quantum Materials (Pro-QM)

Dmitri N. Basov (Columbia University); Class: 2018-2022

MISSION: To discover, characterize, and deploy new forms of quantum matter controllable by gating, magnetic proximity and nano-mechanical manipulation.



https://quantum-materials.columbia.edu

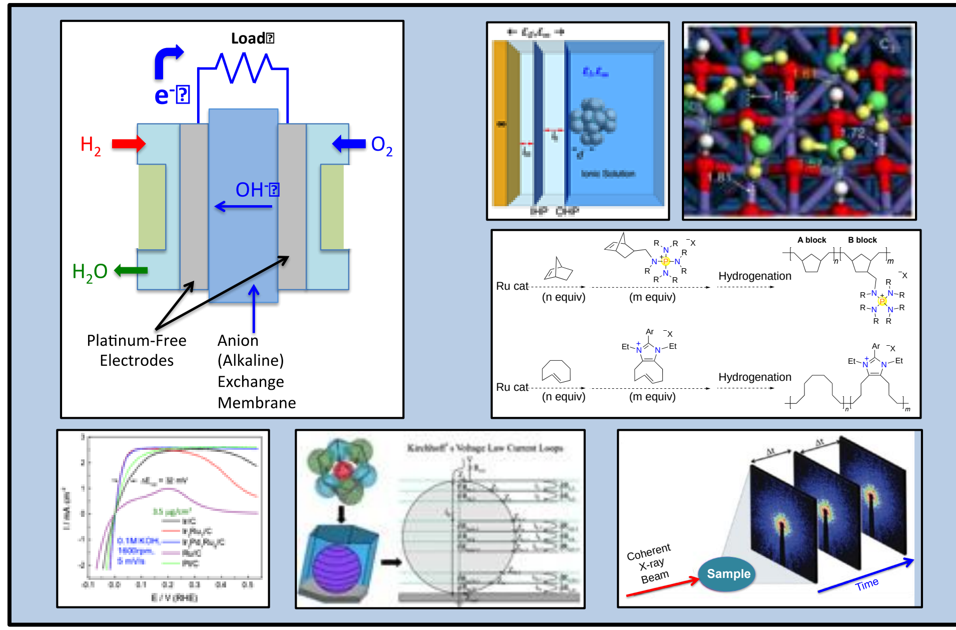
RESEARCH PLAN

Realizing the potential for programmable quantum matter requires a three-pronged approach, combining *i)* the unique suite of driving perturbations, with *ii)* a transformative set of synthesis/device fabrication capabilities and *iii)* nanoscale characterization techniques integrated in a single platform.

Center for Alkaline Based Energy Solutions (CABES)

Héctor D. Abruña (Cornell University); Class: 2018-2022

MISSION: To achieve a detailed understanding of the nature, structure, and dynamics of electrocatalysis in alkaline media.



https://cabes.cornell.edu/

RESEARCH PLAN

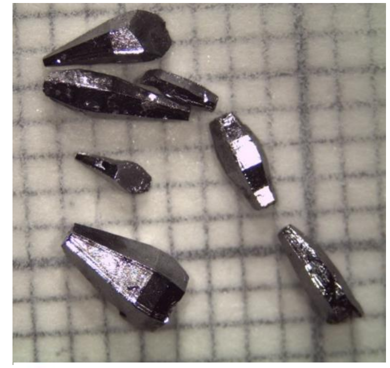
CABES seeks a detailed understanding of the nature, structure, and dynamics of fuel cell systems operating in alkaline media. The center will integrate theory and computational methods, synthesis of electrocatalysts and novel membrane materials, and the development of experimental tools that will provide in situ, spatiotemporal characterization of systems under operation.

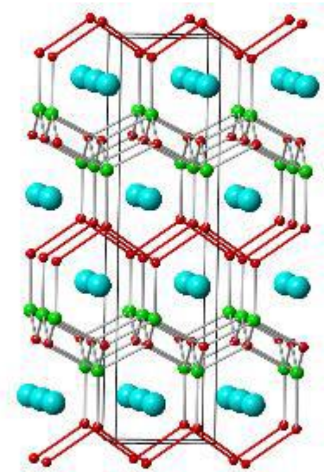
Revised 9/24/2019

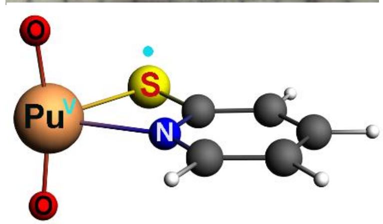
Center for Actinide Science & Technology (CAST)

Thomas E. Albrecht-Schmitt (Florida State University); Class: 2016-2020

MISSION: To advance our understanding of how electronic structure and bonding control the properties of radioactive materials. This knowledge will aid in the development of nuclear technologies that enhance energy security, address nuclear legacy issues, and foster the next generation of nuclear scientists.







https://cast.magnet.fsu.edu/

RESEARCH PLAN

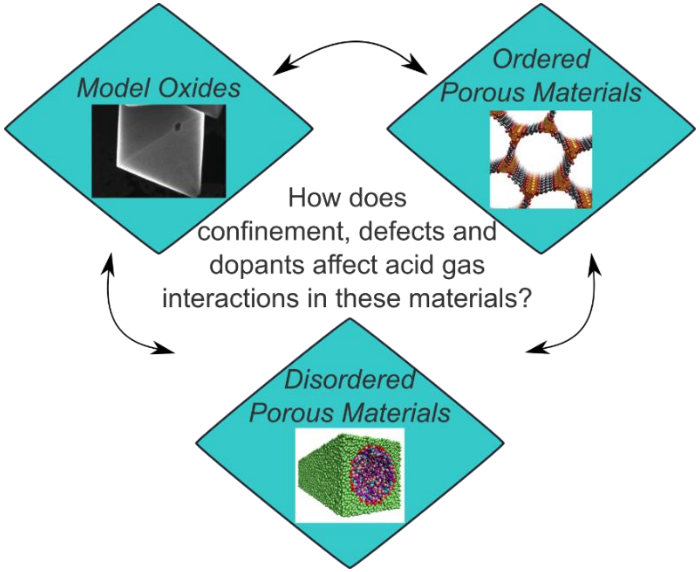
CAST develops new materials that capture radionuclides found within legacy waste from the Cold War. Optimization of these materials requires advances in synthesis, characterization, and theory that provide a deep understanding of the origin of the unusual properties of these nuclear materials.

U.S. DEPARTMENT OF ENERGY | Office of Science

Center for Understanding and Control of Acid Gas-Induced Evolution of Materials for Energy (UNCAGE-ME)

Krista Walton (Georgia Tech); Class: 2014-2022

MISSION: To develop and harness a deep knowledge base in the characterization, prediction, and control of acid-gas interactions with a broad class of materials to accelerate materials discovery in acid gas separations, conversion, and utilization.



http://efrc.gatech.edu

RESEARCH PLAN

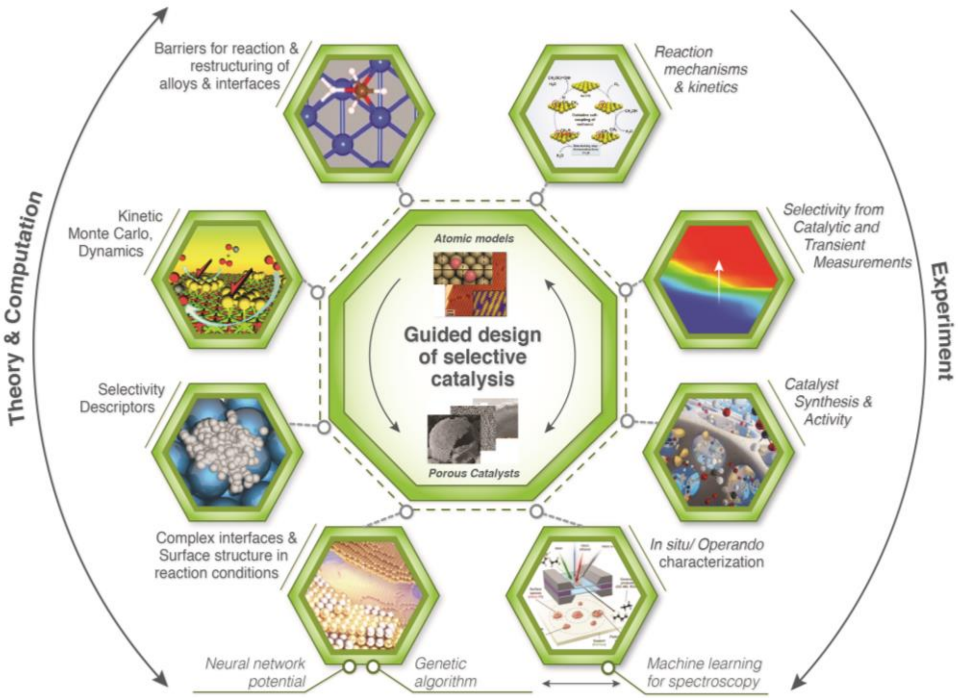
Degradation effects are often decisive factors in the practical use of materials such as sorbents for carbon capture, acid gas conversion, and natural gas purification. Our core research model is to use a variety of in-situ experimental tools coupled with complimentary modeling techniques and machine learning to improve the performance of materials in these environments and advance materials discovery.

U.S. DEPARTMENT OF ENERGY | Office of Science
Georgia Institute of Technology
Oak Ridge National Laboratory
The University of Alabama
Sandia National Laboratories
Penn State
Lehigh University
Wisconsin University of Wisconsin-Madison
Washington University in St. Louis
UNCAGE-ME

Integrated Mesoscale Architectures for Sustainable Catalysis (IMASC)

Cynthia Friend (Harvard University); Class: 2014-2022

MISSION: To establish design principles for highly selective catalytic transformations driven by nanoporous dilute alloys.



https://efrc.harvard.edu/

RESEARCH PLAN

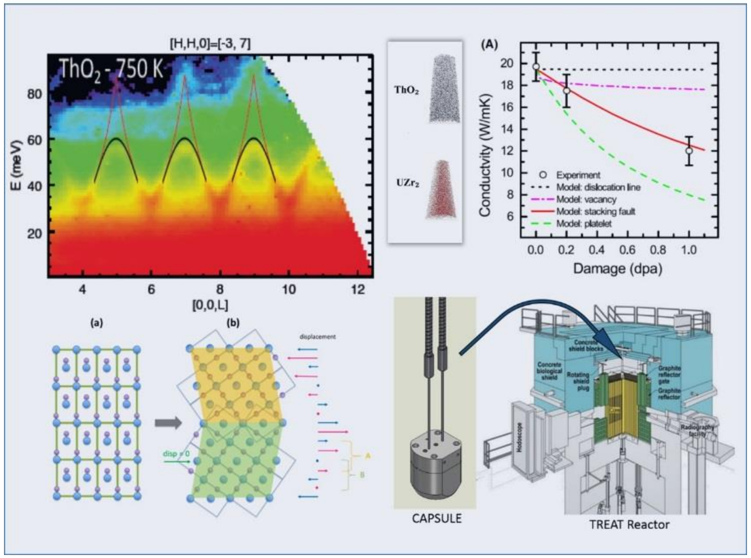
Design principles to improve the selectivity of catalytic reactions will be developed by a combination of experiment and theory. Scale up from fundamental knowledge of the kinetics and mechanism, enabled by advanced methods, will be used to improve selectivity of key synthetic processes.

