

U.S. Department of Energy

Energy Frontier Research Centers

One Page Overviews

Office of Science

August 2016; Revised 01/03/2018

TABLE OF CONTENTS
Ordered by Institution and then by Director

Center for Electrochemical Energy Science (CEES) Paul Fenter, Argonne National Laboratory	1
NorthEast Center for Chemical Energy Storage (NECCES) M. Stanley Whittingham, Binghamton University	2
Center for Emergent Superconductivity (CES) Peter Johnson, Brookhaven National Laboratory	3
Light-Material Interactions in Energy Conversion (LMI) Ralph Nuzzo, California Institute of Technology	4
Energy Frontier Research in Extreme Environments (Efree) Russell Hemley, Carnegie Institution of Washington.....	5
Center for Actinide Science & Technology (CAST) Thomas Albrecht-Schmitt, Florida State University.....	6
Center for Understanding and Control of Acid Gas-induced Evolution of Materials for Energy (UNCAGE-ME) Krista Walton, Georgia Institute of Technology.....	7
Integrated Mesoscale Architectures for Sustainable Catalysis (IMASC) Cynthia Friend, Harvard University	8
Center for Nanoscale Controls on Geologic CO₂ (NCGC) Donald DePaolo, Lawrence Berkeley National Laboratory.....	9
Center for Advanced Solar Photophysics (CASP) Victor Klimov, Los Alamos National Laboratory	10
Center for Excitonics (CE) Marc Baldo, Massachusetts Institute of Technology	11

Solid-State Solar-Thermal Energy Conversion Center (S3TEC) Gang Chen, Massachusetts Institute of Technology	12
Center for Biological Electron Transfer and Catalysis (BETCy) John Peters, Montana State University	13
Center for Next Generation of Materials Design: Incorporating Metastability (CNGMD) William Tumas, National Renewable Energy Laboratory	14
Center for Bio-Inspired Energy Science (CBES) Samuel Stupp, Northwestern University	15
Argonne-Northwestern Solar Energy Research Center (ANSER) Michael Wasielewski, Northwestern University	16
Fluid Interface Reactions, Structures and Transport Center (FIRST) Sheng Dai, Oak Ridge National Laboratory	17
Energy Dissipation to Defect Evolution (EDDE) Yanwen Zhang, Oak Ridge National Laboratory	18
Center for Performance and Design of Nuclear Waste Forms and Containers (WastePD) Gerald Frankel, Ohio State University	19
Center for Molecular Electrocatalysis (CME) R. Morris Bullock, Pacific Northwest National Laboratory	20
Interfacial Dynamics in Radioactive Environments and Materials (IDREAM) Sue Clark, Pacific Northwest National Laboratory	21
Center for Lignocellulose Structure and Formation (CLSF) Daniel Cosgrove, Pennsylvania State University	22
Center for Direct Catalytic Conversion of Biomass to Biofuels (C3Bio) Maureen McCann, Purdue University	23

Center for Mesoscale Transport Properties (m2M) Esther Takeuchi, Stony Brook University	24
Center for the Computational Design of Functional Layered Materials (CCDM) John Perdew, Temple University	25
Center for Gas Separations Relevant to Clean Energy Technologies (CGS) Jeffrey Long, University of California, Berkeley	26
Spins and Heat in Nanoscale Electronic Systems (SHINES) Jing Shi, University of California, Riverside	27
Catalysis Center for Energy Innovation (CCEI) Dionisios Vlachos, University of Delaware	28
Center for Geologic Storage of CO₂ (GSCO₂) Scott Frailey, University of Illinois at Urbana-Champaign	29
Nanostructures for Electrical Energy Storage (NEES) Gary Rubloff, University of Maryland.....	30
Inorganometallic Catalyst Design Center (ICDC) Laura Gagliardi, University of Minnesota.....	31
Center for Solar Fuels (UNC) Thomas Meyer, University of North Carolina	32
Materials Science of Actinides (MSA) Peter Burns, University of Notre Dame	33
Center for Hierarchical Waste Form Materials (CHWM) Hans-Conrad zur Loye, University of South Carolina	34
Center for Frontiers of Subsurface Energy Security (CFSES) Larry Lake, University of Texas at Austin	35

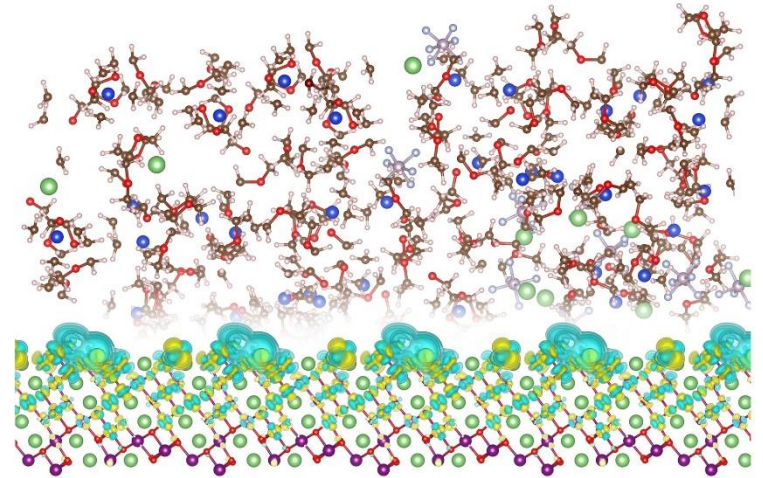
Photosynthetic Antenna Research Center (PARC)	
Robert Blankenship, Washington University in St. Louis.....	36
GRAND CHALLENGES INDEX.....	37
BES REPORTS INDEX	37
TOPICAL INDEX	38
EXPERIMENTAL AND THEORETICAL METHODS INDEX.....	40

Center for Electrochemical Energy Science (CEES) Paul Fenter (Argonne National Laboratory)

The Center's mission is to develop a fundamental understanding and robust control of the reactivity of electrified oxide interfaces, films and materials relevant to lithium-ion battery chemistries.

<http://www.cees.anl.gov>

**CENTER FOR ELECTROCHEMICAL
ENERGY SCIENCE** AN ENERGY FRONTIER
RESEARCH CENTER



ARGONNE NATIONAL LABORATORY • NORTHWESTERN UNIVERSITY
UNIVERSITY OF ILLINOIS AT URBANA-CHAMPAIGN • PURDUE UNIVERSITY

RESEARCH PLAN

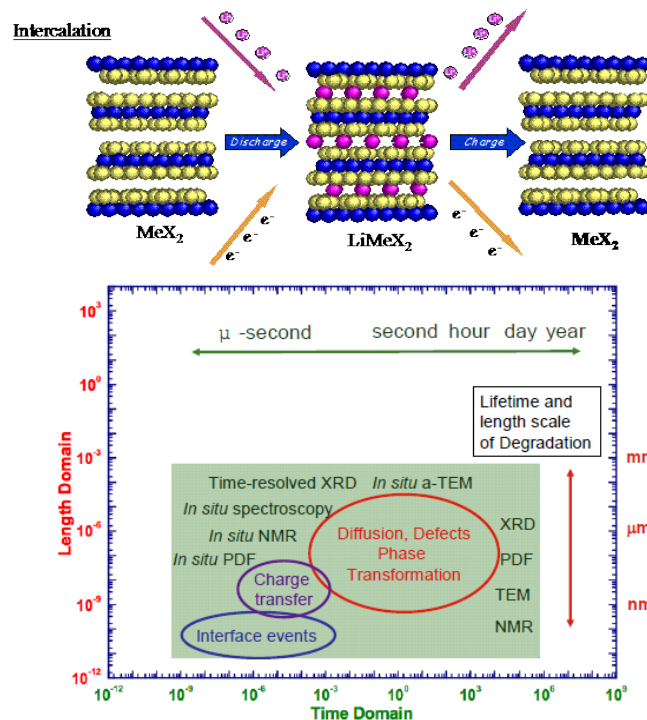
CEES probes the molecular-scale structure and reactivity at electrified oxide-electrolyte interfaces, leverages advanced materials synthesis to create materials with well-defined properties (composition, structure, etc.), and develops novel approaches and chemistries to direct electrochemical reactivity.

Northeast Center for Chemical Energy Storage (NECCES)

M. Stanley Whittingham (Binghamton University)

MISSION: Develop an understanding of how key electrode reactions occur in cathode materials for Li based batteries, 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

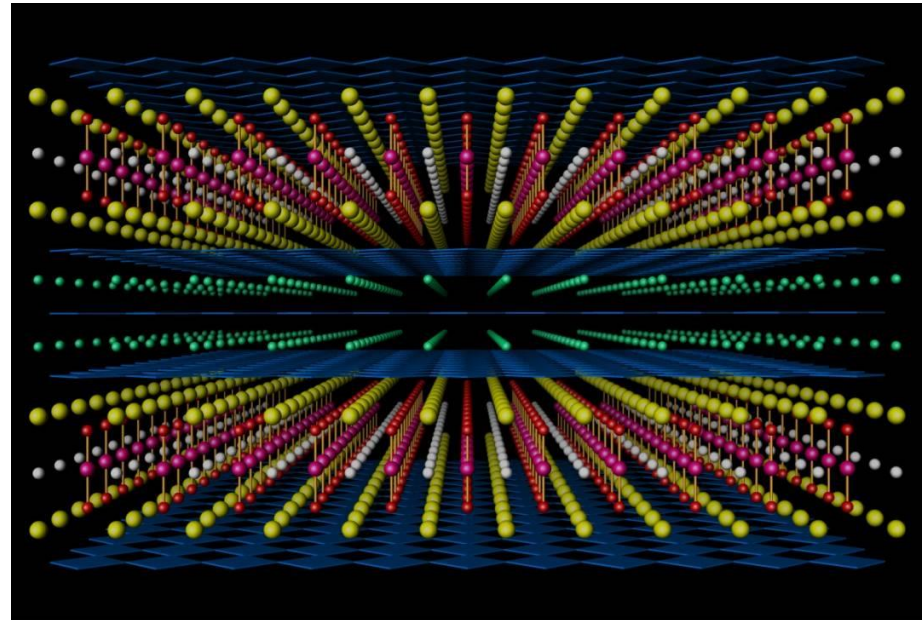
The processes that occur in batteries are complex, spanning a wide range of time and length scales. The team of experimentalists and theorists will make use of, and develop new methodologies to determine how model compound electrodes function in real time, as batteries are cycled.

Center for Emergent Superconductivity (CES)

Peter D. Johnson (Brookhaven National Laboratory)

The central mission of CES is the development of an understanding of High T_c Superconductivity that will enable the prediction and perfection of new High T_c materials for use in a range of energy technologies including applications in generation, storage and transmission.

<http://www.bnl.gov/energy/ces/>



Legend for the 3D model:
● Oxygen (red)
● Mercury (grey)
● Calcium (green)
● Barium (yellow)
● Oxygen (white)
■ Cu-O Sheets (blue)

RESEARCH PLAN

Research to design superconductors with enhanced performance will be directed towards three key areas: (1) develop techniques to create new classes of superconducting materials by design, (2) understand the mechanism of high-temperature superconductivity, and (3) understand the current carrying limiting properties of existing high-temperature superconductors.

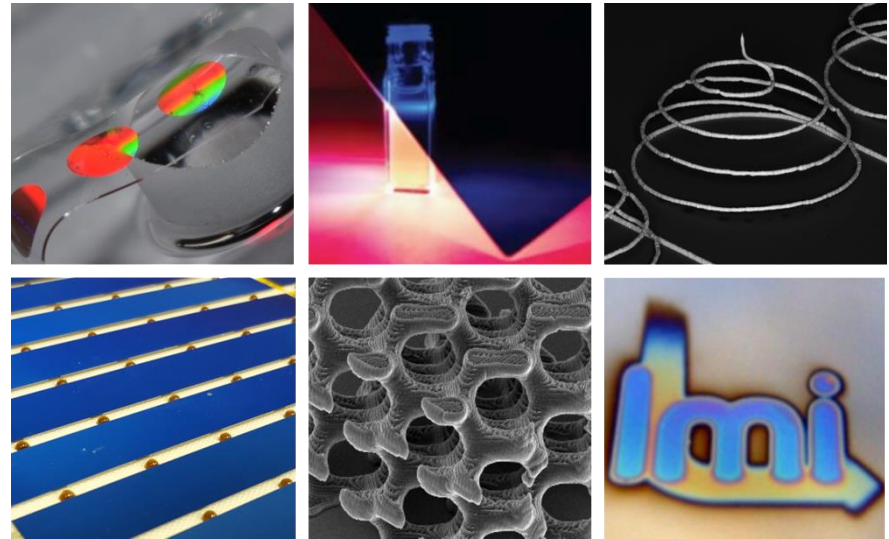
Light-Material Interactions in Energy Conversion (LMI)

Ralph Nuzzo (Caltech)

LMI-EFRC: a national resource for fundamental optical principles and design for solar energy conversion.

