U.S. Department of Energy

Energy Frontier Research Centers

One Page Overviews

Office of Science
8/1/2014
Revised on 08/31/2015

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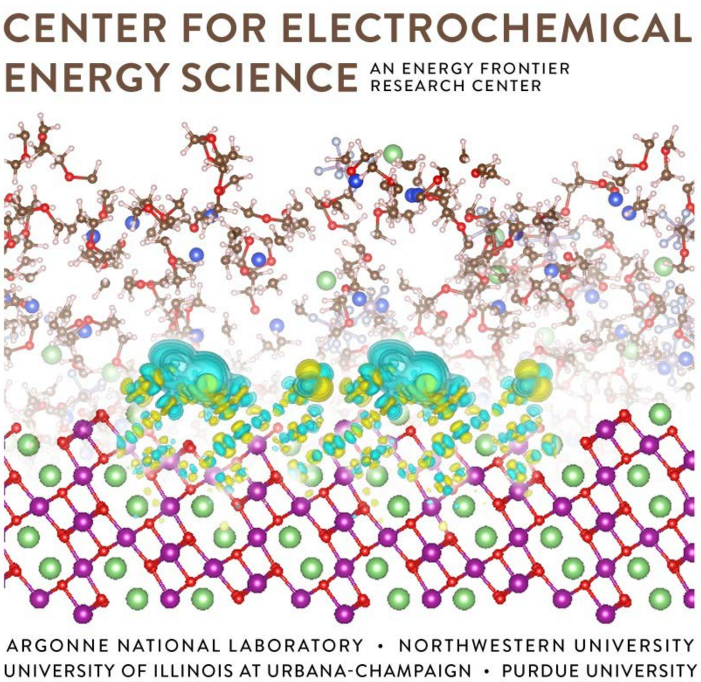
Ordered by Institution and then by Director

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

The Center's mission is 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.

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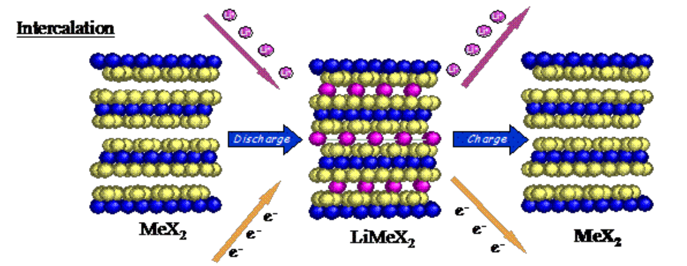
Argonne NATIONAL LABORATORY
ILLINOIS UNIVERSITY OF ILLINOIS AT URBANA-CHAMPAIGN
NORTHWESTERN UNIVERSITY
PURDUE UNIVERSITY

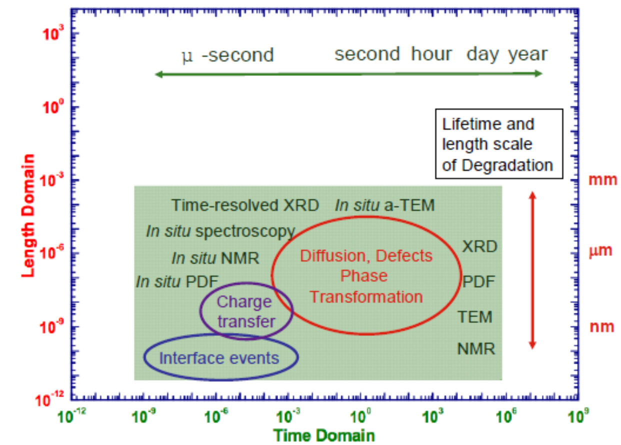
Northeast Center for Chemical Energy Storage (NECCES)
M. Stanley Whittingham (Binghamton University)

EFRC mission statement:

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 make use of, and develop new methodologies to determine how model compound electrodes function in real time, as batteries are cycled.