Center for Thermal Energy Transport under Irradiation (TETI)

David Hurley (Idaho National Laboratory); Class: 2018-2022

MISSION: To provide the foundational work necessary to accurately model and ultimately control electron- and phonon-mediated thermal transport in 5f electron materials in extreme irradiation environments.

Energy Carriers to Mesoscale Transport



http://teti.inl.gov/

RESEARCH PLAN

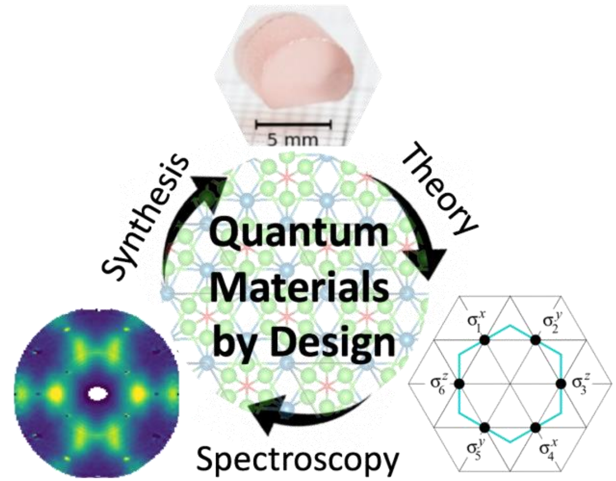
Thermal energy transport under irradiation is directly related to reactor efficiency as well as reactor safety. The aim of TETI is to develop a first principles understanding of electron and phonon transport in advanced nuclear fuels that will provide the necessary tools to enhance thermal transport by tailoring defects and microstructure.

Revised 9/24/2019

Institute for Quantum Matter (IQM)

Collin Broholm (Johns Hopkins University); Class: 2018-2022

MISSION*:* To realize, understand, and control revolutionary quantum materials and structures where quantum effects such as entanglement and coherence find collective macroscopic manifestations.



http://iqm.jhu.edu

RESEARCH PLAN

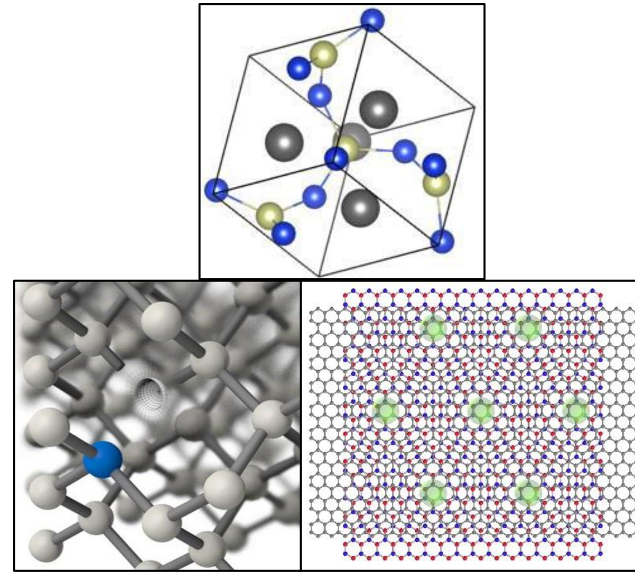
Quantum mechanics successfully describes electrons within atoms as matter waves. IQM will develop “Quantum Materials” where electronic matter waves extend beyond the atomic scale and give rise to unique physical properties. IQM theorists will identify candidate materials and nanoscale structures that will be synthesized and then probed with advanced spectroscopic and transport methods to realize and understand four new quantum states of matter and explore their potential for applications.

U.S. DEPARTMENT OF ENERGY | Office of Science | Johns Hopkins University | Cornell University | PennState | Princeton University | Rutgers

Center for Novel Pathways to Quantum Coherence in Materials (NPQC)

Joel Moore (Lawrence Berkeley National Laboratory); Class: 2018-2022

MISSION: To expand dramatically our understanding and control of coherence in solids by building on recent discoveries in quantum materials along with advances in experimental and computational techniques.



http://npqc.lbl.gov

RESEARCH PLAN

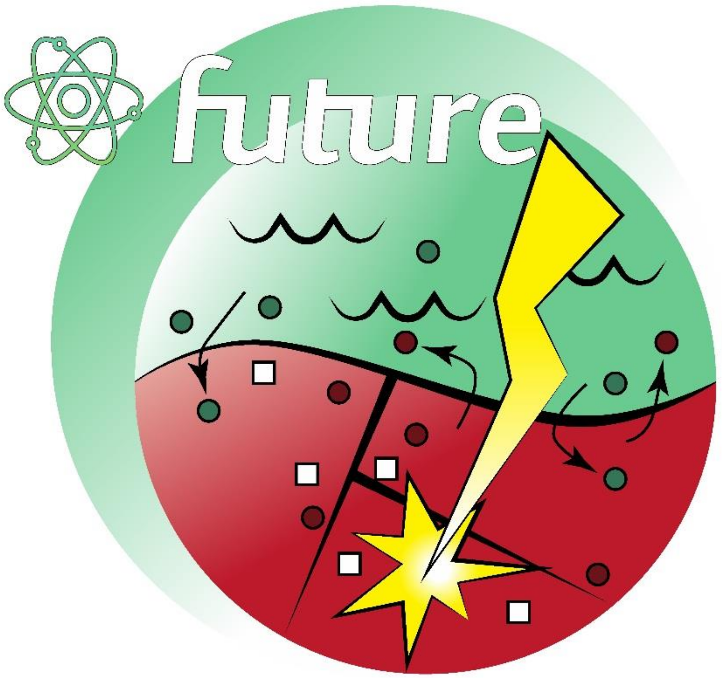
NPQC will study three families of materials in which quantum coherence is especially important, using a variety of advanced characterization techniques and theoretical methods. Major outcomes will include new approaches to solid-state quantum sensing and quantum spectroscopy, along with controllable crossovers between coherent and incoherent behavior in transport and optical properties.

Revised 9/24/2019

Fundamental Understanding of Transport Under Reactor Extremes (FUTURE)

Blas Pedro Uberuaga (Los Alamos National Laboratory); Class: 2018-2022

MISSION: To understand how the coupled extremes of irradiation and corrosion work in concert to modify the evolution of materials by coupling experiments and modeling that target fundamental mechanisms.



http://future.lanl.gov/

RESEARCH PLAN

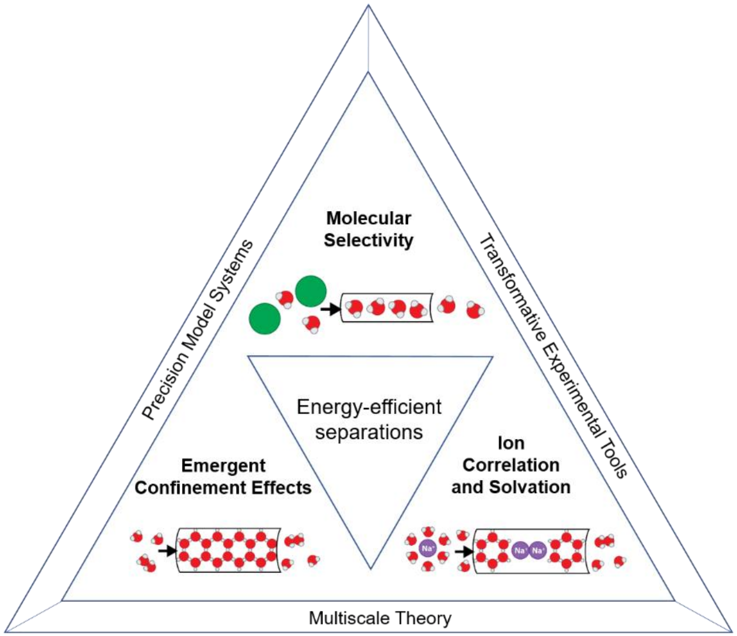
We combine experiment and modeling to understand the fundamental processes responsible for materials evolution under concurrent irradiation and corrosion. Our focus is on point defect production, coupled transport of chemical species in the material, and reactions at and across interfaces.

Revised 9/24/2019

The Center for Enhanced Nanofluidic Transport (CENT)

Michael Strano (MIT); Class: 2018-2022

MISSION: To address emerging and compelling gaps in our knowledge of fluid flow and molecular transport in single digit nanopores and establish the scientific foundation for developing transformative molecular separation technologies impacting the Water-Energy Nexus.



https://cent.mit.edu/

RESEARCH PLAN

CENT will apply precision model systems, transformative experimental tools, and predictive multiscale theories to understand fluid flow and molecular transport in single-digit nanopores, to identify conditions for enhanced flow at extreme confinement, to unravel structure of solid/liquid interfaces, and to design new mechanisms that deliver unprecedented molecular selectivity.