Goal: to tailor the morphology, complex dielectric structure, and electronic properties of matter so as to sculpt the flow of sunlight and heat, enabling light conversion to electrical energy with unprecedented efficiency.

<http://lmi.caltech.edu>



RESEARCH PLAN

Challenge: Solar energy conversion that effectively utilizes the entire solar spectrum. **Approach:** Photonic design combining fundamental limits to solar conversion efficiency, spectrum splitting and control, broad angle light capture and concentration, and thermal photonics. **Outcome:** Photonic principles that enable record photovoltaic conversion efficiency and utilization of the entire visible and infrared solar resource.

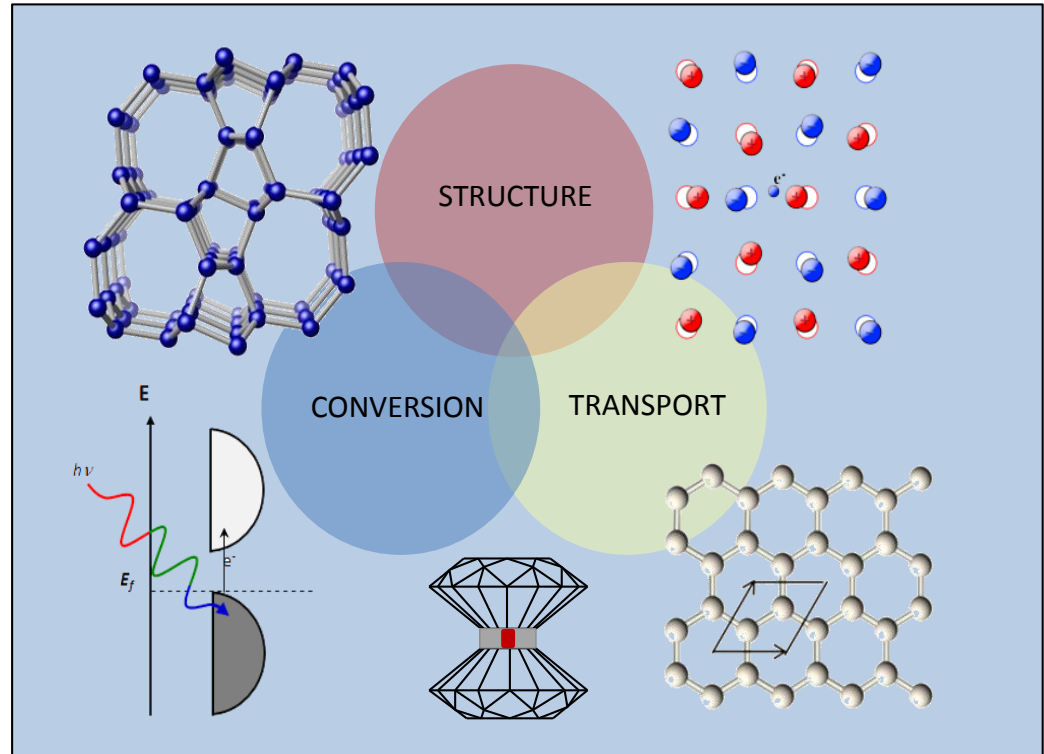
Energy Frontier Research in Extreme Environments (EFree)

Russell J. Hemley (Carnegie Institution of Washington)

EFree Mission Statement:

To accelerate the discovery and synthesis of energy materials using extreme conditions.

<https://efree.carnegiescience.edu/>



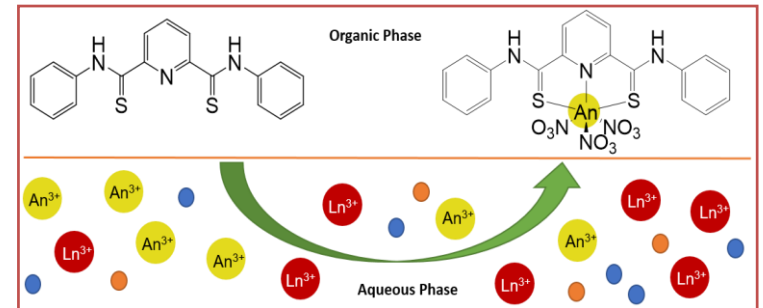
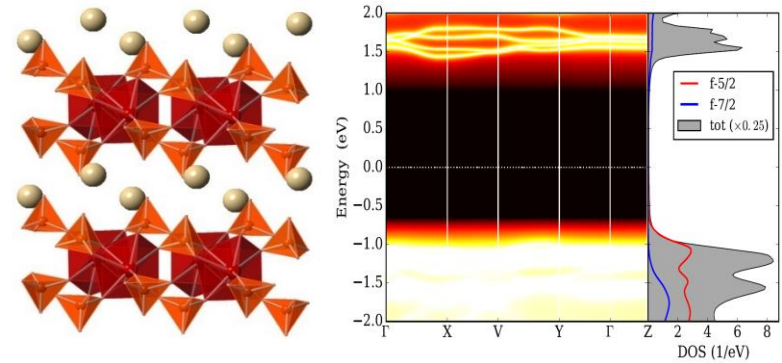
RESEARCH PLAN

By use of advanced extreme conditions techniques, EFree discovers, characterizes, and creates transformative energy materials, including novel structural, energy conversion, and energy transport materials.

Center for Actinide Science & Technology (CAST) Thomas Albrecht-Schmitt (Florida State University)

The mission of CAST is to advance our understanding of how electronic structure and bonding control the properties of heavy element materials. This knowledge will aid in the development of nuclear technologies that enhance energy security, address nuclear legacy issues and environmental concerns, and foster the next generation of nuclear scientists.

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



RESEARCH PLAN

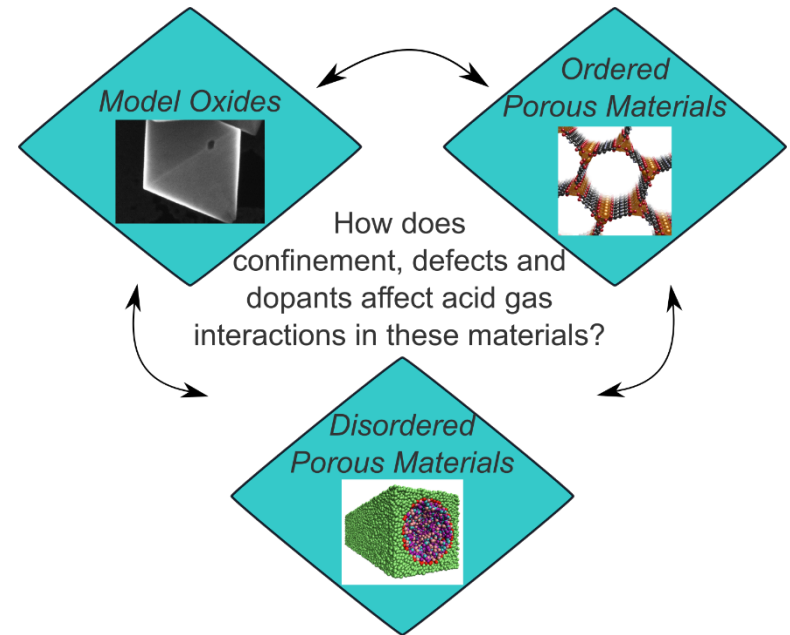
CAST develops new materials that capture radionuclides found within legacy waste from the Cold War. Optimization of these materials requires advances in synthesis, characterization, and theoretical methods that provide a deep understanding of the origin of the unusual properties of these nuclear materials.

Revised 11/14/2017

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

UNCAGE-ME focuses on developing a deep knowledge base in the characterization, prediction, and **control of acid-gas interactions** with a broad class of materials to accelerate **materials development** for large-scale **energy applications**.

<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** to improve the performance of materials in these environments and advance materials discovery.

Integrated Mesoscale Architectures for Sustainable Catalysis (IMASC)

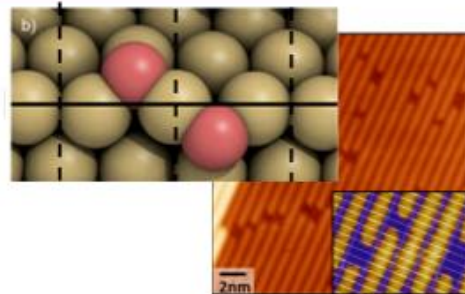
Cynthia Friend (Harvard University)

MISSION STATEMENT:

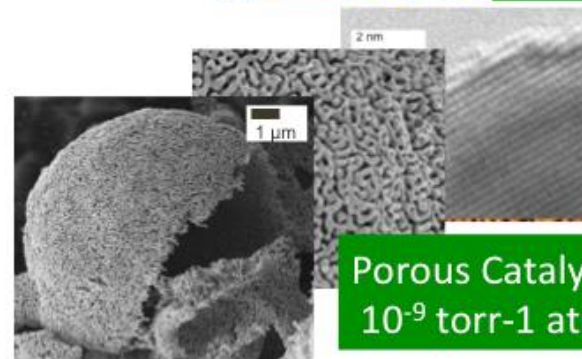
The mission of IMASC is to drive and conduct transformative research in mesoscale science for sustainable catalysis, with full integration of multi-scale experimental, theoretical and computational approaches.

<http://www.efrc.harvard.edu>

Atomistic models



Focus on improving selectivity for selective oxidation and hydrogenation reactions



Porous Catalysts:
 10^{-9} torr-1 atm

RESEARCH PLAN

The plan is to develop principles for designing catalytic processes, based on porous catalyst architectures (non-zeolite), that will reduce energy consumption in producing platform chemicals by carrying out investigations under a wide range of conditions using advanced experiment and theory.

Revised 11/14/2017

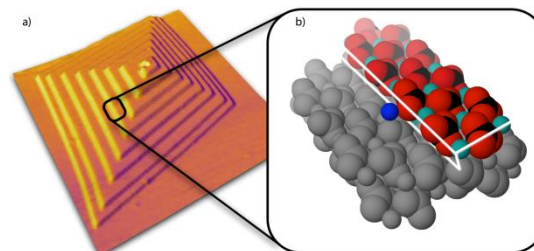
Center for Nanoscale Controls on Geologic CO₂ (NCGC)

Donald J. DePaolo (LBNL)

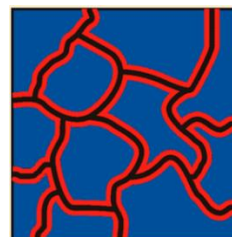
NCGC Mission Statement

Enhance the performance and predictability of subsurface storage systems by understanding the molecular and nanoscale origins of CO₂ trapping processes, and developing computational tools to translate to larger-scale systems

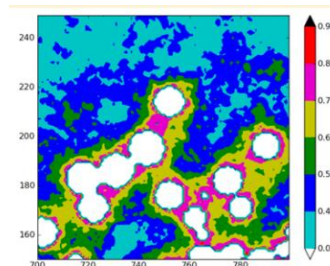
esd1.lbl.gov/research/facilities/ncgc/



Molecular-to-nanoscale characterization and models



Calibration of computer simulations to experiments



RESEARCH PLAN

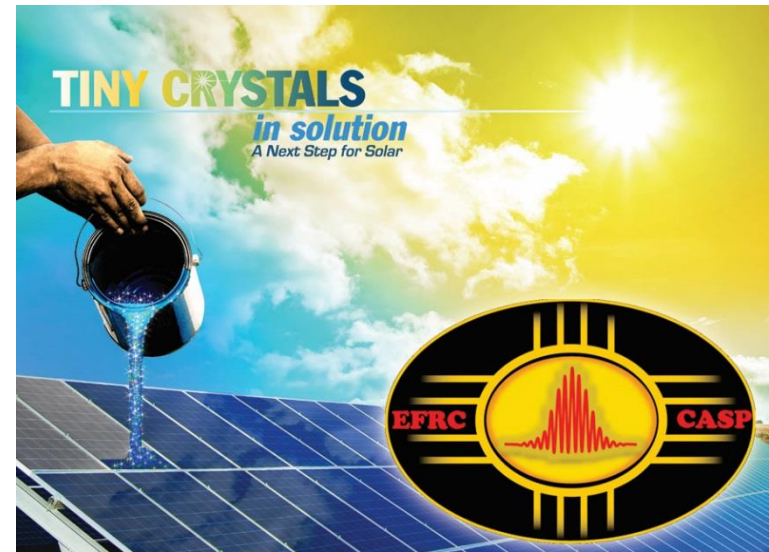
Experimental investigations will probe nanoscale fluid-fluid and fluid-mineral interactions and their effects on subsurface CO₂ trapping. Characterization and experiments will be integrated with mesoscale chemical-mechanical-hydrologic modeling and simulation to achieve a transformational predictive capability for stratigraphic- and reservoir CO₂ trapping efficiency and long-term reliability.