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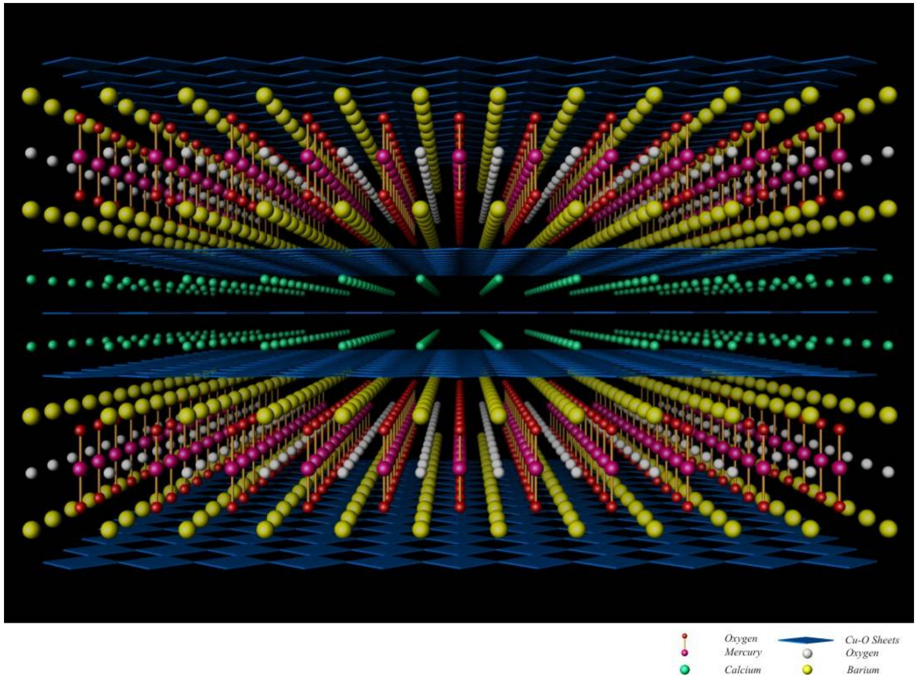
Center for Emergent Superconductivity (CES)
Peter D. Johnson (Brookhaven National Laboratory)

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

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



CES 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.

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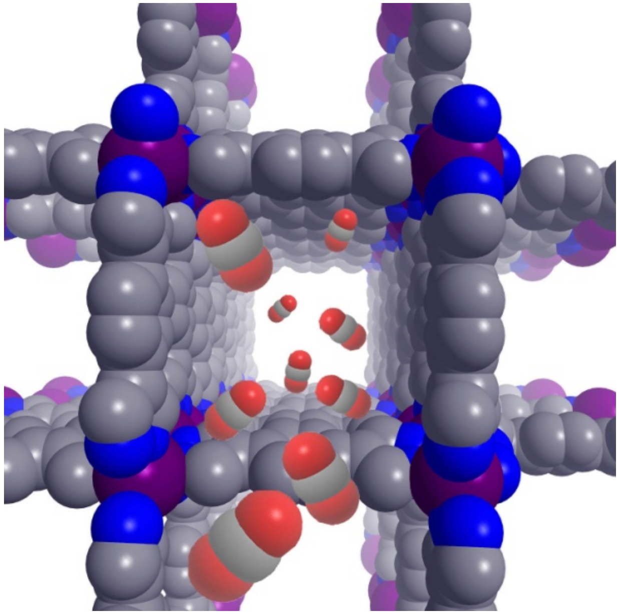
Center for Gas Separations Relevant to Clean Energy Technologies (CGS)
Jeffrey R. Long (University of California, Berkeley)

The aim of the CGS EFRC is to develop new synthesis strategies, combined with novel characterization and computational methods, for tailor-making materials for the efficient separation of gas mixtures, based on a fundamental understanding of the properties and performance of these materials.

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



RESEARCH PLAN

Gas separation requires the molecular control offered by nanoscience and chemical synthesis to tailor-make materials exhibiting exactly the right adsorption and diffusion properties to enable an economic, energy-efficient separation process. New characterization methods and computational tools will be developed to guide and support this quest.

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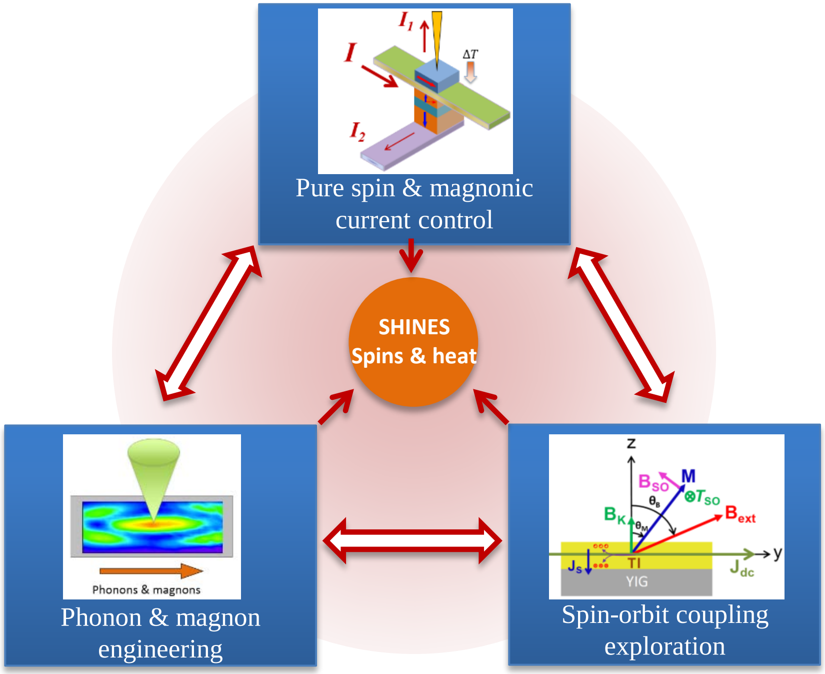
Spins and Heat in Nanoscale Electronic Systems (SHINES)
Jing Shi (University of California, Riverside)