Revised 9/24/2019

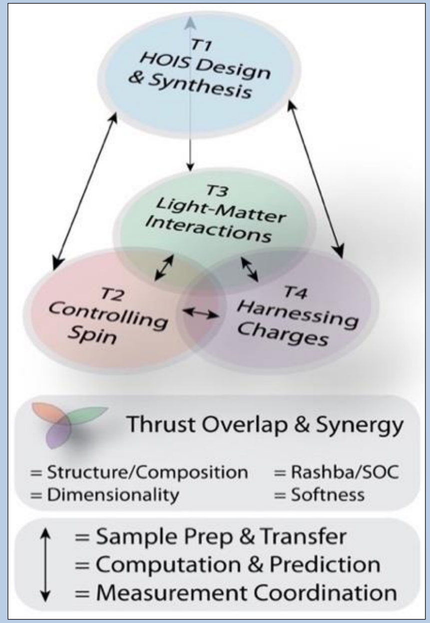
U.S. DEPARTMENT OF ENERGY | Office of Science

Center for Hybrid Organic Inorganic Semiconductors for Energy (CHOISE)

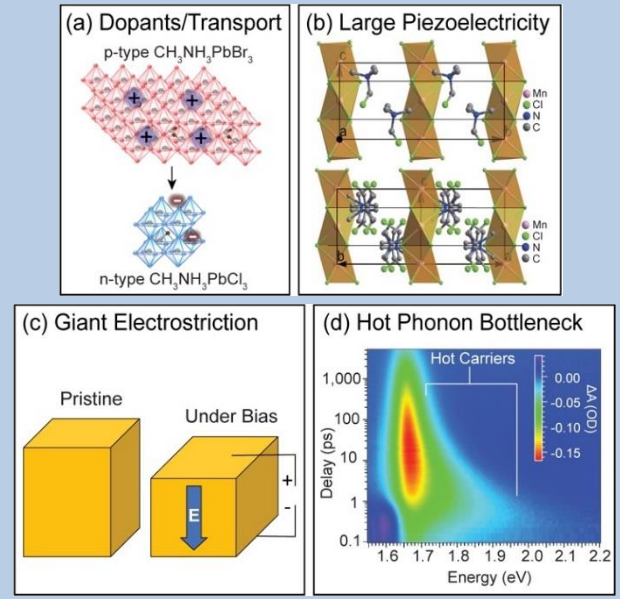
Matthew C. Beard (National Renewable Energy Laboratory); Class: 2018-2022

MISSION: To enable unprecedented synthetic control over the emergent phenomena of spin, charge, and light-matter interactions, in tailored organic-inorganic perovskite-inspired systems for energy science.

CHOISE Plan:



Example emergent phenomena



https://www.choise-efrc.org/

RESEARCH PLAN

CHOISE will employ the full flexibility of organic and inorganic chemistry to design and demonstrate HOIS with unique and controllable spin, electronic, and optical properties. Key structural parameters will include metal selection, halide/psuedohalide choice, overall stoichiometry, and organic cation choice.

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U.S. DEPARTMENT OF ENERGY | Office of Science
CHOISE Center for Hybrid Organic Inorganic Semiconductors for Energy
NREL NATIONAL RENEWABLE ENERGY LABORATORY
Duke UNIVERSITY
THE UNIVERSITY OF UTAH
THE UNIVERSITY OF TOLEDO
THE UNIVERSITY OF CHICAGO
THE UNIVERSITY of NORTH CAROLINA at CHAPEL HILL
SLAC NATIONAL ACCELERATOR LABORATORY
SAN DIEGO STATE UNIVERSITY

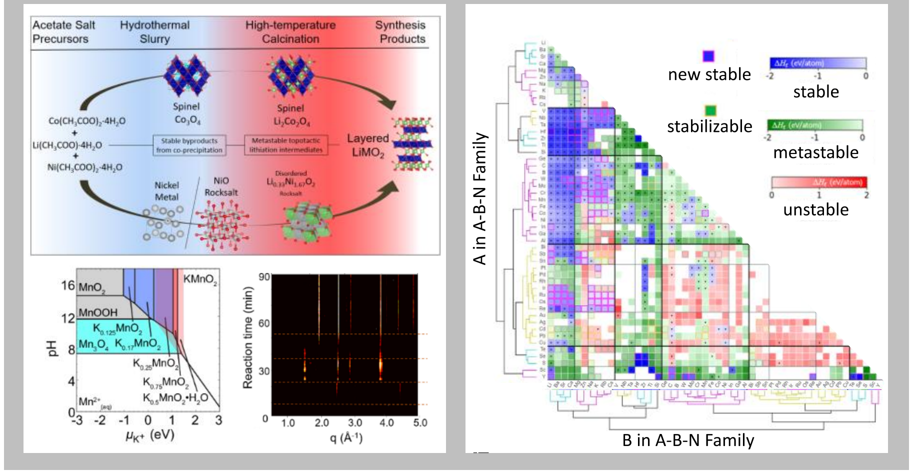
Center for Next Generation of Materials by Design (CNGMD)

William Tumas (National Renewable Energy Laboratory); Class: 2014-2020

MISSION*:* To dramatically transform the discovery of functional energy materials through multiple-property search, incorporation of metastable materials into predictive design, and the development of theory to guide materials synthesis.

Predictive Design & Synthesis of

Complex Metal Oxides | **New Functional Nitrides**



www.cngmd-efrc.org

RESEARCH PLAN

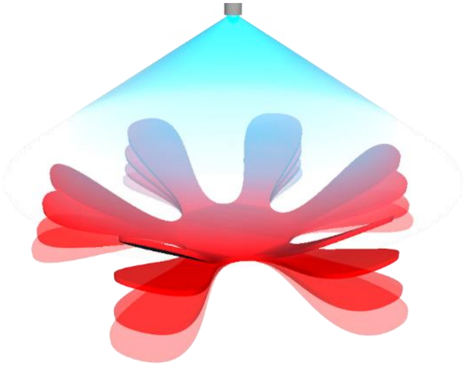
Integrate theory, synthesis, characterization and data analytics to establish the foundational science for metastability and theory-guided synthesis.

- Quantify the synthetically accessible limit of metastability
- Predict synthetic pathways for high-energy polymorphs & metastable materials
- Determine functionality and synthetic pathways for new oxides and nitrides

Center for Bio-Inspired Energy Science (CBES)

Samuel I. Stupp (Northwestern University); Class: 2009-2022

MISSION: To develop the next frontier in soft materials relevant to energy challenges by designing structures that emulate functions we see in biological systems.



http://cbes.northwestern.edu

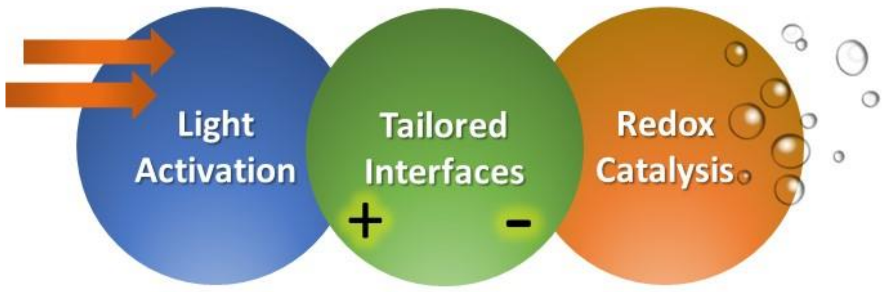
RESEARCH PLAN

CBES tackles the challenge of encoding synthetic soft materials with the ability to transduce energy forms and move autonomously in ways that are characteristic of "living matter". The main goals are to develop new opportunities around the concepts of "robotic soft matter", denoting the ability to rapidly perform mechanical, optical, or chemical tasks with only small inputs of energy, and "photosynthetic matter", which requires systems structured holistically to enable efficient chemical production using visible light. We approach these enormous bio-inspired challenges through bottom-up chemical design and synthesis combined with top-down engineering strategies, computation, and theory.

Center for Light Energy Activated Redox Processes (LEAP)

Michael R. Wasielewski (Northwestern University); Class: 2018-2020

MISSION: To develop the fundamental scientific understanding needed to use efficient light-driven multi-electron redox processes to power energy-demanding chemistry.



http://www.LEAP-Center.org

RESEARCH PLAN

Within the LEAP Center, researchers will:

- Produce charges at high potentials with new light absorbers
- Control charge flow from light absorbers to catalysts
- Perform energy-intensive reactions with new catalysts

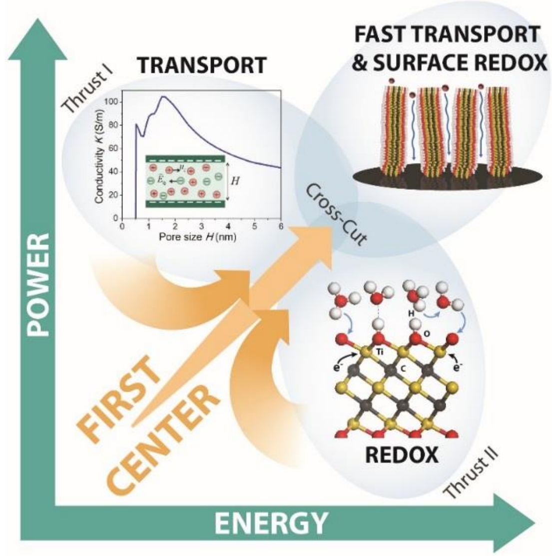
Reactions LEAP researchers will target are power-critical energy storage and chemical synthesis reactions such as water splitting, carbon dioxide and nitrogen reduction, and carbon-carbon bond formation.

U.S. DEPARTMENT OF ENERGY | Office of Science | Center for Light Energy LEAP Activated Redox Processes | Northwestern | Argonne NATIONAL LABORATORY | Yale

Fluid Interface Reactions, Structures and Transport (FIRST)

Sheng Dai (Oak Ridge National Laboratory); Class: 2009-2022

MISSION: To achieve fundamental understanding and validated, predictive models of the atomistic origins of electrolyte and coupled electron transport under nanoconfinement that will enable transformative advances in capacitive electrical energy storage and other energy-relevant interfacial systems.



www.ornl.gov/sci/first/

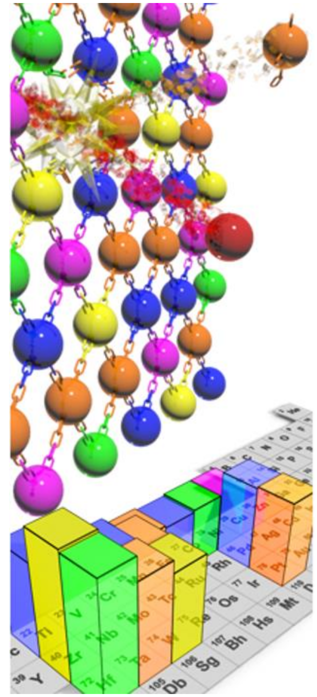
RESEARCH PLAN:

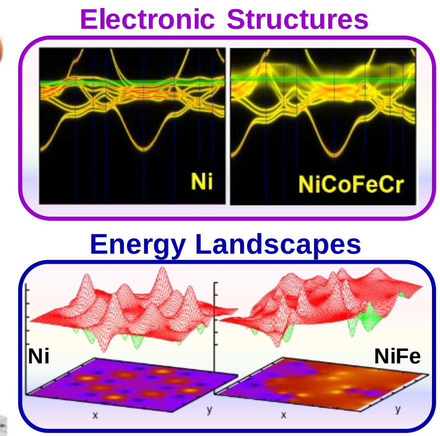
Thrust I integrates novel experimental and computational approaches to determine how electrolyte transport is affected by composition, nano-confinement and surface chemistry/charge. Thrust II considers how fast surface redox reactions proceed in pseudocapacitive electrode/electrolyte systems. The Cross-Cutting Theme uses these fundamental insights to achieve simultaneous high power and energy density.