Center for Advanced Solar Photophysics (CASp) Victor I. Klimov (Los Alamos National Laboratory)

The purpose of this center is to explore, design and apply the unique interactions of *nanomaterials* with light to enable *disruptive advances* in the efficiency of solar energy capture and conversion.

<http://casp.lanl.gov>

<http://www.centerforadvancedsolarphtophysics.org>



RESEARCH PLAN

Our focus is on fundamental physics and chemistry of solution-processible semiconductor nanocrystals specifically designed to exhibit novel phenomena that will enhance the conversion of sunlight into electricity. The desired outcomes of this work are effective, low-cost schemes for light harvesting and conversion using approaches such as up- and down-conversion, carrier multiplication, and controlled coupling in mesoscopic nanocrystal assemblies.

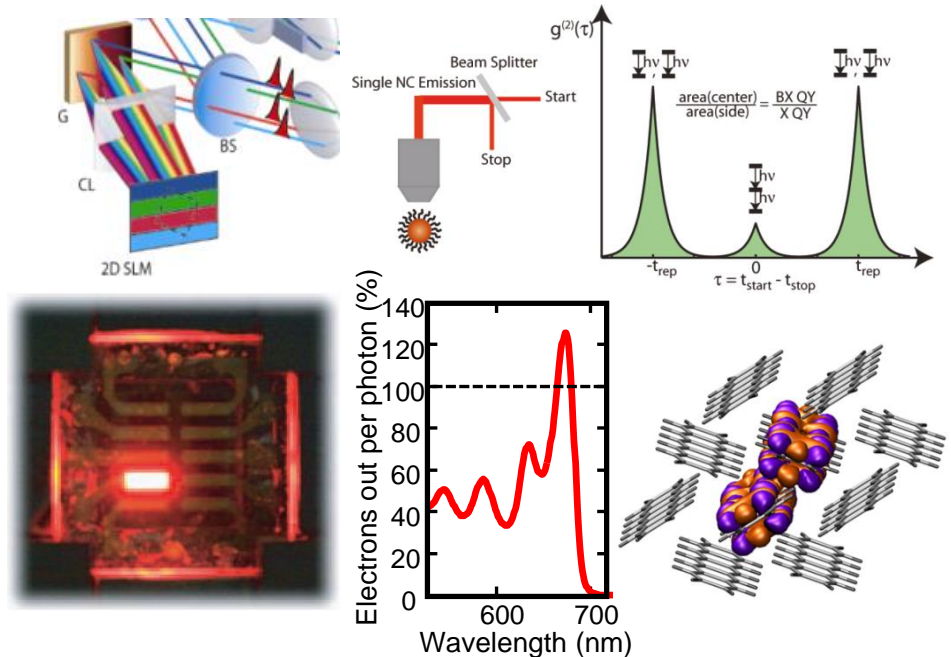
Center for Excitonics (CE)

Marc Baldo (MIT)

Electronics vs Excitonics

Excitons are nanoscale packets of energy that are characteristic of low-cost materials for solar cells and solid state lighting. The CE EFRC seeks to supersede traditional electronics with devices that use excitons to mediate the flow of energy.

<http://www.rle.mit.edu/excitonics/>



RESEARCH PLAN

The CE EFRC addresses the two grand challenges in excitonics:

- (1) Understand, control and exploit exciton transport
- (2) Understand and exploit energy conversion between excitons, electrons, and photons.

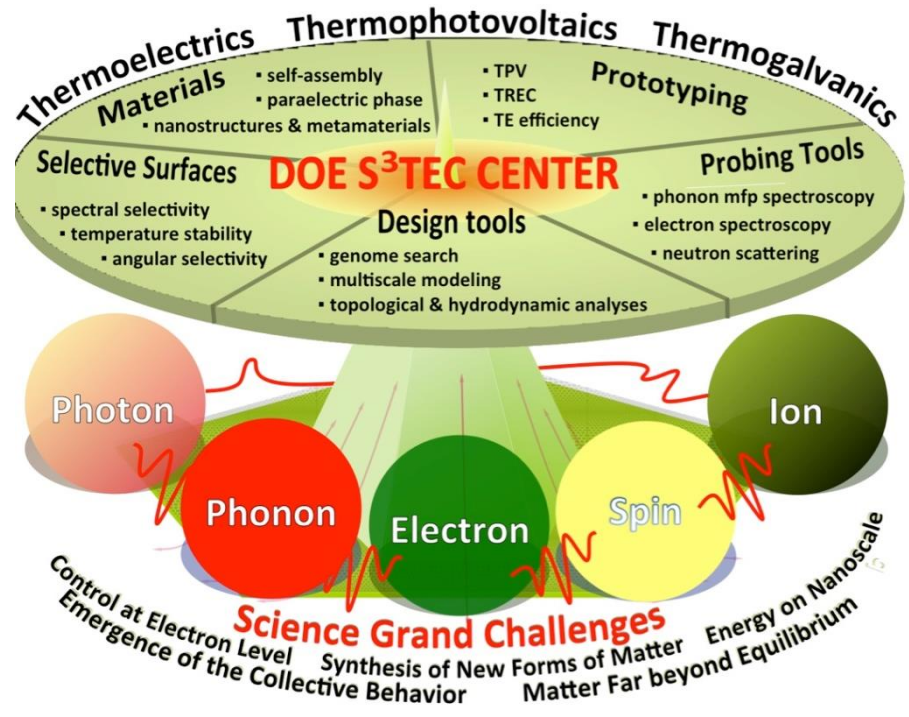
CE's advances will be applied to low-cost solar cells and solid state lighting.

Solid-State Solar-Thermal Energy Conversion Center (S³TEC)

Gang Chen (Massachusetts Institute of Technology)

EFRC Mission: To advance fundamental science and materials for harnessing heat from the Sun and terrestrial sources and for converting this heat into electricity via thermoelectric, thermophotovoltaic, and thermogalvanic technologies.

<http://s3tec.mit.edu/>

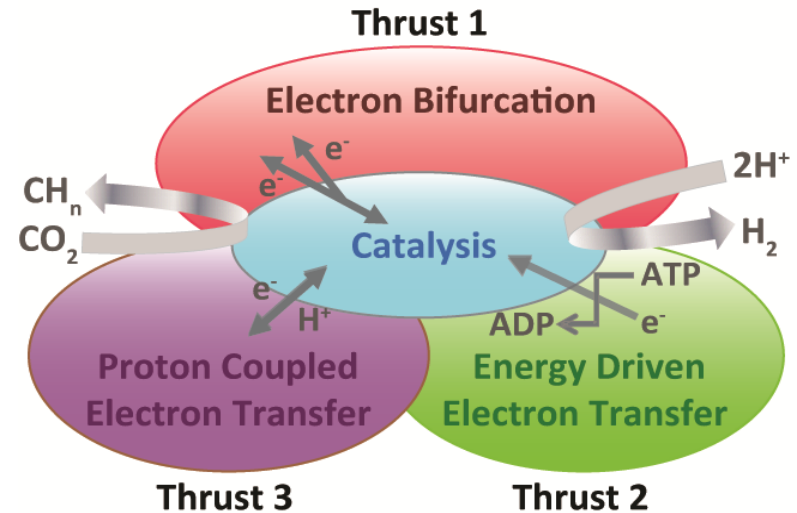


RESEARCH PLAN

The Center combines experiments, modeling, and simulation to study and optimize the properties of elementary energy carriers involved in heat-to-electricity energy conversion, which will guide design and synthesis of new materials and demonstration of proof-of-principles prototypes.

Biological Electron Transfer and Catalysis (BETCy) John Peters (Montana State University)

EFRC mission: The focus of the Biological Electron Transfer and Catalysis (*BETCy*) EFRC research is elucidating mechanisms of conversion of electrochemical potential into chemical bond energy through investigating the basis for controlling electron bifurcation, electron-ion coupling, and redox catalysis in model enzymes.



<http://eu.montana.edu/betcy-efrc/>

RESEARCH PLAN

The research plan of the *BETCy* EFRC has been designed to provide the basis to exploit the unique features of biochemical mechanisms that have yet to be explored substantively in the context of energy production but have the potential for innovative solutions and game-changing advancement.

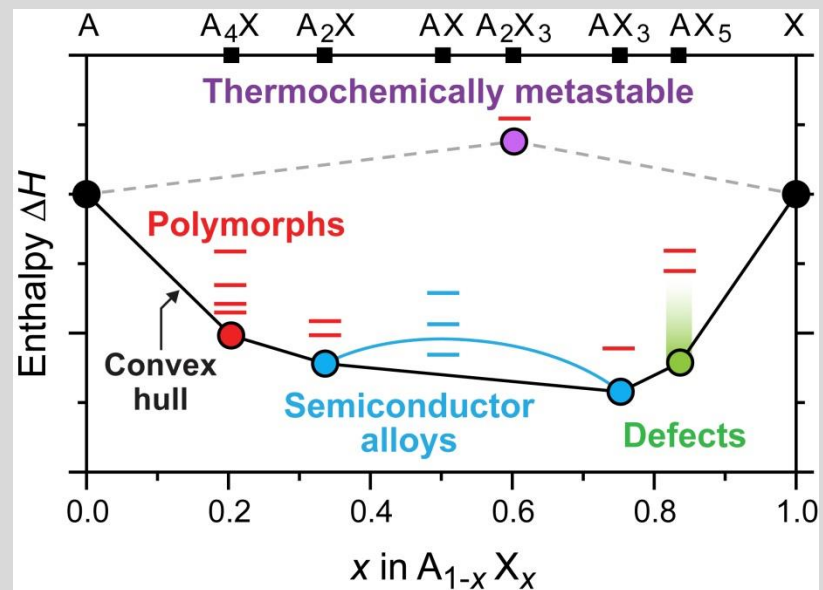
Revised 11/14/2017

Center for Next Generation of Materials Design (CNGMD)

William Tumas (National Renewable Energy Laboratory)

The mission of CNGMD is to dramatically transform the discovery of functional energy materials using high-throughput multiple-property search, incorporation of metastable materials into predictive design, and the development of theory to guide materials synthesis.

www.cngmd-efrc.org



Four classes of metastable materials (shown in color) targeted for theory-driven synthesis in the CNGMD EFRC.

RESEARCH PLAN

- Integrate high-throughput theory, synthesis, characterization, and data mining to rapidly *discover new functional semiconductor materials for energy applications*.
- Develop new theory and experimental *tools* to accelerate materials discovery.
- Discover and study *metastable materials* including polymorphs, alloys, defects.
- Identify *synthesis pathways* by coupling theory and *in-situ* characterization.