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 superconducting condensate for dissipationless spin and energy transport

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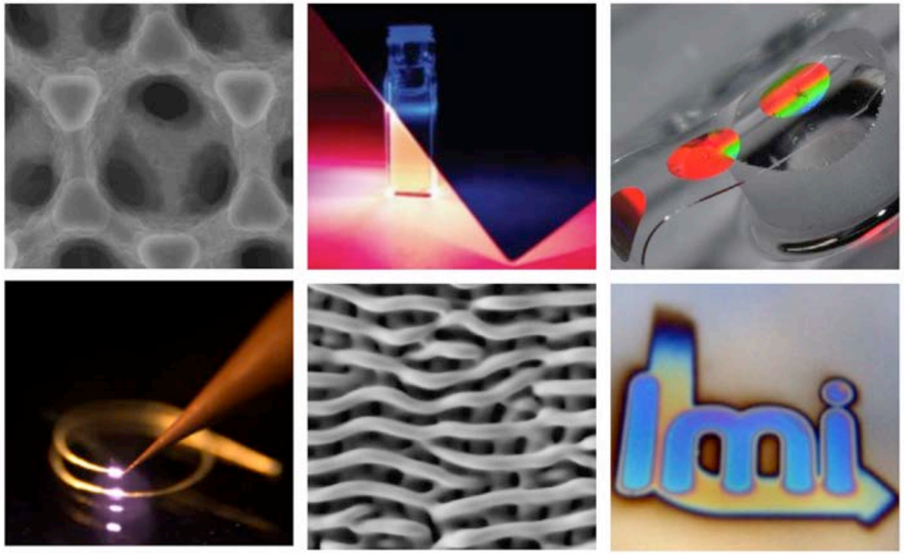
U.S. DEPARTMENT OF ENERGY | Office of Science | UC RIVERSIDE | University of California Irvine | UCLA | Johns Hopkins University | The University of Texas at Austin | Colorado State University | ASU

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, high quality optoelectronic and thermal materials, and new electromagnetic design ideas including plasmonics and photonic crystals. ***Outcome:*** **Photonic principles that enable record photovoltaic conversion efficiency and utilization of the entire visible and infrared solar resource.**

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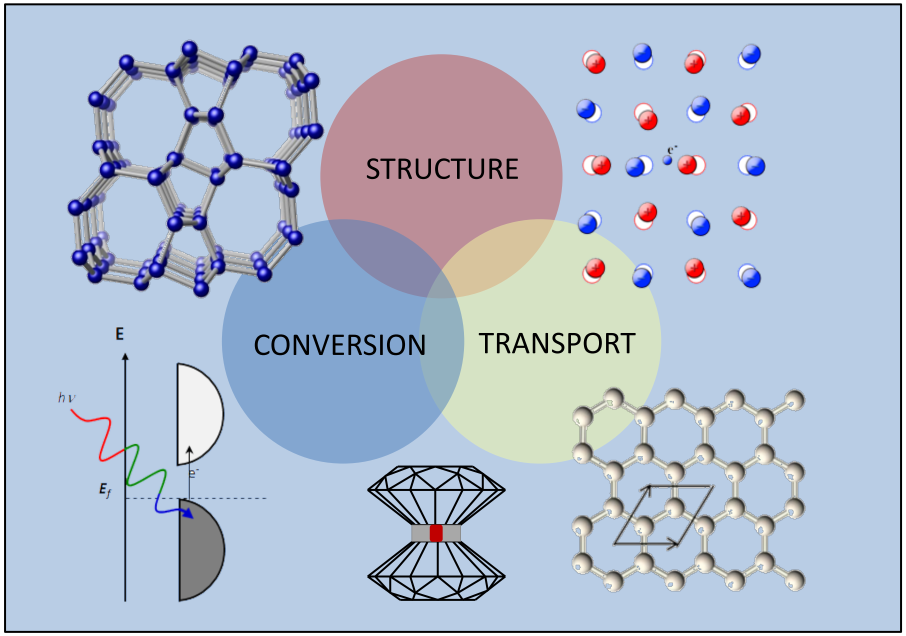
Energy Frontier Research in Extreme Environments (EFree)
Russell J. Hemley (Carnegie Institution of Washington)