Energy Dissipation to Defect Evolution (EDDE)

Yanwen Zhang (Oak Ridge National Laboratory); Class: 2014-2020

MISSION: To understand how extreme chemical complexity can be exploited to control energy dissipation and defect evolution under equilibrium and non-equilibrium conditions, and to guide the development of radiation-tolerant alloys with unique magnetic and thermal properties.





Tailoring chemical complexity (left) is a powerful tool to modify electronic (top right) and atomic (bottom right) properties.

http://edde.ornl.gov/

RESEARCH PLAN

Tailoring chemical complexity dramatically modifies material properties at the level of electrons and atoms. We will understand and modify chemical complexity to ultimately enhance radiation tolerance by reducing the rate of Energy Dissipation (Thrust 1) and controlling Defect Evolution (Thrust 2).

U.S. DEPARTMENT OF ENERGY | Office of Science | Oak Ridge National Laboratory | University of Michigan | The University of Tennessee Knoxville | University of Wyoming | Virginia Tech

Center for Performance and Design of Nuclear Waste Forms and Containers (WastePD)

Gerald Frankel (Ohio State University); Class: 2016-2020

MISSION: To understand the fundamental mechanisms of waste form performance, and apply that understanding to develop design approaches for new waste forms with improved and predictable performance.

https://efrc.engineering.osu.edu

RESEARCH PLAN

WastePD is studying the mechanisms of corrosion of glass, ceramic and metallic waste forms and containers and developing the underlying science required to design materials with improved properties and to accurately predict long term performance.

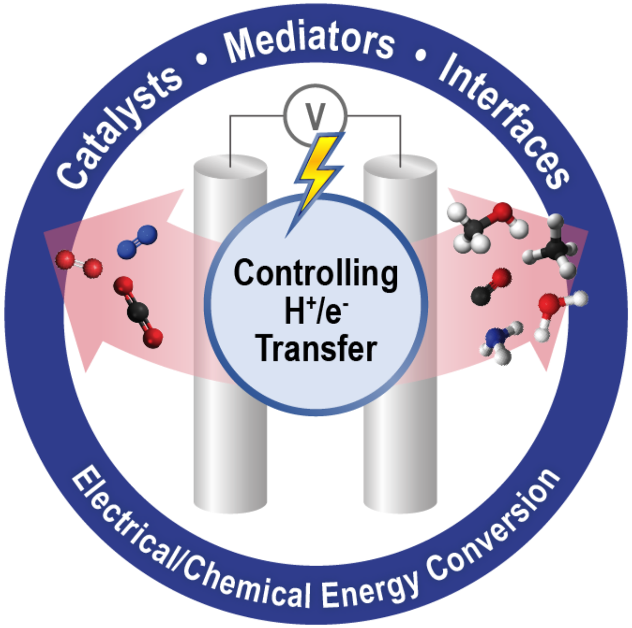
Revised 9/24/2019

U.S. DEPARTMENT OF ENERGY | Office of Science | The Ohio State University | cea | LSU | Pacific Northwest National Laboratory | PennState | RPI | University of Virginia | QuesTek Innovations LLC | CITRINE | UNT

Center for Molecular Electrocatalysis (CME)

Morris Bullock (Pacific Northwest National Laboratory); 2009-2022

MISSION: To establish the fundamental principles needed for efficient interconversion of electrical energy and chemical bonds through precise control of electron and proton transfers.



https://efrc.pnnl.gov/cme/

RESEARCH PLAN

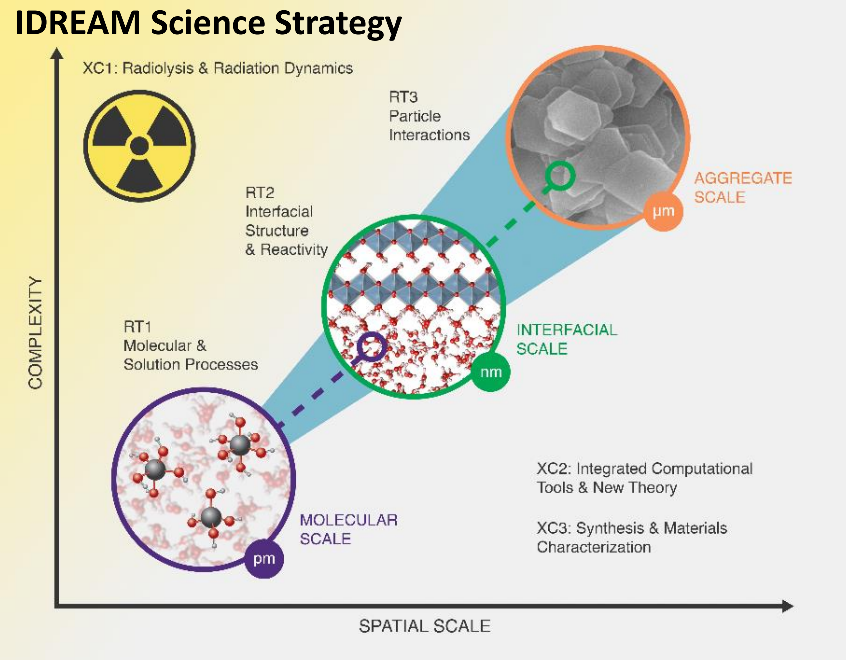
We target fundamental discoveries in molecular electrocatalysis and interfacial reactivity to achieve fast, energy-efficient interconversion of electrical and chemical energy. Our approach to the design of electrocatalysts exploits the emerging area of electron-proton transfer mediators and takes a molecular approach to heterogeneous interfaces.

U.S. DEPARTMENT OF ENERGY | Office of Science | Pacific Northwest National Laboratory | Yale | The University of Wisconsin Madison | MIT Massachusetts Institute of Technology | University of Washington | Purdue University

Interfacial Dynamics in Radioactive Environments and Materials (IDREAM)

Sue Clark (Pacific Northwest National Laboratory); Class: 2016-2020

MISSION: To master molecular–to–mesoscale chemical and physical phenomena at interfaces in complex environments characterized by extremes in alkalinity and low-water activity, and driven far from equilibrium by ionizing (γ,β) radiation.



https://efrc.pnnl.gov/idream/

RESEARCH PLAN

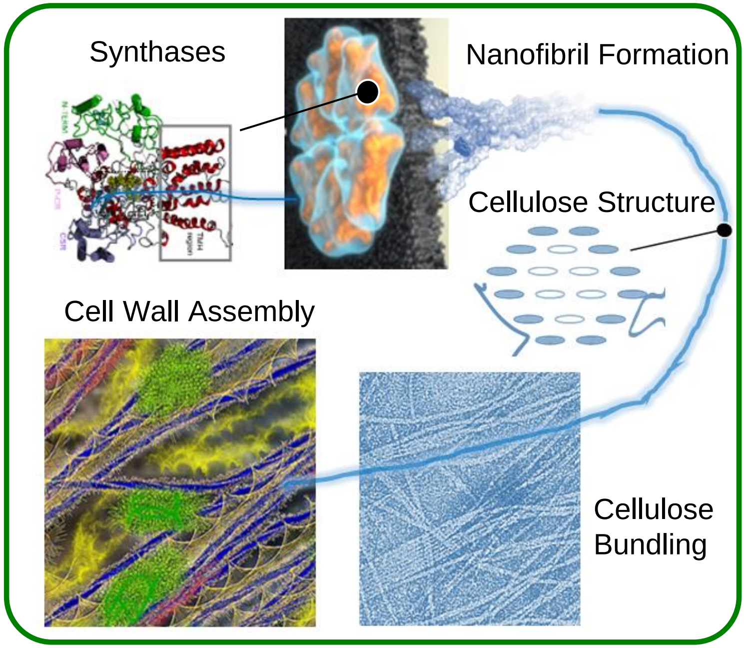
IDREAM is conducting fundamental studies to support innovations in processing high-level radioactive wastes (HLW). This work facilitates the transformation of HLW processing by elucidating the basic chemistry and physics required to control and manipulate interfacial phenomena in extreme HLW environments.

U.S. DEPARTMENT OF ENERGY | Office of Science | Pacific Northwest National Laboratory | Washington State University | University of Washington | Oak Ridge National Laboratory | University of Notre Dame | Georgia Tech | EFRC: IDREAM

Center for Lignocellulose Structure and Formation (CLSF)

Daniel J. Cosgrove (Penn State University); Class: 2009-2022

MISSION: To develop a nano- to meso-scale understanding of cellulosic cell walls, the energy-rich structural material in plants, and the physical mechanisms of wall assembly, forming the foundation for new technologies in sustainable energy and novel biomaterials.



www.lignocellulose.org

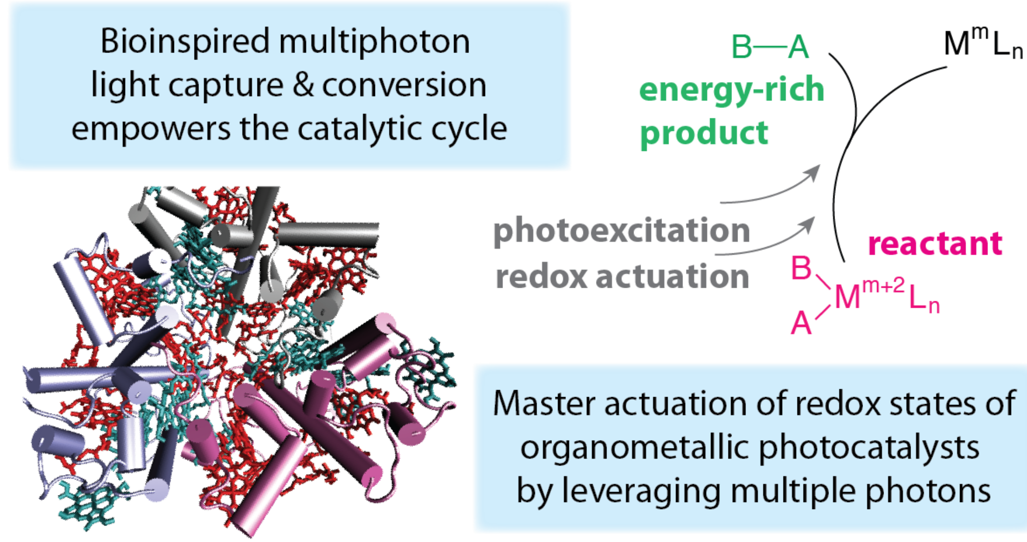
RESEARCH PLAN

Combining cutting-edge tools of biology and physics, CLSF is elucidating (a) the nano-machinery that transforms simple sugars into cellulose microfibrils and (b) the physical processes by which cellulose interacts with matrix polysaccharides and lignin to produce hierarchically-ordered cell walls with diverse physical, chemical and material properties.