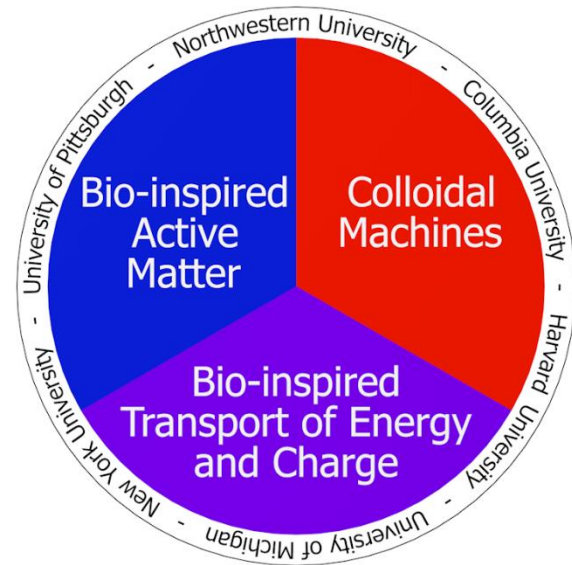
Revised 1/3/2018

Center for Bio-inspired Energy Science (CBES) Samuel Stupp (Northwestern University)

CBES mission statement:

To discover and develop bio-inspired systems that reveal new connections between energy and matter.

<http://cbes.northwestern.edu/>



RESEARCH PLAN

Combining theory and experiments, the Center will develop artificial materials and systems that take inspiration from biology. These systems will include materials with bio-inspired functions (artificial muscles, organelles, and adaptive materials), colloidal machines (motors, ensembles of motors, and artificial cells), and energy and charge transport (quantum ratchets and ion pumps).

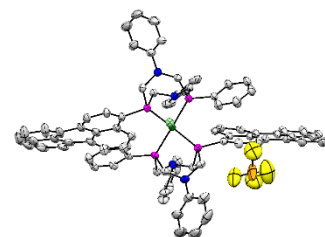
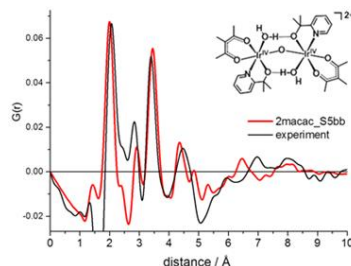
Argonne-Northwestern Solar Energy Research (ANSER) Center

Michael R. Wasielewski (Northwestern University)

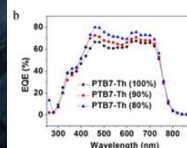
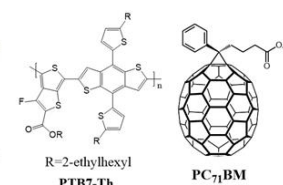
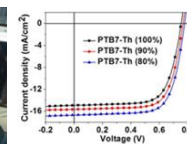
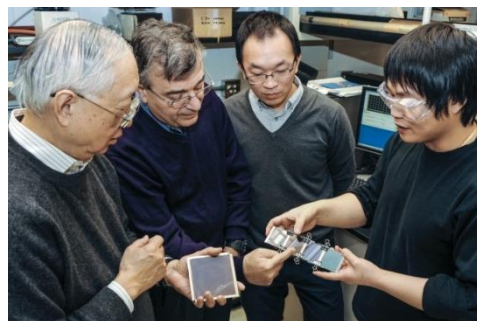
The mission of the ANSER Center is to revolutionize our understanding of molecules, materials, and methods necessary to create dramatically more efficient technologies for solar fuels and electricity production.

<http://www.AnserCenter.org>

Solar Fuels



Solar Electricity



RESEARCH PLAN

Develop a fundamental understanding of how to:

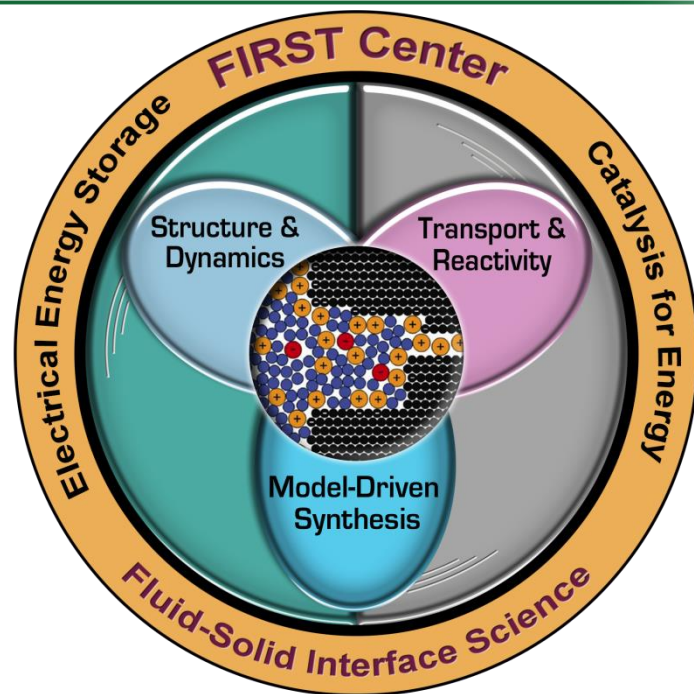
- Design, fabricate, and characterize new catalysts to split water to hydrogen and oxygen and to convert carbon dioxide into liquid fuels using sunlight.
- Design, fabricate, and characterize new materials for low-cost, earth-abundant, next generation solar cells and powering solar fuels catalysts.

Fluid Interface Reactions, Structures and Transport (FIRST) Sheng Dai (Oak Ridge National Laboratory)

FIRST Center Mission Statement:

To develop fundamental understanding and validated, predictive models of the unique nanoscale environment at fluid-solid interfaces that will enable transformative advances in electrical energy storage and electrocatalysis

<http://web.ornl.gov/sci/first/>



RESEARCH PLAN

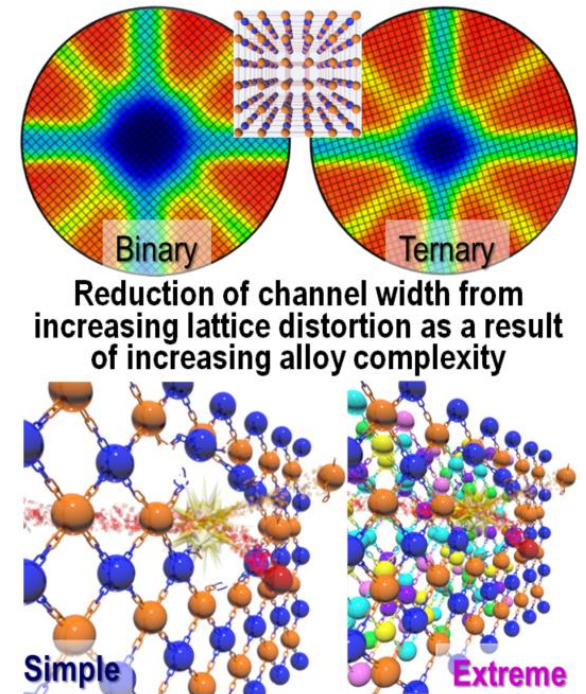
FIRST integrates novel experimental and analytical approaches, advanced materials synthesis and characterization, and multiscale computational modeling to achieve a level of understanding of the structures, dynamics, transport properties and reactivity of fluid-solid interfaces sufficient to design and test novel interfacial systems with transformative properties.

Energy Dissipation to Defect Evolution (EDDE)

Yanwen Zhang (Oak Ridge National Laboratory)

EFRC Mission: To develop a foundation of energy dissipation mechanisms in tunable concentrated solid-solution alloys, to control the early stage processes of radiation damage formation and defect evolution, and to yield new design principles and accelerate science-based material discovery of radiation-tolerant structural alloys for energy applications.

<http://edde.ornl.gov/>



RESEARCH PLAN

Challenge: To improve structural alloy performance in a radiation environment for safe and economical operation.

Approach: To understand energy dissipation through electron and phonon interactions, and how they are influenced by alloy complexity.

Outcome: New design principles for radiation-tolerant structural alloys.

The mission of WastePD is to understand the fundamental mechanisms of waste form performance, and apply that understanding to develop tools for design of waste forms with improved performance.



<https://efrc.osu.edu>

RESEARCH PLAN

- Science of Environmental Degradation of Waste Form Materials
- Roles of Surface Films and Material Reactivity
- Impact of Environment on Degradation of Waste Form Materials

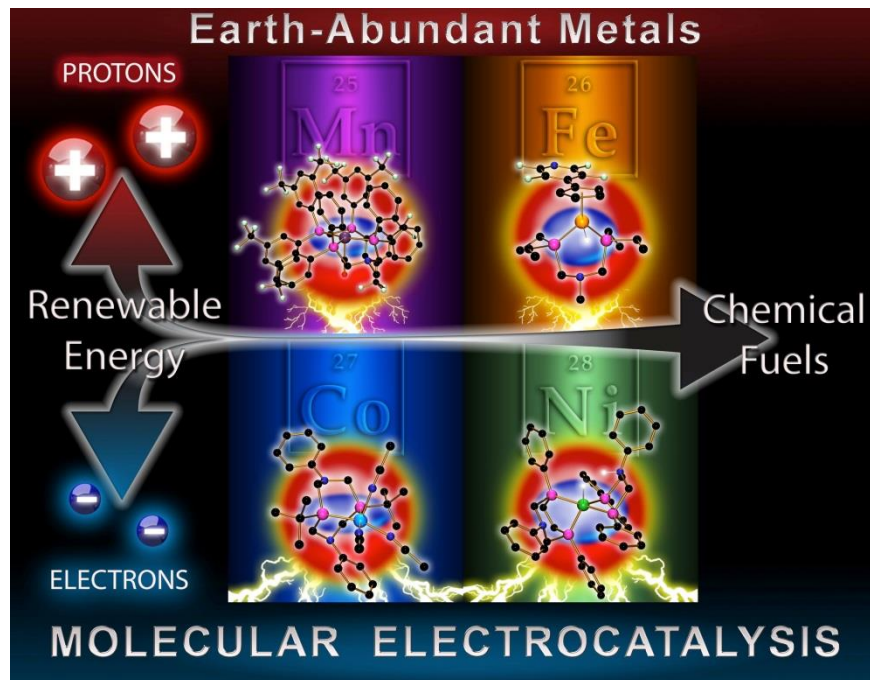
Revised 11/14/2017

The Center for Molecular Electrocatalysis (CME)

R. Morris Bullock (Pacific Northwest National Laboratory)

CME's vision is to develop a comprehensive understanding of **proton transfer reactions** that will lead to transformational changes in the ability to **design molecular electrocatalysts** that rapidly and efficiently convert between electrical energy and chemical energy (bonds) in fuels.

<http://efrc.pnnl.gov>



RESEARCH PLAN

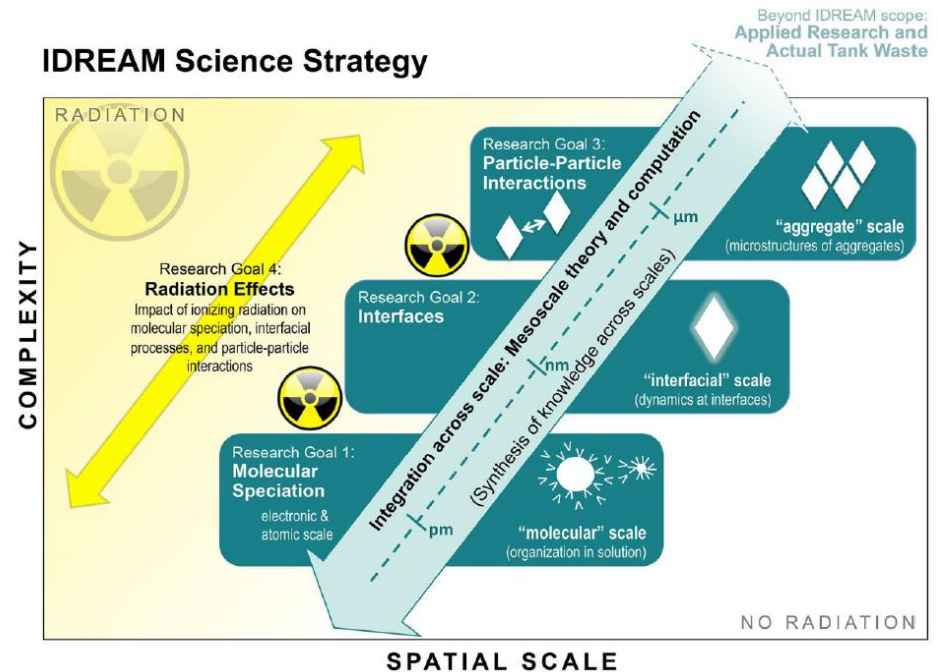
Catalysts facilitate the conversion of electricity obtained from carbon-neutral, sustainable energy sources (such as solar and wind) into chemical bonds in fuels. CME's research addresses the precise control of movement of protons and electrons to enhance the rate and efficiency of electrocatalysts.