EFRC Mission Statement:

To accelerate the discovery and synthesis of kinetically stabilized, energy materials utilizing extreme conditions.

https://efree.carnegiescience.edu/

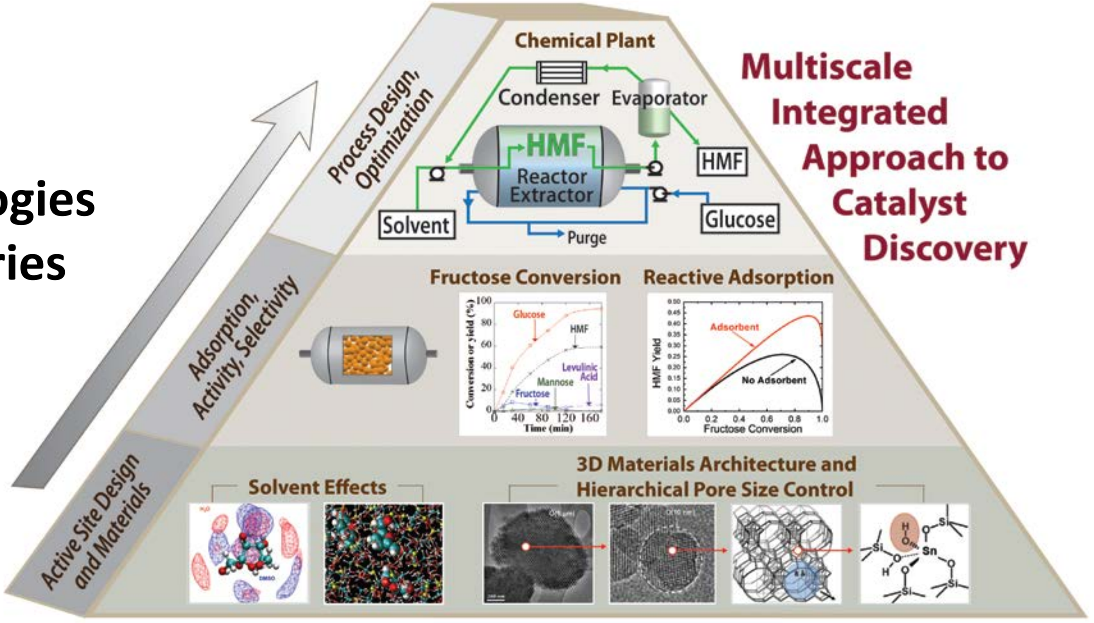


RESEARCH PLAN

By use of advanced extreme conditions techniques, EFree discovers, creates, and characterizes paradigm-shifting, transformative energy materials, including the synthesis and recovery of novel structural, energy conversion, and energy transport materials.

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

CCEI focuses on developing innovative, transformational heterogeneous catalytic technologies for utilization in future biorefineries to convert lignocellulosic (non-food-based) biomass into economically viable chemicals and fuels.



www.efrc.udel.edu

RESEARCH PLAN

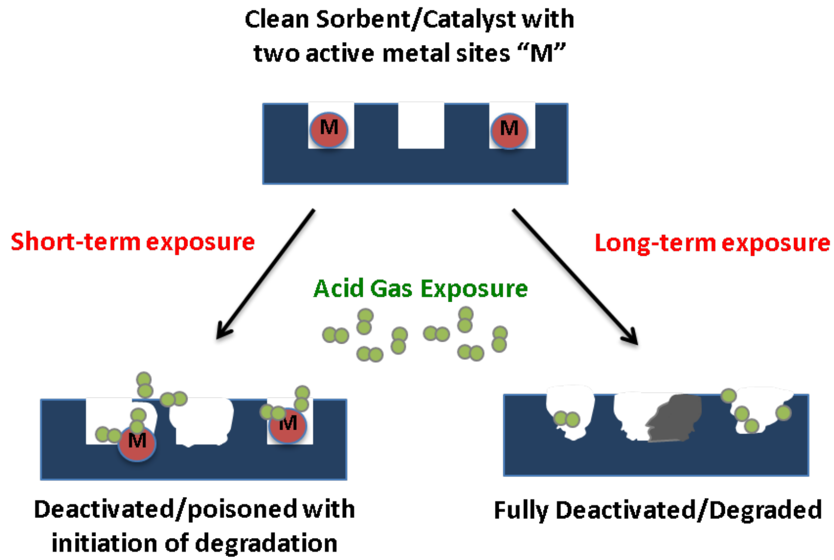
Biomass feedstocks vary considerably by source, and their transformation entails complex, multiscale reactions and processes. Based on a fundamental understanding of the underlying chemistry, CCEI develops novel catalytic materials and processes to set the foundations for the operation of modern biorefineries for carbon neutral production of chemicals and fuels.