Bioinspired Light-Escalated Chemistry (BioLEC)

Gregory Scholes (Princeton University); Class: 2018-2022

MISSION: To employ light harvesting and advances in solar photochemistry to enable unprecedented photoinduced cross-coupling reactions that valorize abundant molecules.



http://chemlabs.princeton.edu/biolec/

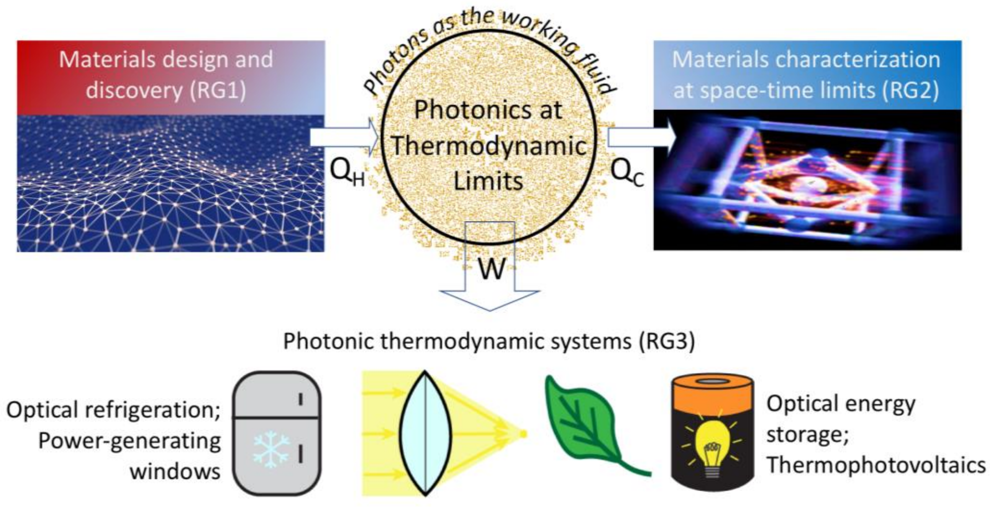
RESEARCH PLAN

The fundamental advance of the BioLEC EFRC will be to establish a platform for directing difficult chemical transformations that are enabled by combining the energies of multiple photons. The resulting breakthroughs will yield energy-relevant chemicals, fuels, and materials.

Photonics at Thermodynamic Limits (PTL)

Jennifer Dionne (Stanford University); Class: 2018-2022

MISSION: To achieve photonic operations at thermodynamic limits by controlling the flow of photons, electrons, and phonons in atomically-architected materials, enabling entirely new energy conversion systems.



http://ptl.stanford.edu

RESEARCH PLAN

CHALLENGE: To design photonic conversion systems for energy and information that operate at thermodynamic limits.

APPROACH: Theory provides insights to guide materials and systems design that are in turn validated by novel, state-of-the-art characterization techniques.

OUTCOME: New theory, new forms of matter, and novel characterization techniques that achieve unprecedented levels of optical efficiency.

Revised 9/24/2019

U.S. DEPARTMENT OF ENERGY | Office of Science

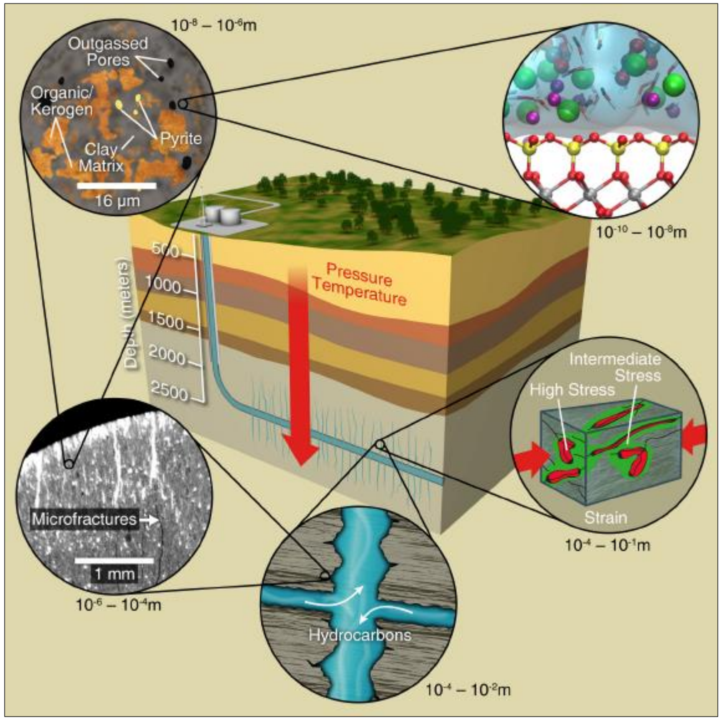
PTL PHOTONICS AT THERMODYNAMIC LIMITS

Stanford University · Berkeley University of California · Harvard University · Caltech · Illinois

Center for Mechanistic Control of Water-Hydrocarbon-Rock Interactions in Unconventional and Tight Oil Formations (CMC - UF)

Anthony R. Kovscek (Stanford University); Class: 2018-2022

MISSION: To seek fundamental mechanistic understanding to achieve control over the various non-equilibrium chemical and physical processes occurring in shale that increases hydrocarbon production while decreasing the amount of produced water, contaminants, and the number of wells drilled.



https://cmc-uf.stanford.edu/

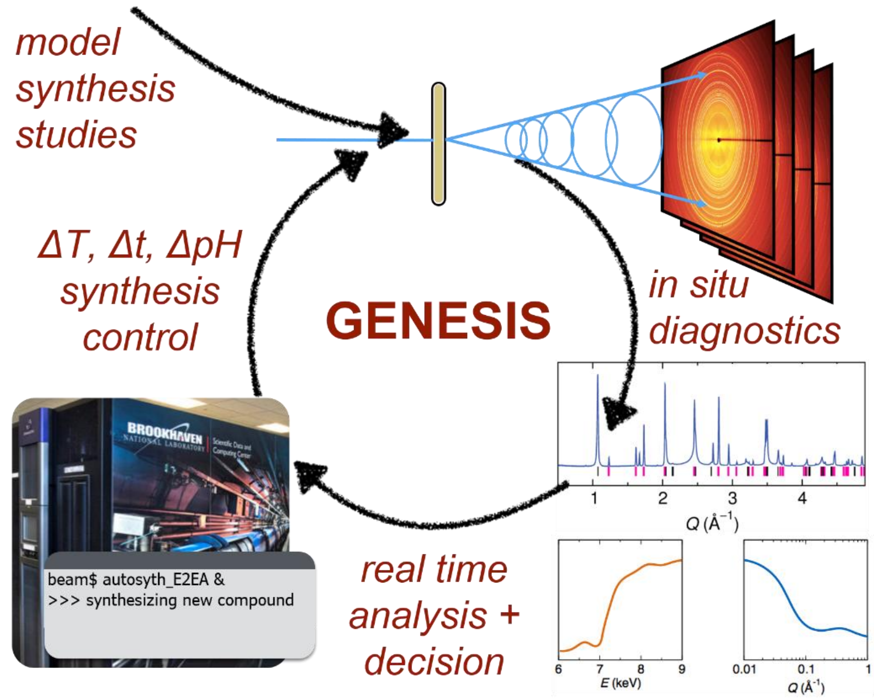
RESEARCH PLAN

Conduct a bottom-up, multiscale, multiphysics, multiphase, and multidisciplinary investigation of transport processes in nanoporous shales incorporating reactions with fracture fluids and the mechanics of geomaterials.

A Next Generation Synthesis Center (GENESIS)

John Parise (Stony Brook University); Class: 2018-2022

MISSION: To develop a new paradigm for synthesis that accelerates the discovery of materials, by understanding how key structural and chemical transformations during synthesis are governed by the synthesis variables.



https://www.stonybrook.edu/genesis/

RESEARCH PLAN

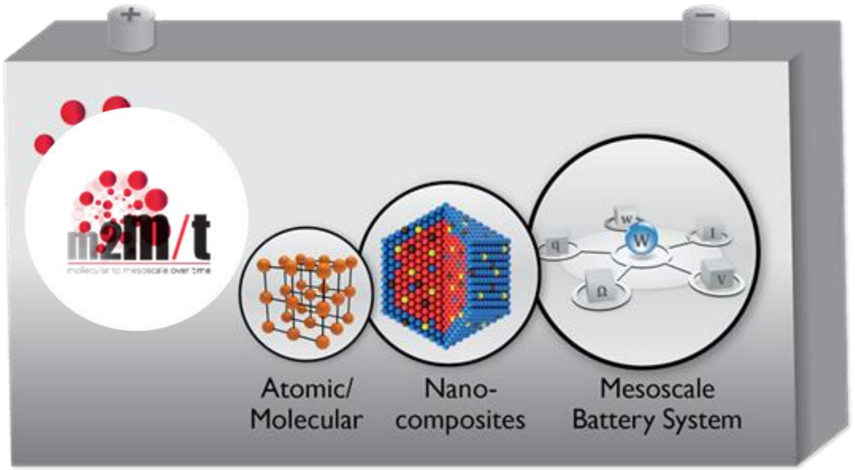
GENESIS will accelerate the mapping of reaction space by integrating advanced in situ diagnostics and data science tools to interrogate, predict, and control reaction pathways. This will enable guided navigation of the pathways leading to new functional material targets.