Revised 11/14/2017

Interfacial Dynamics in Radioactive Environments and Materials (IDREAM)

Sue Clark (Pacific Northwest National Laboratory)

Mission: 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.



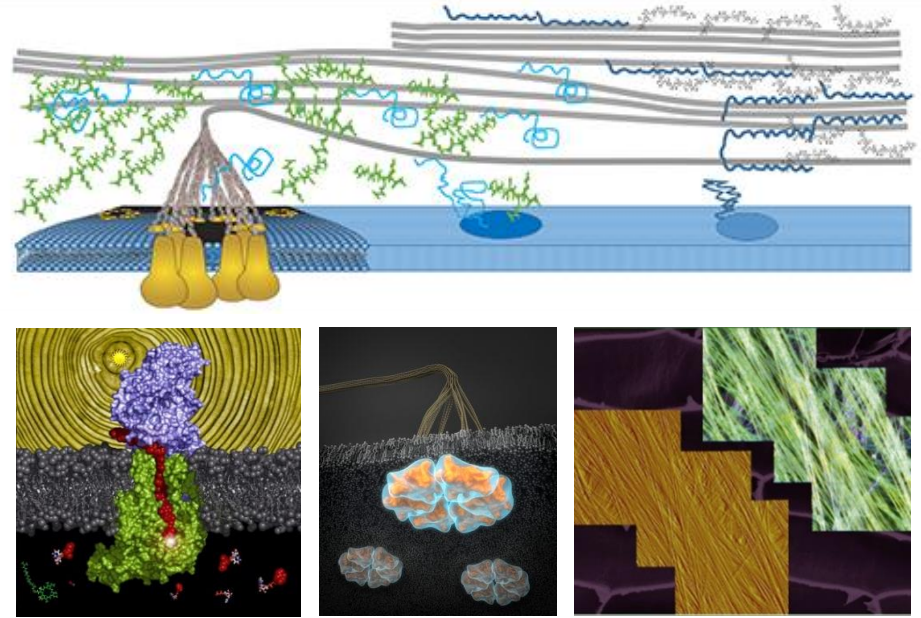
RESEARCH PLAN

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.

Center for Lignocellulose Structure and Formation (CLSF) Daniel J. Cosgrove (Penn State University)

Mission: to develop a nano- to meso-scale understanding of plant cell walls, the main structural material in plants, and the mechanisms of their assembly, forming the foundation for significant advances in sustainable energy and novel biomaterials.

www.lignocellulose.org



RESEARCH PLAN

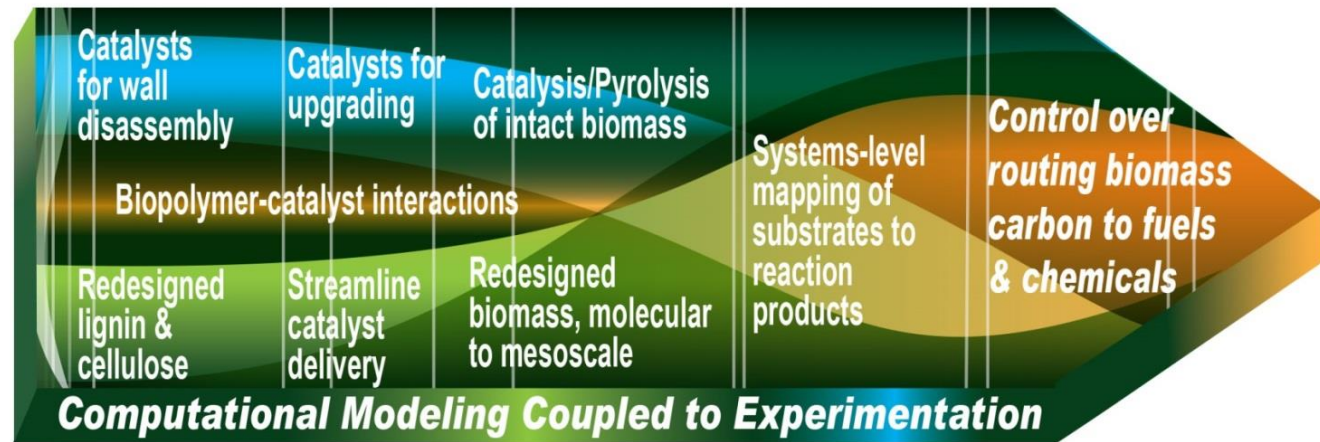
With a unique mix of molecular biologists, chemists, physicists, engineers and computational modelers, CLSF is developing a molecular understanding of the nano-machinery that transforms simple sugars into cellulose microfibrils and the 'rules of assembly' that enable scaffolds of cellulose microfibrils to interact with water, matrix polysaccharides, and lignin to produce hierarchically-ordered cell walls with diverse physical and material properties.

Revised 11/14/2017

Center for Direct Catalytic Conversion of Biomass to Biofuels (C3Bio)

Maureen McCann (Purdue University)

The C3Bio mission is to master the ability to reconfigure all partially reduced carbon from plant cell walls into desired molecules.



<http://www.purdue.edu/discoverypark/c3bio/>

RESEARCH PLAN

C3Bio develops fundamental understanding of how biomass structural complexity impacts the yields and selectivities of liquid hydrocarbon fuels and high-value chemicals during catalytic or pyrolytic transformations of plant cell walls. We modify cell wall composition and catalytically transform intact biomass to specify both the structures within, and the reaction products from, lignocellulosic biomass.

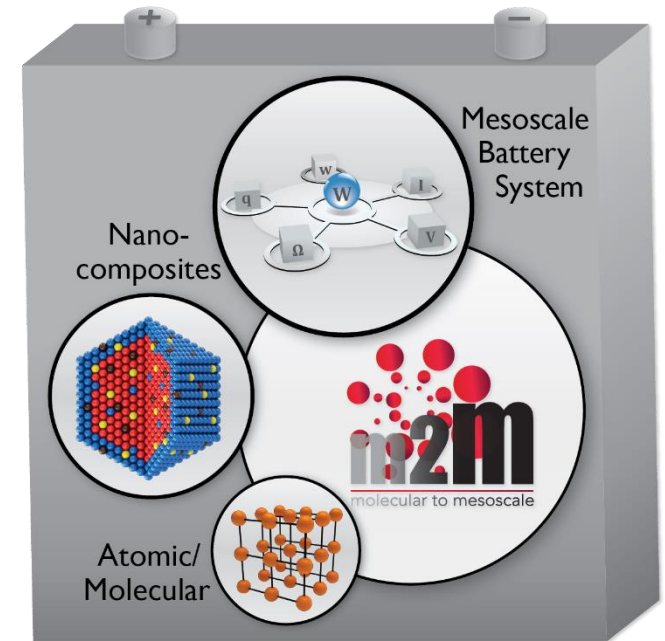
Center for Mesoscale Transport Properties (*m2m*)

Esther S. Takeuchi (Stony Brook University)

m2m EFRC mission statement:

to understand and to provide control of transport properties in complex battery systems with respect to multiple length scales, from molecular to mesoscale (*m2m*); to minimize heat and maximize work of electrical energy storage devices.

<http://www.stonybrook.edu/m2m/>



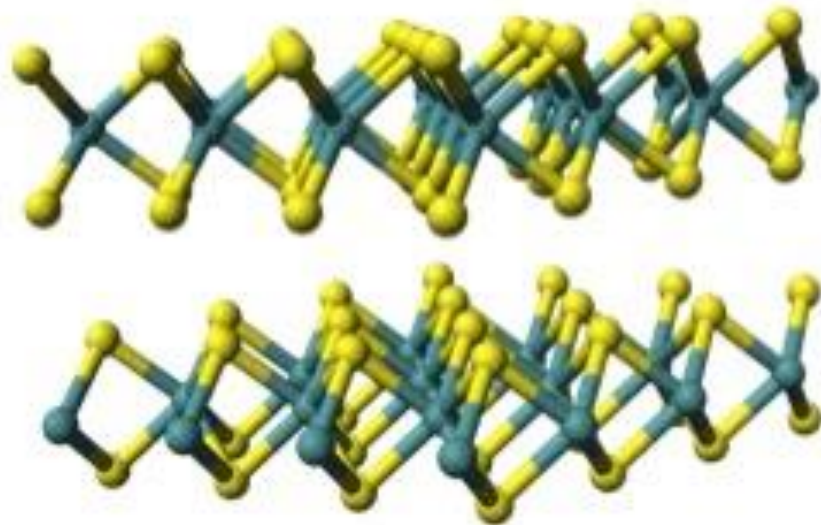
RESEARCH PLAN

Construct and probe battery-relevant systems over a range of dimensional scales, from the molecular to mesoscale (*m2m*); to provide an iterative theory and application based process to expedite understanding and optimization of functional energy delivery; to minimize heat and maximize work of energy storage devices under genuine use conditions.

EFRC mission statement

To develop, apply, and validate methods to calculate the electronic structure of materials. While these methods can be useful for the design of many new materials, we focus on the layered and two-dimensional materials that have potential for clean-energy technologies.

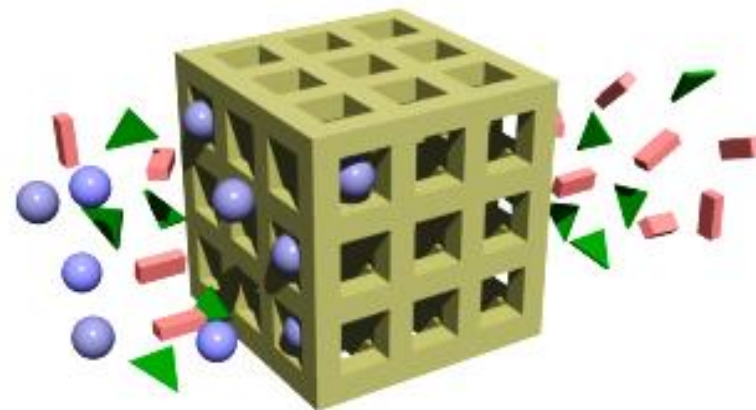
<http://efrc.cst.temple.edu>



RESEARCH PLAN

We are developing efficient and accurate density functionals including intermediate or full-range van der Waals interaction, and higher-level methods. These methods are being applied to understand how properties of layered materials are affected by composition, structure, defects, interfaces, and strain, and to the catalysis of hydrogen evolution.

The aim of the CGS is to develop new materials and membranes that enable energy-efficient separation of gas mixtures, as required in the clean use of fossil fuels and in reducing emissions from industry. Particular emphasis is placed on (i) separations that reduce CO₂ emissions from power plants and (ii) energy-intensive gas separations in industry and agriculture.



<http://www.cchem.berkeley.edu/co2efrc/>

RESEARCH PLAN

To reduce the industrial separation energy costs by employing more effective materials, new materials for the efficient separation of industrially-relevant gases will be developed. In particular, CGS is targeting novel adsorbents for CO₂ capture, the separation of O₂ from air and N₂ from methane, and for the shape-selective separation of hydrocarbons. New characterization methods and computational tools will be developed to guide and support these quests.