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. A variety of in-situ experimental tools coupled with complimentary modeling techniques will improve the performance of materials in these environments and advance materials discovery.

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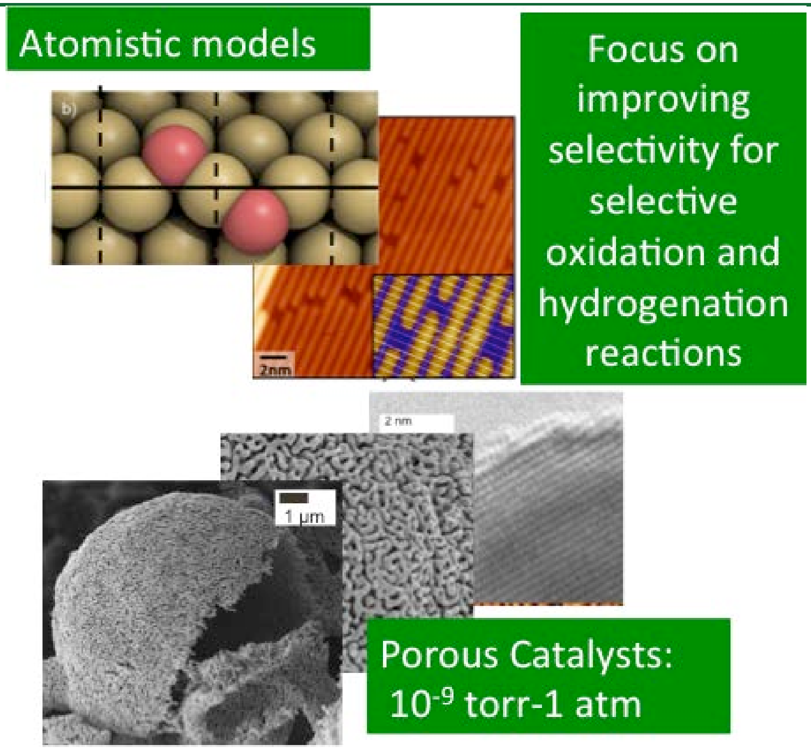
Integrated Mesoscale Architectures for Sustainable Catalysis (IMASC)

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

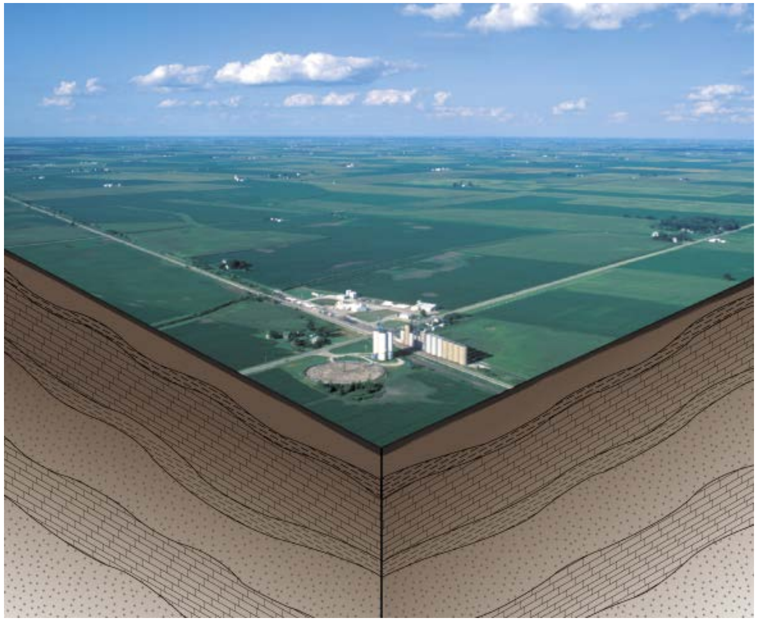


RESEARCH PLAN

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.