Revised 9/24/2019

Center for Mesoscale Transport Properties(m2m/t)

Esther S. Takeuchi (Stony Brook University); Class: 2014-2022

MISSION: To build the scientific knowledge to enable creation of scalable electrochemical energy storage systems with high energy, power, and long life.



http://stonybrook.edu/m2m

RESEARCH PLAN

The mission will be accomplished through the following initiatives:

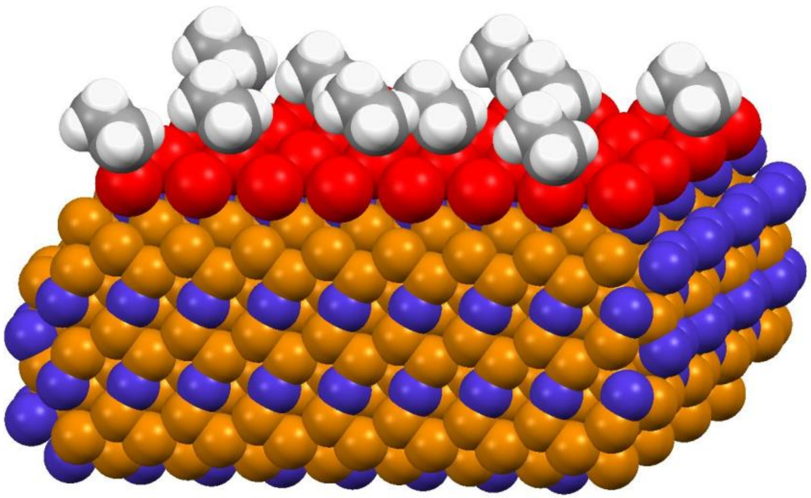
- Synthesis and investigation of multifunctional materials and heterostructures.
- Understand and control kinetically driven interfacial phenomena.
- Rational design of electrode architectures to facilitate transport.

Revised 9/24/2019

Center for Complex Materials from First Principles (CCM)

John P. Perdew (Temple University); Class: 2014-2020

MISSION: To develop, test, apply, and experimentally validate improved methods of electronic structure calculation for both simple and complex materials (including quantum materials).



http://efrc.cst.temple.edu/

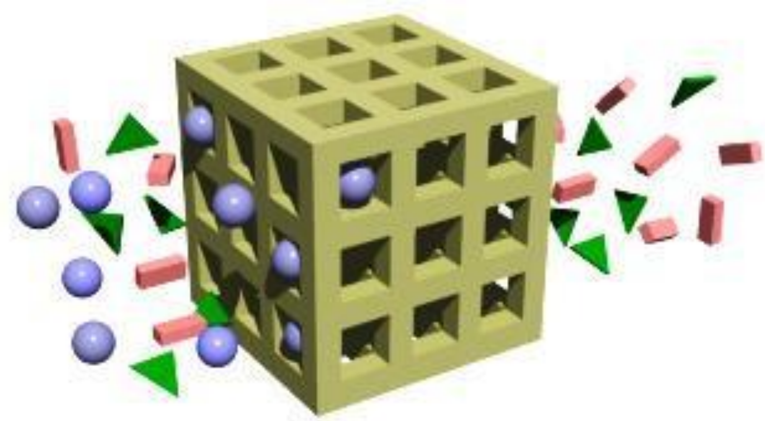
RESEARCH PLAN

CCM will develop more accurate but still computationally-efficient density functionals from first principles, testing and applying them to layered and two-dimensional materials, water at interfaces, catalysis, and cuprate high-temperature superconducting materials.

Center for Gas Separations (CGS)

Jeffrey R. Long (University of California, Berkeley); Class: 2009-2020

MISSION: To develop new metal–organic frameworks and membranes that enable energy-efficient separations of gas mixtures, as required in the clean use of fossil fuels and in reducing emissions from industry. Particular emphasis is placed on separations that reduce CO_2 emissions from power plants on energy-intensive gas separations in industry and agriculture.



www.cchem.berkeley.edu/co2efrc/

RESEARCH PLAN

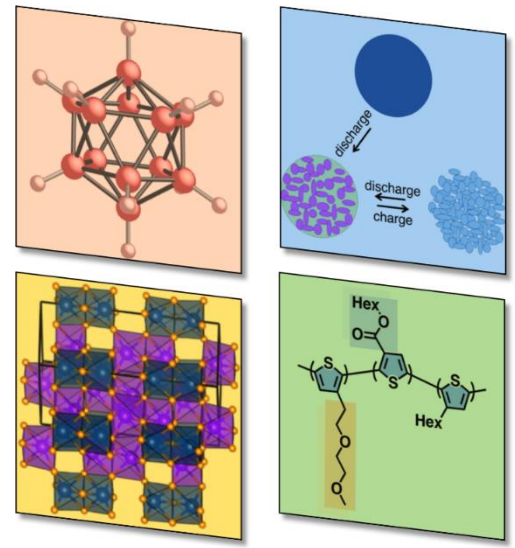
New adsorbent materials will be developed that are capable of substantially reducing the energy costs associated with industrial gas separations. The CGS is targeting adsorbents for CO_2 capture, the separation of O_2 from air and N_2 from methane, and for the shape-selective separation of hydrocarbons, among other applications. New characterization methods and computational tools will be developed to guide and support these materials design efforts.

Revised 9/24/2019

Synthetic Control Across Length-scales for Advancing Rechargeable (SCALAR)

Sarah Tolbert (University of California, Los Angeles); Class: 2018-2022

MISSION: To use the power of synthetic materials chemistry to design materials, interfaces, and architectures that help solve long-standing problems in electro-chemical energy storage



http://www.chem.ucla.edu/SCALAR

RESEARCH PLAN

The SCALAR center aims to take a holistic approach to the design of new functional materials that bridges the atomistic, nanometer, and macro length-scales in the quest to improve battery performance. To achieve this goal, the team will leverage molecular and solid-state synthetic methods, combined with solution phase self-assembly, to create new electrode materials that increase capacity, reduce losses, and improve reversibility in rechargeable batteries.

Revised 9/24/2019

U.S. DEPARTMENT OF ENERGY | Office of Science

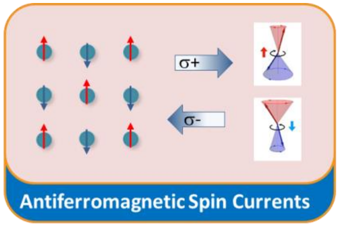
SYNTHETIC CONTROL ACROSS LENGTH-SCALES
SCALAR
FOR ADVANCING RECHARGEABLES

UCLA UCSB UC San Diego
Caltech USC SLAC

Spins and Heat in Nanoscale Electronic Systems (SHINES)

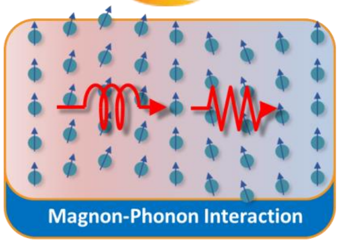
Jing Shi (University of California, Riverside); Class: 2014-2020

MISSION: To control interactions involving spins and lattice to achieve high energy efficiency in nanoscale electronic devices.



SHINES

Spins and Heat in Nanoscale Electronic Systems



http://efrcshines.ucr.edu

RESEARCH PLAN

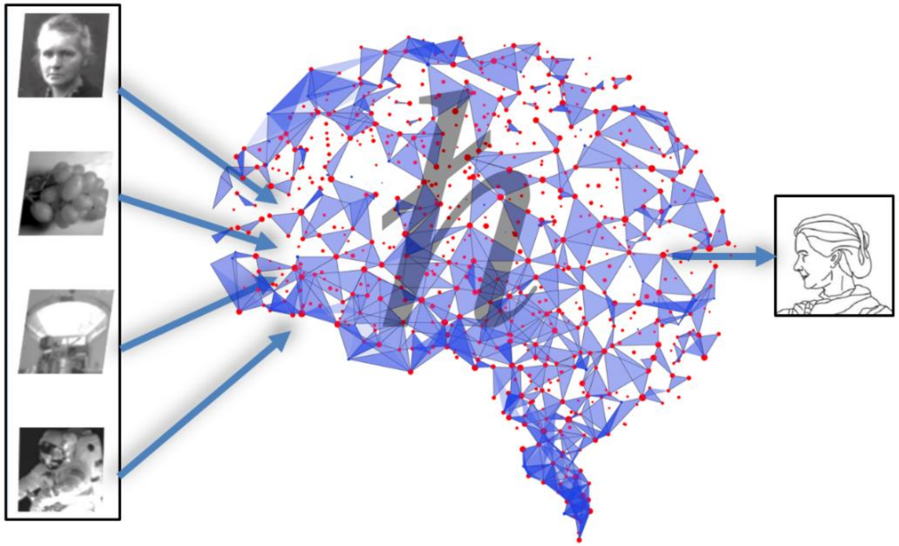
SHINES EFRC will design and synthesize novel magnetic thin films and heterostructures, control microscopic interactions via material synthesis and application of external stimuli, and discover and understand new phenomena arising from tailored interactions that will result in new functionalities and high energy efficiency in nanoscale spintronics devices.

U.S. DEPARTMENT OF ENERGY | Office of Science | UC Riverside | UCLA | Johns Hopkins University | The University of Texas at Austin | SHINES Spins and Heat In Nanoscale Electronic Systems

Quantum-Materials for Energy Efficient Neuromorphic-Computing (Q-MEEN-C)

Ivan K. Schuller (University of California, San Diego); Class: 2018-2022

MISSION: To lay down the quantum-materials-based foundation for the development of an energy-efficient, fault-tolerant, computer that is inspired and works like a brain ("neuromorphic").



A neuromorphic computer readily distills the image of a famous scientist from multiple inputs.

http://efrc.ucsd.edu

RESEARCH PLAN

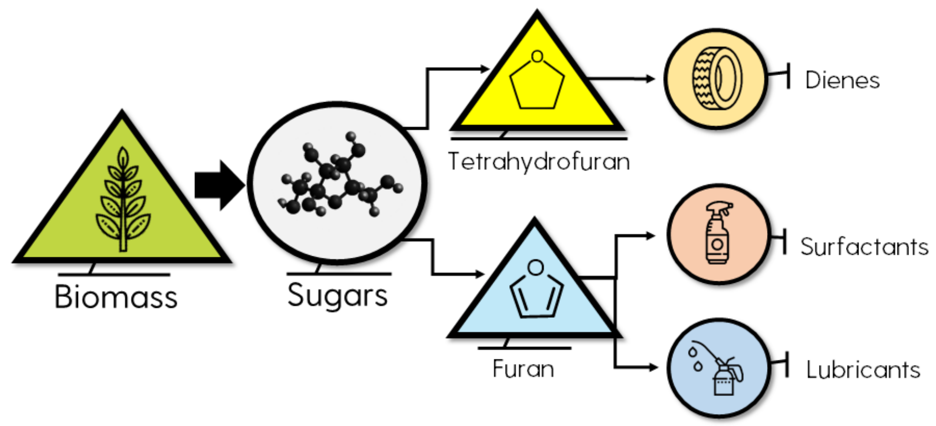
Q-MEEN-C will breakaway from the conventional Turing-von Neumann paradigm by developing quantum materials for new types of bio-inspired ("neuromorphic") devices. Their exotic properties will be harnessed to develop completely novel functionalities: artificial synapses, neurons, axons, and dendrites that can be used to construct machines with artificial intelligence.