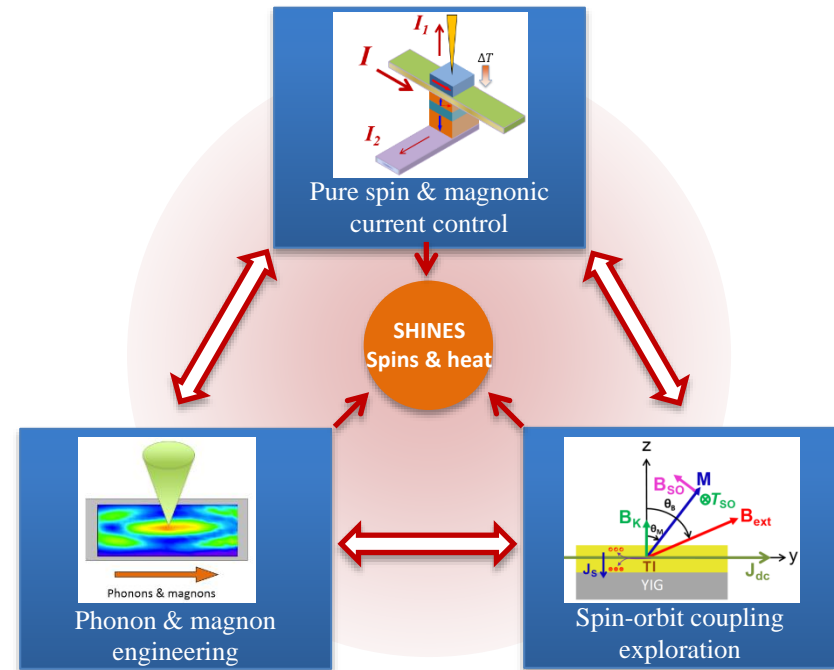
Spins and Heat in Nanoscale Electronic Systems (SHINES)

Jing Shi (University of California, Riverside)

EFRC mission:

To explore the interplay of spin, charge, and heat and to control the transport of spin and energy for achieving significantly higher energy efficiencies in nanoscale electronic devices

<http://efrcshines.ucr.edu/>



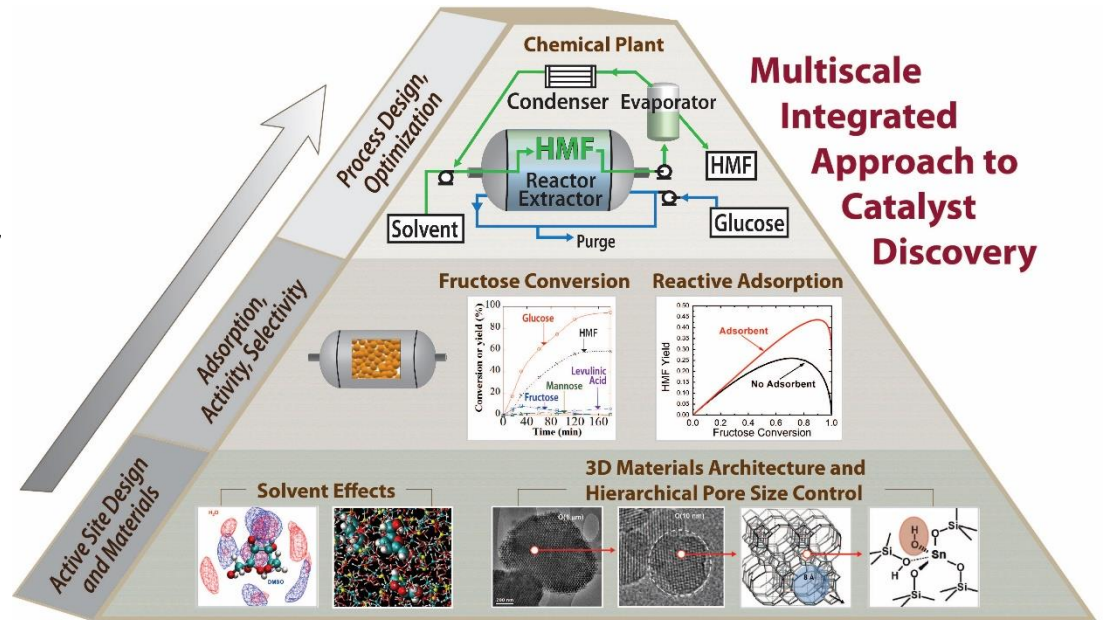
RESEARCH PLAN

Developing better understanding of and significantly improving pure spin current effects in nanoscale electronic devices; engineering acoustic phonon and magnon transport in nano-structured materials via controlling their dispersions and interactions; and exploring spin-orbit coupling for low energy effects and spin superfluidity for dissipationless spin and energy transport.

Catalysis Center for Energy Innovation (CCEI) Dionisios G. Vlachos (University of Delaware)

CCEI focuses on developing innovative, transformational heterogeneous catalytic technologies to economically convert lignocellulosic (**non-food-based**) biomass into chemicals and fuels.

www.efrc.udel.edu



**Multiscale
Integrated
Approach to
Catalyst
Discovery**

RESEARCH PLAN

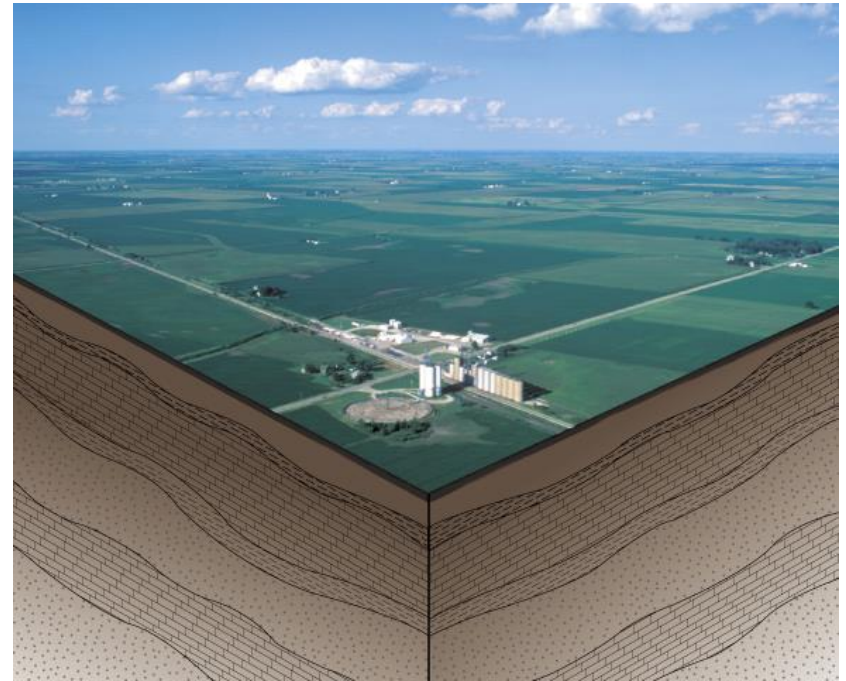
CCEI develops novel catalytic materials and processes for the operation of modern biorefineries for carbon neutral production of chemicals and fuels. It advances fundamental knowledge by developing methods that can tackle the complexity of biomass feedstock and the multiscale nature of chemical reactions.

Center for Geologic Storage of CO₂ (GSCO2)

Scott M. Frailey (University of Illinois at Urbana-Champaign)

The goal of the GSCO2 is to generate new conceptual, mathematical, and numerical models applicable to geologic storage systems in specific and strategically identified research areas, based on uncertainty and limitations observed in field pilots and CO₂ injection demonstration projects, laboratory experiments, and the experience of researchers.

<http://www.gsco2.org/>



RESEARCH PLAN

The GSCO2 will use fundamental and basic scientific principles as the basis for investigating recognized CO₂ storage challenges. Our focus is on the mechanism of injection-induced microseismicity and controlling and predicting its occurrence.

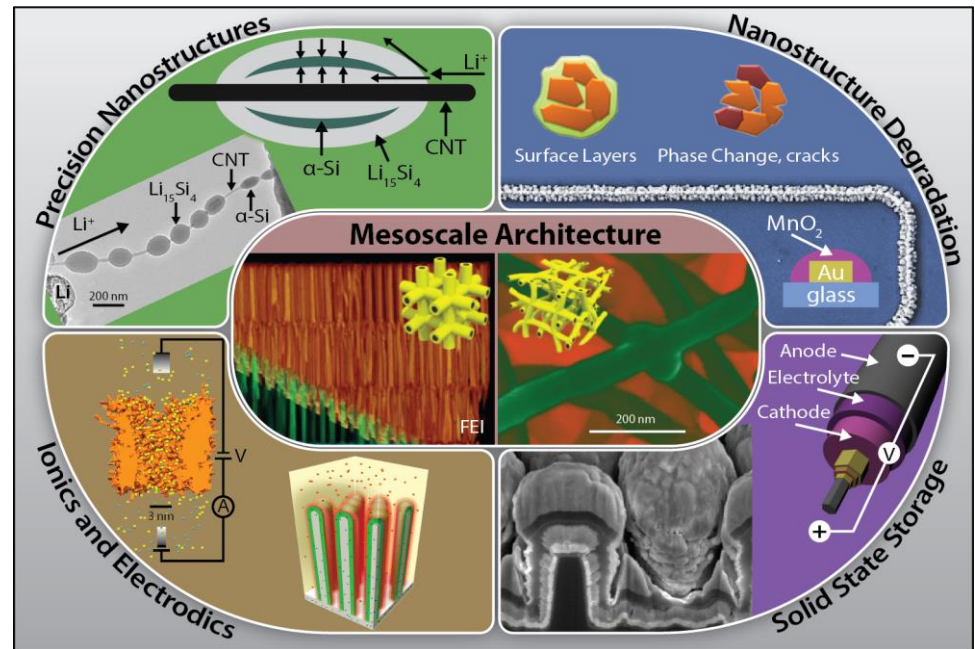
Revised 11/14/2017

Nanostructures for Electrical Energy Storage (NEES)

Gary W. Rubloff (University of Maryland)

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

www.efrc.umd.edu



RESEARCH PLAN

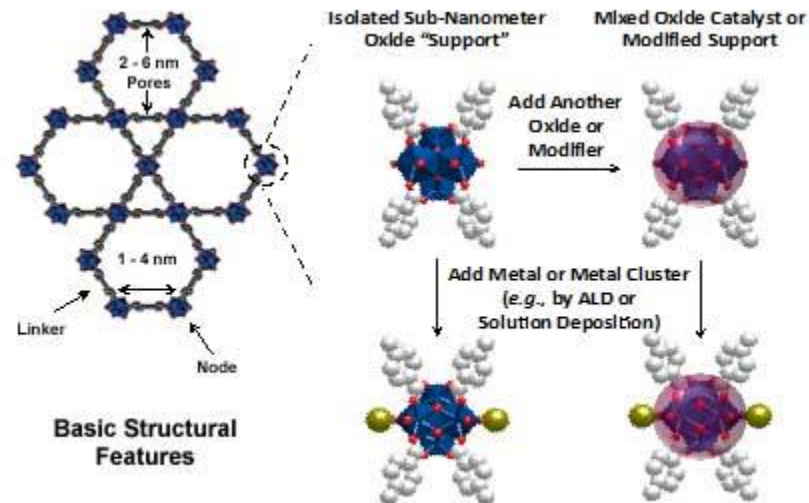
- arrange **precision nanostructures** into **mesoscale architectures** in regular & random configurations,
- investigate **mesoscale ionics & electrodelectrics consequences**,
- pursue a **science of dynamic nanostructure degradation** addressing both short & long term time scales,
- enable **solid-state nanostructured batteries** for safety, high power & energy.

Inorganometallic Catalyst Design Center (ICDC)

Laura Gagliardi (University of Minnesota)

ICDC is devoted to guiding the discovery of superior catalysts by integrating computational modeling with experiments in well-defined systems that are amenable to high-throughput search and discovery methods.