Center for Geologic Storage of CO_2 (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 reservoir geologic storage systems in specific and strategically identified research areas, based on uncertainty and limitations observed in field pilots and demonstration CO_2 injection projects, laboratory experiments, and previous experience of researchers in industry-sponsored applied research.



http://www.gsco2.org/

RESEARCH PLAN

GSCO2 will use fundamental and basic scientific principles as the basis for investigating existing CO_2 storage technology gaps in two areas: (1) predicting and controlling the distribution of CO_2 within the storage reservoir and (2) the occurrence of microseismicity during CO_2 storage.

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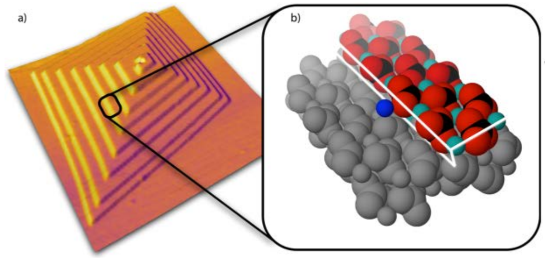
Center for Nanoscale Controls on Geologic CO_2 (NCGC)
Donald J. DePaolo (LBNL)

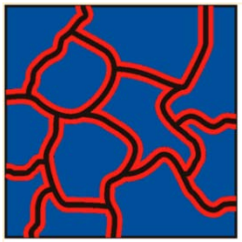
NCGC Mission Statement

Enhance the performance and predictability of subsurface storage systems by understanding the molecular and nanoscale origins of CO_2 trapping processes, and developing computational tools to translate to larger-scale systems

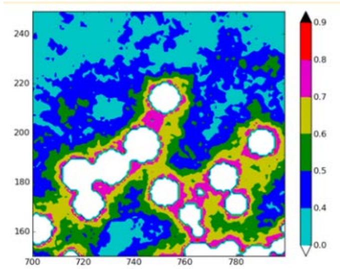
esd1.lbl.gov/research/facilities/ncgc/



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 CO_2 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 CO_2 trapping efficiency and long-term reliability.

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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.centerforadvancedsolarphotophysics.org

RESEARCH PLAN

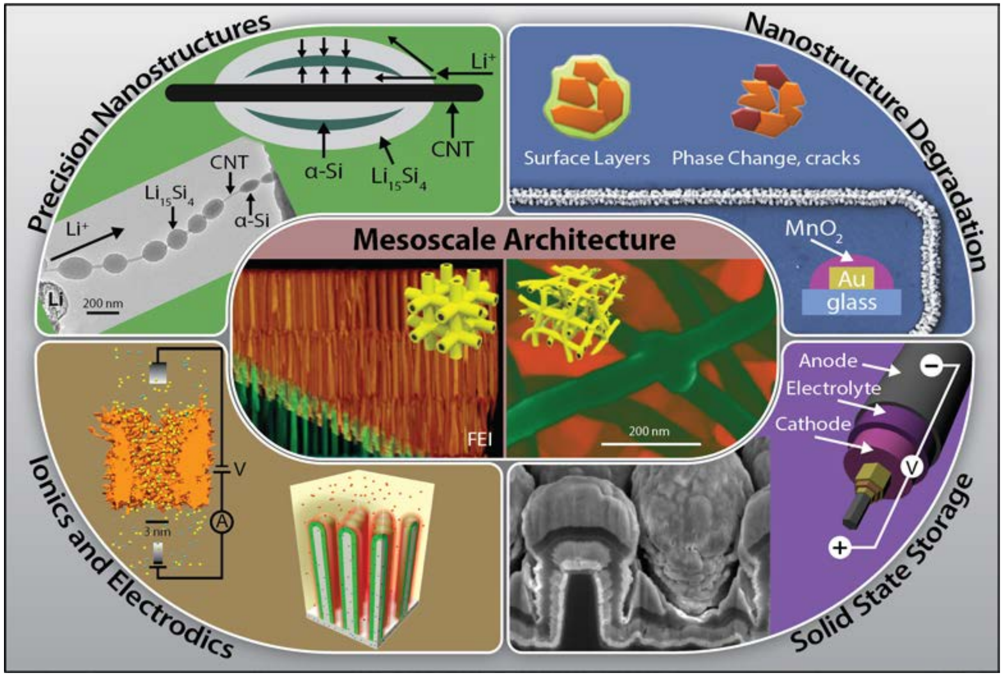
Our focus is on fundamental physics and chemistry of solution-processible semiconductor nanocrystals specifically designed to exhibit novel phenomena that will enhance the conversion of sunlight into electricity. The desired outcomes of this work are effective, low-cost schemes for light harvesting and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