U.S. DEPARTMENT OF ENERGY | Office of Science | UC San Diego | UCSB | UC DAVIS | THE UNIVERSITY OF CHICAGO | BROOKHAVEN NATIONAL LABORATORY | PURDUE UNIVERSITY | Northwestern University | NYU | cnrs | NIST | Argonne NATIONAL LABORATORY

Catalysis Center for Energy Innovation (CCEI)

Dionisios G. Vlachos (University of Delaware); Class: 2009-2022

MISSION: To advance the catalysis science of complex systems with a focus on thermocatalytic transformation of lignocellulosic (non-food-based) biomass into chemicals and transportation fuels.



www.ccei.udel.edu

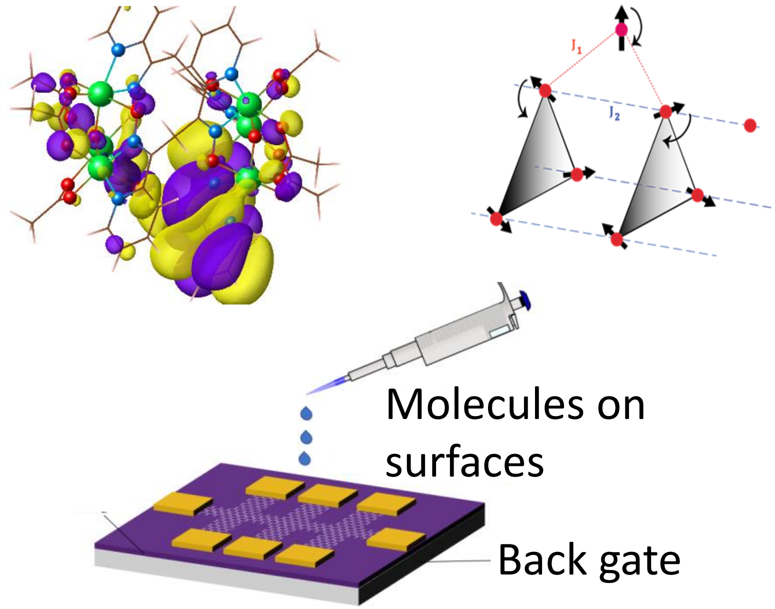
RESEARCH PLAN

Development of multifunctional, multiscale materials for enhanced energy efficiency by integrating kinetics and catalysis, synthesis of new and model materials with tailored architectures, development of imaging and operando spectroscopic techniques for characterizations, and multiscale computations.

Molecular Magnetic Quantum Materials (M^2QM)

Hai-Ping Cheng (University of Florida); Class: 2018-2022

MISSION: To provide the materials physics and chemistry understanding of molecular magnetic quantum materials essential for quantum and conventional computing beyond Moore's Law, with an overarching goal of turning molecular magnets into quantum materials useful for both quantum computing and quantum current conventional devices.



www.efrc.ufl.edu

RESEARCH PLAN

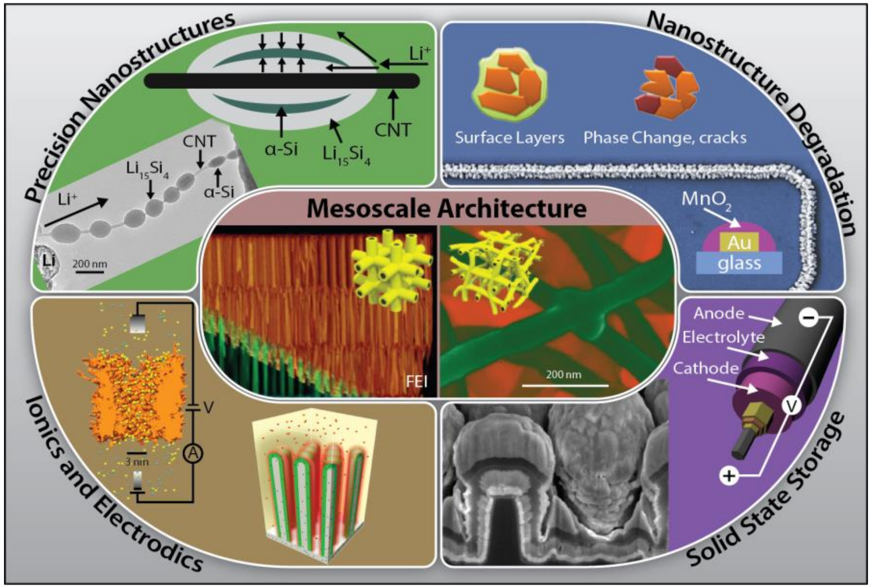
Synthesize and characterize (experimentally and computationally) linked molecular magnets with various coupling strength, and study their resulting quantum properties and coupling to surfaces and junction interfaces. Study magneto-electric couplings and exotic spin phenomena in molecular solids.

Revised 9/24/2019

Nanostructures for Electrical Energy Storage (NEES)

Gary W. Rubloff (University of Maryland); Class: 2009-2020

MISSION: To reveal scientific insights and design principles that enable a next-generation electrical energy storage technology based on dense mesoscale architectures of multifunctional solid state nanostructures.



www.efrc.umd.edu

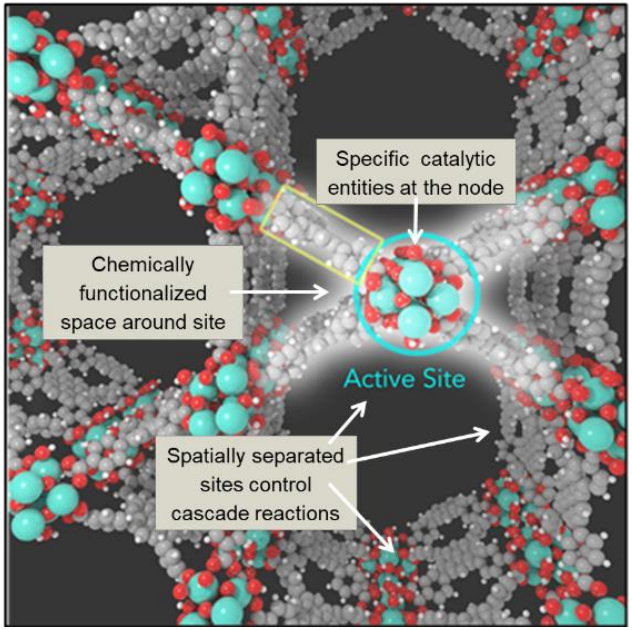
RESEARCH PLAN

- Synthesizes precision nanostructures and mesoscale architectures for solid state electrochemical energy storage
- Reveals interacting roles of ions and electrons in transport and energetics
- Elucidates and controls interfacial chemistry during synthesis and operation
- Enables nanostructure-based all-solid-state batteries for safety and simultaneous high power and energy.

Inorganometallic Catalyst Design Center (ICDC)

Laura Gagliardi (University of Minnesota); Class: 2014-2022

MISSION: To discover new classes of energy-science relevant catalytic materials, especially through the exploitation of computational modeling to identify underlying structure-function relationships that are critical to advancing further, predictive catalyst discovery.



http://www1.chem.umn.ezdu/icdc/

RESEARCH PLAN

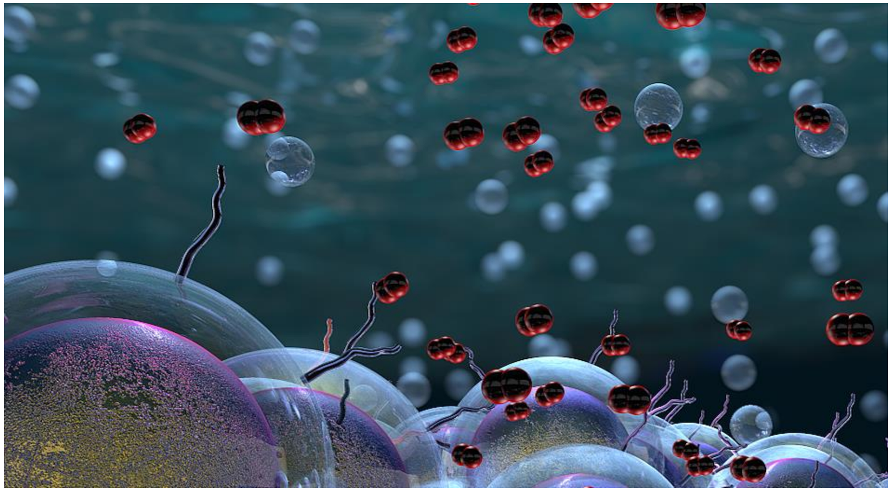
We will advance computational and synthetic methods to create electronically and structurally well defined catalysts in mesoscale, hierarchically structured and uniform environments. Using rigorous theoretical and experimental techniques, we will discover and rationalize structure/function relationships for atomically precise active sites and their surroundings.