<http://www.chem.umn.edu/icdc/>



RESEARCH PLAN

ICDC designs a new class of catalysts consisting of inorganometallic clusters supported by metal-organic frameworks. ICDC computationally predicts such cluster catalysts for conversions of natural gas into methanol and oligomers, with new quantum and classical simulation techniques. The coupling between the experimental and the theoretical efforts ensures that the discovery of these novel materials and the understanding of their properties occurs through a truly iterative theoretical/experimental loop.

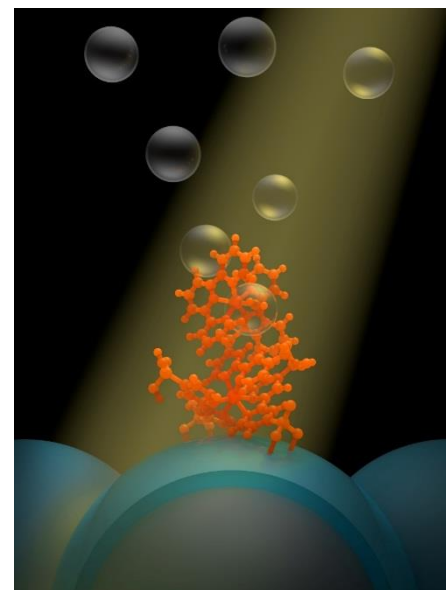
Center for Solar Fuels (UNC EFRC)

Thomas J. Meyer (University of North Carolina at Chapel Hill)

UNC EFRC MISSION:

The **Center for Solar Fuels** conducts research on the dye sensitized photoelectrosynthesis cell (DSPEC) for water splitting and tandem cells for the reduction of carbon dioxide to carbon-based solar fuels.

www.efrc.unc.edu



RESEARCH PLAN

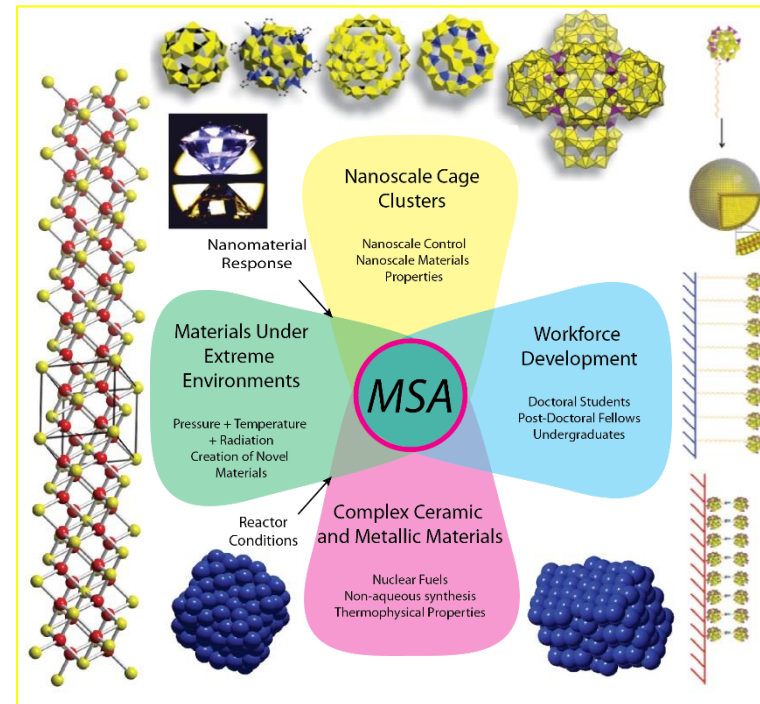
A modular approach is applied to design, test, and evaluate high efficiency DSPEC device prototypes for solar water oxidation and CO₂ reduction to formate or syngas H₂:CO mixtures. Results are being integrated from research on water oxidation, CO₂ reduction, light-harvesting chromophores and chromophore arrays, chromophore-catalyst assemblies, mesoporous nanoparticle semiconductor oxide and transparent conducting oxide films, and core/shell structures to create efficient DSPEC device prototypes.

Materials Science of Actinides (MSA)

Peter C. Burns (University of Notre Dame)

The MSA EFRC seeks to conduct transformative research in the actinide sciences with full integration of experimental and computational approaches, and an emphasis on research questions that are important to the energy future of the nation. Workforce development is a motivating goal.

<http://msa-efrc.com>



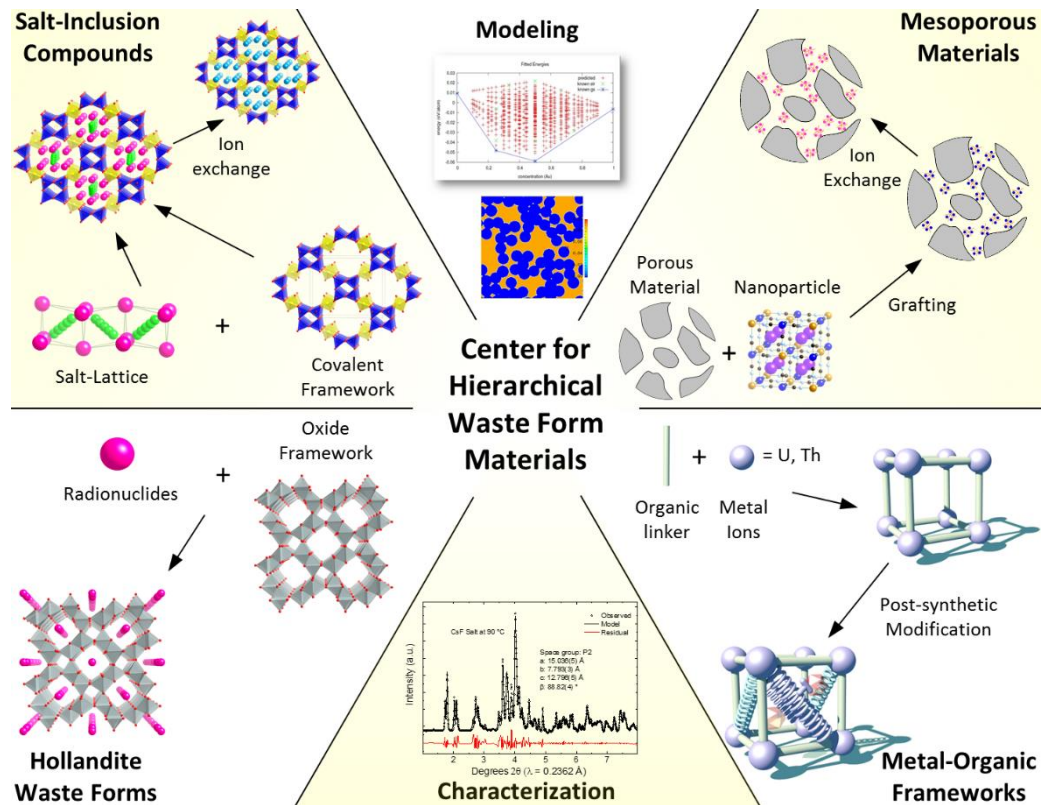
RESEARCH PLAN

This EFRC blends experimental and computational approaches to study highly complex actinide materials (such as materials for fuels, waste forms, or separations), with an emphasis on the nanoscale. The behaviors and properties of such materials in extreme environments of radiation and pressure is a major focus of this research.

Center for Hierarchical Waste Form Materials (CHWM) Hans-Conrad zur Loye (University of South Carolina)

CHWM 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>



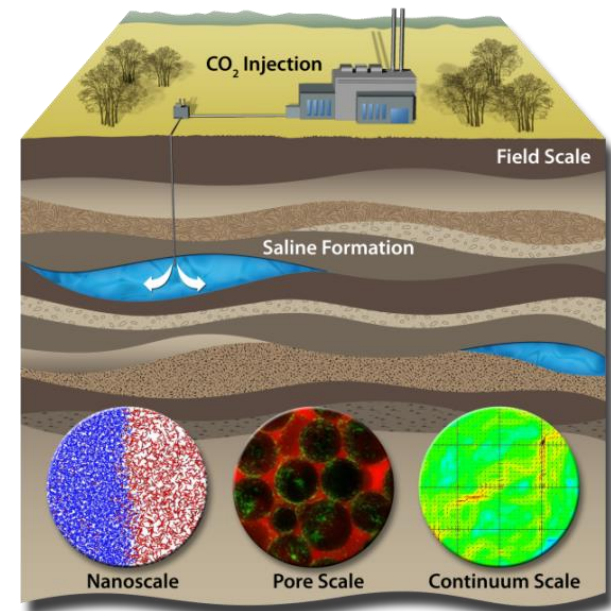
RESEARCH PLAN: Fundamental knowledge necessary to create new materials to safely sequester nuclear waste will be developed through the computationally-informed design of novel hierarchical materials, generating innovative chemical approaches and structure motifs through the use of advanced synthesis and characterization methods.

Revised 11/14/2017

Center for Frontiers of Subsurface Energy Security (CFSES) Larry W. Lake (University of Texas at Austin)

CFSES Mission: to understand and control emergent behavior arising from coupled physics and chemistry in heterogeneous geomaterials, particularly during the years to decades time scale over which injection for geologic CO₂ storage will drive natural systems far-from-equilibrium.

<http://www.utefrc.org/>

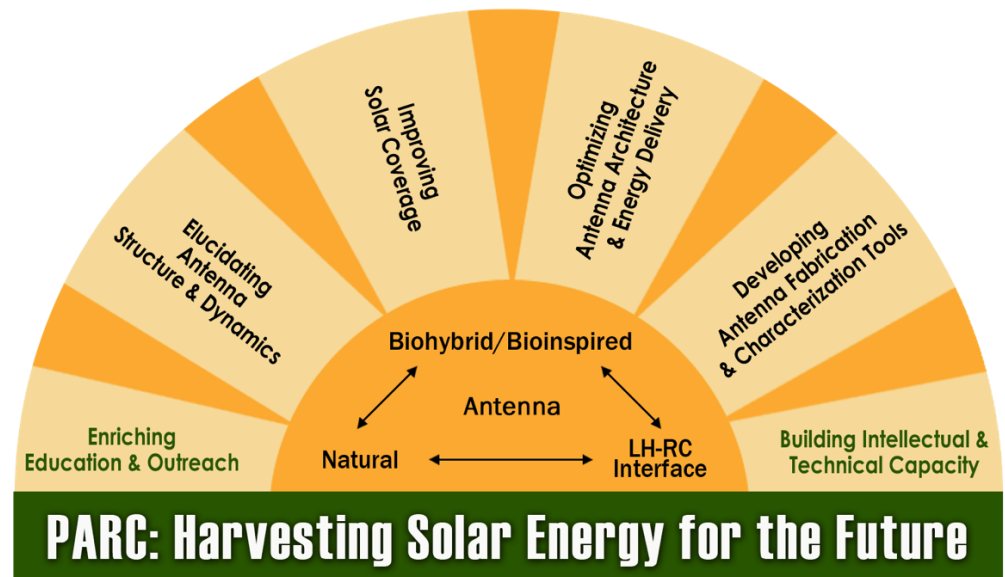


RESEARCH PLAN

CFSES will pursue scientific advances with the goal to (i) establish scientific understanding of far-from-equilibrium processes in heterogeneous geologic media, and (ii) develop novel materials and methods for controlling those processes.

Photosynthetic Antenna Research Center (PARC) Robert Blankenship (Washington Univ. in St. Louis)

The objective of PARC is to understand the basic scientific principles that underpin the efficient functioning of natural photosynthetic antenna systems as a basis for design of biohybrid and bioinspired architectures for next-generation systems for solar-energy conversion.