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

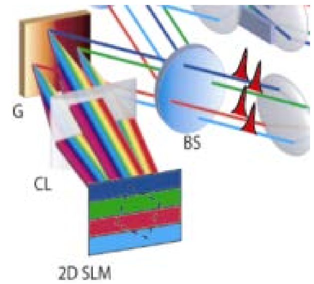
The NEES EFRC …

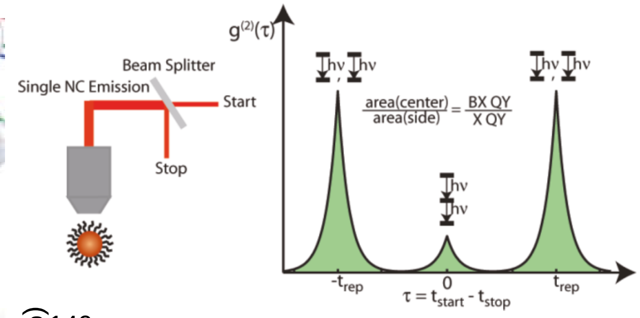


- arranges ***precision nanostructures*** into ***mesoscale architectures*** in regular & random configurations,
- investigates ***mesoscale ionics & electrodics consequences***,
- pursues a ***science of dynamic nanostructure degradation*** addressing both short & long term time scales,
- enables ***solid-state nanostructured batteries*** for safety, high power & energy.

U.S. DEPARTMENT OF ENERGY | Office of Science | NEES NANOSTRUCTURES for ELECTRICAL ENERGY STORAGE | University of Maryland | Sandia National Laboratories | UCI | Yale | UF University of Florida | The University of Utah | Michigan State University | UCLA

Center for Excitonics (CE)
Marc Baldo (MIT)

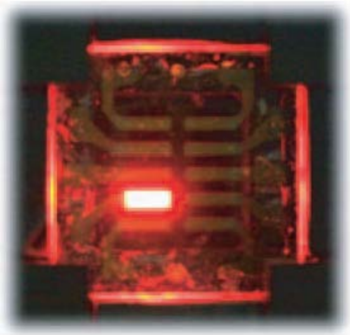


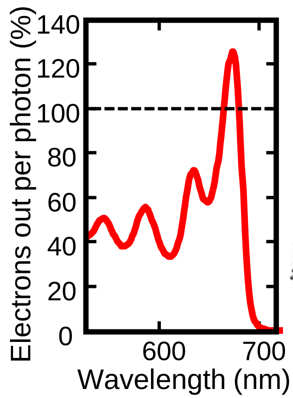


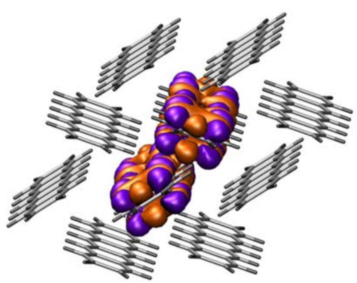
<u>Electronics vs Excitonics</u>

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.

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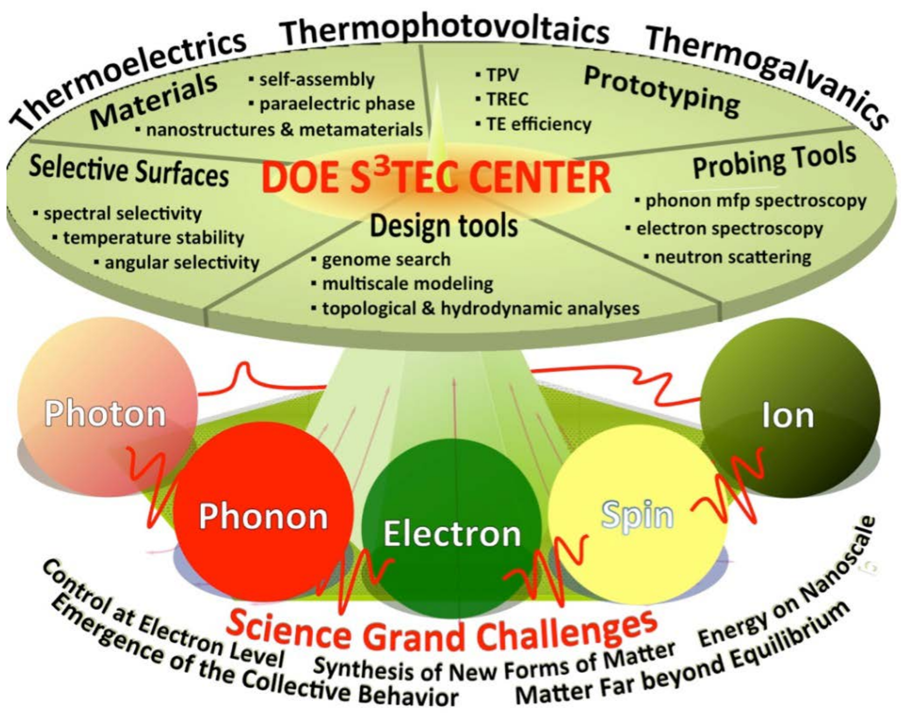
BROOKHAVEN NATIONAL LABORATORY