U.S. DEPARTMENT OF ENERGY | Office of Science | ICDC INORGANOMETALLIC CATALYST DESIGN CENTER | Northwestern University | MIT | NuMat Technologies | Stony Brook University | Clemson University | Argonne National Laboratory | Pacific Northwest National Laboratory | UC Davis

Alliance for Molecular PhotoElectrode Design for Solar Fuels (AMPED)

Gerald J. Meyer (University of North Carolina at Chapel Hill); Class: 2018-2020

MISSION: To develop the fundamental molecular basis for solar-driven water oxidation and carbon dioxide reduction catalysis



www.amped.unc.edu

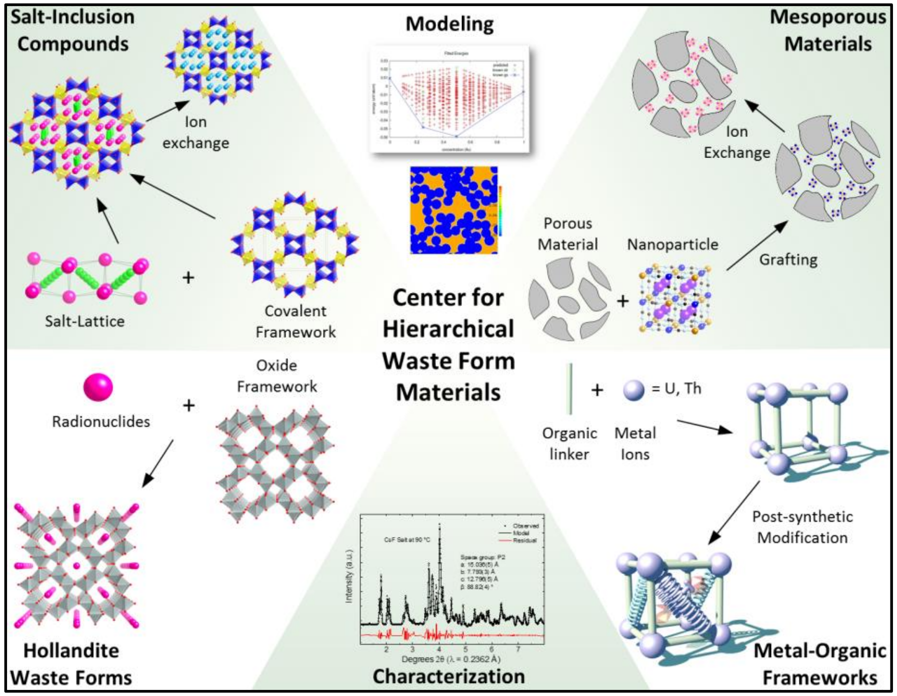
RESEARCH PLAN

The AMPED EFRC will focus on molecular approaches to dye-sensitized synthesis of solar fuels, with an emphasis on the fundamental energy science underpinning photocatalytically active materials. A variety of individual photoelectrode architectures are being mechanistically examined using diverse solution and surface characterization techniques to provide an unparalleled depth in understanding of light-driven chemistry at material–molecule–electrolyte interfaces.

Center for Hierarchical Waste Form Materials (CHWM)

Hans-Conrad zur Loye (University of South Carolina); Class: 2016-2020

MISSION: To combine experiment and modeling to develop the chemistry and structure motifs needed to create hierarchical materials that effectively immobilize nuclear waste in persistent architectures.



http://CHWM.sc.edu

RESEARCH PLAN

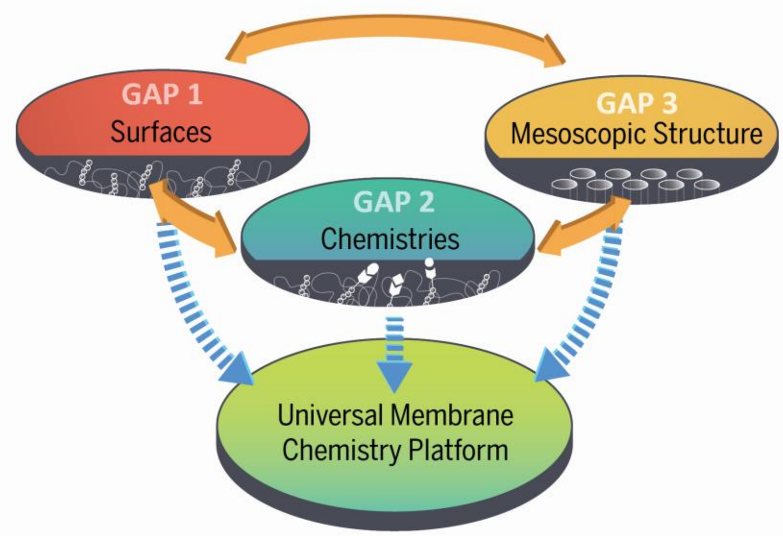
To create new materials to safely sequester nuclear waste, the center will combine experiment and modeling to develop the chemistry and structure motifs that can lead to advanced hierarchical materials that effectively immobilize nuclear waste and prevent it from re-entering the environment.

Center for Materials for Water and Energy Systems (M-WET)

Benny D. Freeman (The University of Texas at Austin); Class: 2018-2022

MISSION: To discover and understand fundamental science to design new membrane materials, develop tools and knowledge to predict new materials' interactions with targeted solutes from recalcitrant water sources, provide fit for purpose water, and recover valuable solutes with less energy.

Integrating Framework



www.mwet.utexas.edu

RESEARCH PLAN

M-WET will integrate polymer synthesis, characterization and modeling to fill basic science gaps in the understanding of fluids and materials to design novel surfaces, highly selective solute/fluid interactions, mesoscopic structures, and membranes for energy applications.

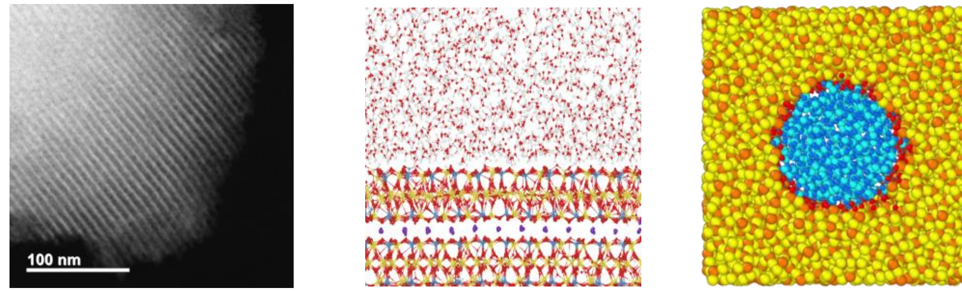
U.S. DEPARTMENT OF ENERGY | Office of Science | MWET CENTER FOR MATERIALS FOR WATER AND ENERGY SYSTEMS | TEXAS The University of Texas at Austin | UCSB | BERKELEY LAB

Multi-scale Fluid-Solid Interactions in Architected and Natural Materials (MUSE)

Darryl P. Butt (University of Utah); Class: 2018-2022

MISSION: To synthesize geomaterials with repeatable hierarchical heterogeneity and develop an understanding of transport and interfacial properties of fluids confined within these materials.

Synthesis, characterization of geomaterials
Understanding properties of fluids in confined media



www.EFRCMUSE.utah.edu

RESEARCH PLAN

Synthesized heterogeneous geomaterials will be used as substrates for determining the transport and interactions of multi-phase fluids over many length scales, including at the nanometer scale. Dynamic in-operando determination of material and fluid properties will be performed, and these measurements will be used for the development of experimentally-validated, atomistically-informed modeling tools and frameworks.

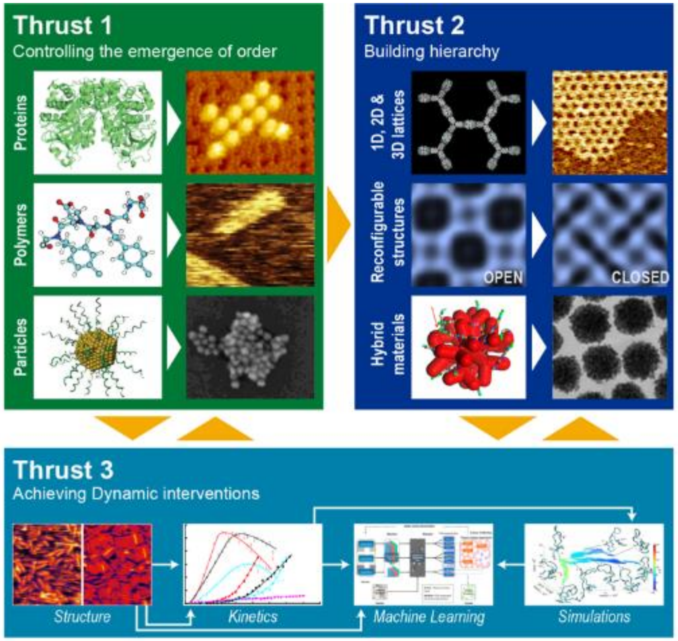
Revised 9/24/2019

U.S. DEPARTMENT OF ENERGY | Office of Science | MUSE | Idaho National Laboratory

Center for the Science of Synthesis Across Scales (CSSAS)

François Baneyx (University of Washington); Class: 2018-2022

MISSION: To harness the complex functionality of hierarchical materials by mastering the design of high-information-content building blocks that predictively self-assemble into responsive, reconfigurable, self-healing materials, and direct the formation and organization of inorganic components.



https://www.cssas-efrc.com/

RESEARCH PLAN

CSSAS will predict how the chemistry and sequence of inorganic, polymer and protein building blocks gives rise to ordered templates; master free energy landscapes to control the assembly of these templates into hierarchical and hybrid materials; and access new states of matter through the integration of data science, *in situ* characterization, and simulations.

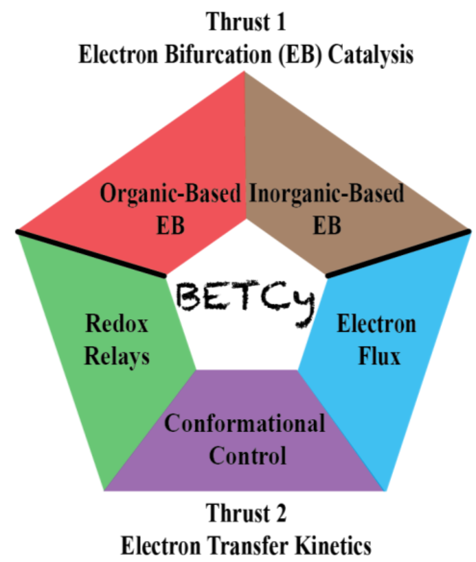
Revised 9/24/2019

U.S. DEPARTMENT OF ENERGY | Office of Science
UNIVERSITY of WASHINGTON
THE UNIVERSITY OF CHICAGO
Pacific Northwest NATIONAL LABORATORY
UC San Diego
OAK RIDGE National Laboratory

Biological Electron Transfer and Catalysis Center (BETCy)

John W. Peters (Washington State University); Class: 2014-2020

MISSION: To understand the means by which biology controls the kinetics and thermodynamics of electron bifurcation at both organic and inorganic centers, electron transfer relays, allosteric coupling, and cooperative conformational dynamics.



http://betcy-efrc.org/

RESEARCH PLAN

Develop a collective knowledge of metalloenzymes as models for redox reactions by applying physical science and computational tools to characterize biochemical reactions catalyzed by multi-subunit enzymes harboring arrays of iron-sulfur clusters and flavin cofactors. Understanding these mechanisms is central to overcoming the thermodynamic barriers that currently limit production of reduced products and fuels.

U.S. DEPARTMENT OF ENERGY | Office of Science

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TRANSFORMATIVE OPPORTUNITIES INDEX

BES REPORTS INDEX

TOPICAL INDEX

EXPERIMENTAL AND THEORETICAL METHODS INDEX