<http://parc.wustl.edu/>

RESEARCH PLAN

PARC will investigate:

- Natural Antennas: Structure and Efficiency
- Biohybrid and Bioinspired Antennas: Design and Characterization
- Antenna-Reaction Center Interface: Organization and Delivery

Revised 11/14/2017

GRAND CHALLENGES INDEX

- How can we master energy and information on the nanoscale to create new technologies with capabilities rivaling those of living things?.....4, 10, 11, 12, 15, 16, 22, 23, 28, 32, 36
- How do remarkable properties of matter emerge from the complex correlations of atomic or electronic constituents and how can we control these properties?.....1, 3, 5, 6, 7, 9, 10, 12, 15, 16, 17, 19, 21, 23, 25, 28, 32, 33, 35
- How do we characterize and control matter away—especially very far away—from equilibrium?.....1, 2, 3, 5, 6, 9, 10, 12, 13, 14, 15, 16, 18, 19, 21, 22, 24, 28, 29, 32, 33, 34, 35
- How do we control materials processes at the level of electrons?.....2, 3, 4, 5, 6, 10, 11, 12, 13, 14, 16, 18, 19, 20, 22, 24, 25, 27, 30, 31, 32, 33
- How do we design and perfect atom- and energy-efficient syntheses of revolutionary new forms of matter with tailored properties?.....2, 3, 4, 5, 6, 7, 8, 10, 11, 12, 13, 14, 16, 17, 18, 19, 20, 24, 25, 26, 28, 30, 31, 32, 33, 34, 36

BES REPORTS INDEX

- Advanced Nuclear Energy Systems.....6, 18, 21, 33
- Carbon Capture: Beyond 2020.....7, 9, 26, 35
- Catalysis for Energy.....5, 7, 8, 13, 15, 16, 17, 20, 23, 25, 28, 31, 32
- Clean and Efficient Combustion of 21st Century Transportation Fuels.....16, 25, 26
- Computational Materials Science and Chemistry: Accelerating Discovery and Innovation through Simulation-Based Engineering and Science.....2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 14, 15, 16, 17, 20, 21, 22, 25, 26, 28, 30, 31, 32, 33, 34, 35, 36
- Electrical Energy Storage.....1, 2, 5, 17, 24, 25, 30
- Environmental Management.....6, 19, 21, 33, 34, 35
- From Quanta to Continuum: Mesoscale Science.....2, 3, 4, 5, 8, 9, 10, 11, 12, 14, 15, 16, 17, 20, 21, 22, 23, 24, 26, 28, 29, 30, 31, 32, 33, 35, 36
- Geosciences: Facilitating 21st Century Energy Systems.....5, 9, 26, 29, 35
- Hydrogen Economy.....5, 13, 14, 16, 20, 25, 26, 28, 32
- Materials under Extreme Environments.....4, 5, 6, 12, 17, 18, 21, 25, 33
- New Science for a Secure and Sustainable Energy Future.....4, 6, 8, 10, 12, 14, 15, 16, 17, 20, 22, 23, 27, 28, 29, 32, 35
- Science for Energy Technology: Strengthening the Link between Basic Research and Industry.....4, 5, 6, 10, 12, 14, 15, 16, 17, 23, 24, 25, 26, 28, 29, 30, 31, 32, 33, 35
- Solar Energy Utilization.....4, 5, 10, 11, 12, 13, 14, 15, 16, 20, 23, 25, 32, 36
- Solid-State Lighting.....4, 11, 12, 14
- Superconductivity.....3, 5

TOPICAL INDEX

- biofuels (including algae and biomass).....13, 22, 23, 28, 36
- bio-inspired.....13, 15, 16, 20, 22, 28, 36
- carbon capture.....7, 9, 26
- carbon sequestration.....9, 22, 29, 35
- catalysis
 - heterogeneous.....5, 7, 8, 16, 17, 23, 25, 28, 30, 31, 32
 - homogeneous.....15, 16, 20, 23, 28, 32
- charge transport.....1, 2, 3, 4, 5, 10, 11, 12, 14, 15, 16, 17, 24, 30, 32
- corrosion.....19, 30, 33
- defects.....2, 4, 5, 6, 7, 10, 12, 14, 17, 18, 25, 29, 30, 32, 33
- energy storage (including batteries and capacitors).....1, 2, 5, 17, 20, 24, 25, 30
- hydrogen and fuel cells.....5, 13, 14, 16, 20, 25, 26, 28, 32
- interface
 - gas/liquid.....9, 28, 29
 - gas/solid.....5, 7, 9, 12, 19, 23, 25, 26, 28, 29, 30, 31
 - liquid/solid.....1, 2, 9, 10, 12, 14, 16, 17, 19, 20, 21, 23, 24, 25, 28, 29, 30, 31, 32, 33, 36
 - metal/oxide.....4, 7, 8, 10, 12, 14, 16, 19, 21, 24, 27, 28, 30, 31, 32, 33
 - metal/semiconductor.....4, 10, 12, 14, 16, 24, 30, 32, 36
 - organic/metal.....4, 12, 16, 23, 24, 30, 32
 - organic/organic.....4, 9, 15, 16, 22, 23, 24, 26, 36
 - organic/oxide.....2, 4, 7, 11, 12, 16, 24, 26, 30, 32, 33
 - organic/semiconductor.....4, 11, 12, 14, 15, 16, 17, 24, 30, 32
 - semiconductor/semiconductor.....4, 10, 11, 12, 14, 16, 25, 32
 - solid/solid.....1, 2, 4, 9, 10, 12, 14, 16, 23, 24, 28, 29, 30, 32, 33
- materials
 - actinide.....6, 19, 33, 34
 - biological (DNA, protein).....13, 15, 22, 23, 36
 - cellulose.....22, 23, 28, 30
 - ceramic.....2, 3, 4, 5, 6, 19, 30, 33
 - glass.....4, 5, 6, 19, 34
 - ionic liquid.....6, 12, 15, 17, 30
 - metal.....4, 6, 8, 12, 14, 16, 17, 18, 19, 24, 27, 28, 30, 31, 32, 33
 - optoelectronic and metamaterial.....4, 5, 10, 11, 12, 14, 25, 32
 - organic semiconductor.....11, 12, 14, 16, 32
 - oxide.....1, 2, 3, 4, 5, 6, 7, 8, 10, 12, 14, 16, 17, 19, 24, 25, 27, 28, 30, 31, 32, 33, 34
 - polymer.....4, 7, 11, 12, 15, 16, 22, 23, 24, 26, 30, 32, 33, 36
 - porous.....2, 4, 5, 6, 7, 8, 12, 16, 17, 26, 28, 29, 30, 31, 32, 33, 34
 - rare earth elements.....4, 6, 11, 12, 33, 34
 - semiconductor.....4, 5, 6, 10, 11, 12, 14, 15, 16, 17, 25, 30, 32
 - transparent conductor.....4, 10, 11, 12, 14, 16, 17, 32
 - wide band-gap semiconductor.....4, 5, 6, 10, 11, 12, 14, 16, 32
- materials and chemistry by design.....1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 14, 15, 16, 17, 18, 19, 20, 22, 23, 25, 26, 28, 30, 31, 32, 33, 34, 36
- mechanical behavior.....4, 9, 12, 17, 22, 25, 26, 29, 30
- membrane.....7, 16, 26, 30
- mesostructured materials.....2, 4, 5, 6, 8, 9, 10, 11, 12, 15, 16, 17, 22, 23, 24, 28, 29, 30, 32, 33, 36
- nanostructured materials
 - 0D.....4, 10, 11, 12, 15, 17, 24, 30, 32, 33, 34
 - 1D.....4, 5, 10, 11, 12, 14, 15, 16, 17, 24, 30, 32, 33
 - 2D.....1, 2, 4, 7, 10, 11, 12, 14, 15, 16, 17, 24, 25, 27, 30, 32, 33
 - 3D.....2, 4, 7, 8, 10, 11, 12, 14, 15, 16, 17, 22, 23, 24, 26, 28, 30, 31, 32, 33, 36
 - nanocomposites.....2, 4, 5, 10, 12, 16, 22, 23, 24, 27, 30, 32, 33
- nuclear (including radiation effects).....6, 18, 19, 21, 33, 34
- optics.....4, 10, 11, 12, 14, 16
- phonons.....4, 5, 12, 14, 16, 18, 27
- photosynthesis (natural and artificial).....11, 16, 20, 32, 36
- separations.....6, 7, 17, 21, 23, 26, 28, 33

solar
 fuels.....5, 13, 14, 16, 20, 32, 36
 photovoltaic.....4, 5, 10, 11, 12, 14, 15, 16, 25, 32
 thermal.....4, 12, 14
solid state lighting.....4, 11, 12, 14
spin dynamics.....3, 11, 12, 16, 18, 27
spintronics.....11, 12, 27
superconductivity.....3, 5
synthesis

atomic layer deposition.....3, 10, 14, 16, 30, 32
novel materials.....1, 2, 3, 4, 5, 6, 7, 8, 10, 12, 14, 15, 16, 17, 18, 20,
 22, 23, 25, 26, 28, 30, 31, 32, 33, 34, 36
scalable processing.....4, 6, 7, 10, 12, 16, 26, 28, 30, 33
self-assembly.....4, 6, 7, 10, 15, 16, 17, 22, 26, 28, 30, 32, 33, 34,
 36
thermal conductivity.....4, 5, 12, 18, 27
thermoelectric.....5, 12, 14, 27

EXPERIMENTAL AND THEORETICAL METHODS INDEX

- classical mechanics.....9, 10, 12, 13, 15, 16, 17, 20, 22, 26, 29, 31, 33
continuum modeling.....2, 4, 9, 15, 16, 17, 20, 22, 24, 28, 29, 30, 31,
35, 36
density functional theory (DFT).....1, 2, 3, 5, 6, 7, 8, 10, 11, 12, 13, 14,
15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32,
33, 34, 36
electron microscopy.....1, 2, 3, 4, 5, 7, 8, 9, 10, 12, 14, 15, 17, 18, 19,
22, 23, 24, 28, 29, 30, 31, 33, 36
extreme scale computing.....9, 29
finite element method.....4, 10, 16, 22, 29, 30, 32, 35
high-throughput screening methods.....2, 11, 14, 16, 25, 26, 28, 30,
31
laser diagnostics.....10, 12, 14, 16, 33
lithography.....4, 10, 11, 12, 15, 16, 30, 36
mesoscale modeling.....2, 3, 4, 8, 9, 10, 11, 12, 15, 16, 17, 22, 23, 24,
26, 28, 29, 30, 31, 34, 36
molecular dynamics (MD).....2, 5, 6, 7, 8, 10, 11, 12, 14, 15, 16, 17,
18, 19, 20, 21, 22, 23, 25, 26, 28, 29, 30, 31, 32, 33, 34, 36
monte carlo (MC).....2, 3, 4, 5, 6, 7, 10, 11, 12, 15, 16, 18, 19, 21, 22,
26, 27, 28, 29, 30, 31, 33, 34, 36
multiscale modeling.....2, 3, 4, 7, 8, 9, 10, 12, 14, 15, 16, 17, 18, 19,
21, 22, 23, 24, 25, 26, 28, 29, 30, 31, 34, 36
near-field scanning optical microscopy.....2, 4, 12, 14, 16, 22, 36
neutron diffraction and scattering.....2, 5, 6, 7, 9, 12, 17, 18, 21, 22,
26, 30, 33, 34, 36
neutron spectroscopy.....2, 5, 7, 12, 17, 21, 36
next generation optimization methods.....4, 5, 6, 10, 14, 31
quantum mechanics.....3, 4, 5, 6, 7, 8, 10, 11, 12, 13, 14, 15, 16, 17,
18, 19, 20, 22, 23, 25, 26, 27, 28, 31, 32, 33, 36
scanning probe microscopy.....2, 3, 4, 5, 7, 8, 10, 12, 14, 15, 16, 17,
19, 21, 22, 23, 24, 25, 28, 30, 31, 33, 36
surface science.....1, 7, 8, 10, 12, 14, 15, 16, 17, 19, 21, 22, 24, 25, 28,
29, 30, 31, 32, 33, 35, 36
ultrafast physics.....3, 10, 16, 18, 25, 32, 36
X-ray diffraction and scattering.....1, 2, 3, 5, 6, 7, 9, 10, 12, 13, 14, 15,
16, 17, 18, 20, 22, 23, 24, 26, 28, 29, 30, 31, 33, 34, 36
X-ray imaging.....1, 2, 5, 6, 16, 23, 24, 29, 30, 33
X-ray spectroscopy.....2, 5, 6, 8, 9, 12, 14, 16, 18, 22, 23, 24, 26, 28,
30, 31, 33, 34