center for excitonics

Solid-State Solar-Thermal Energy Conversion Center (S^3TEC)
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 will combine 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.

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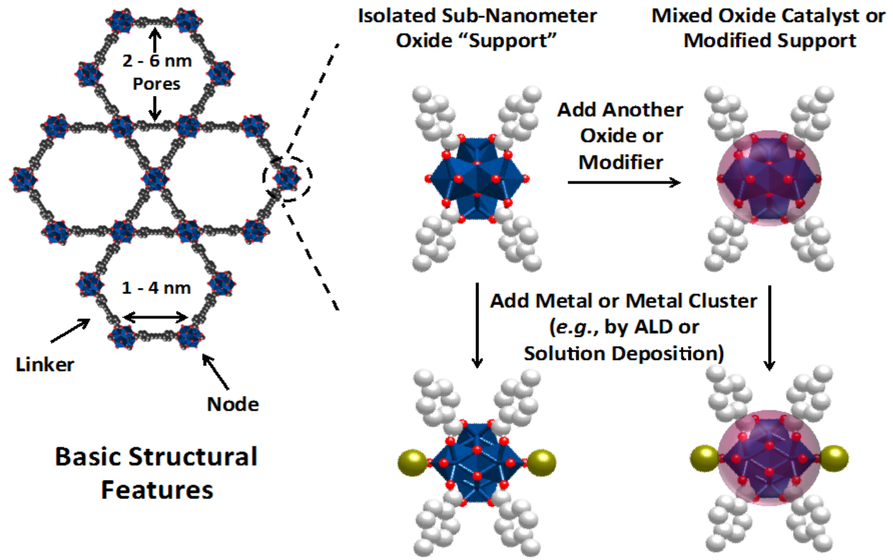
Inorganometallic Catalyst Design Center (ICDC)
Laura Gagliardi (University of Minnesota)

ICDC is devoted to *computationally guided discovery of a new class of energy-science-relevant catalytic materials and the underlying structure-function relationships that will guide further catalyst discovery*.



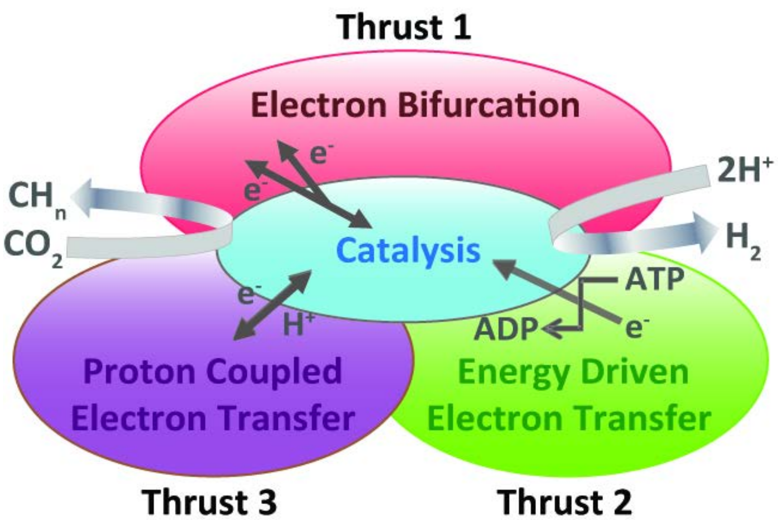
http://www.chem.umn.edu/icdc/

RESEARCH PLAN

ICDC will design a new class of catalysts consisting of inorganometallic clusters supported in uniform arrays by organic linkers based on metal-organic frameworks or surface-supported porphyrins. ICDC will computationally predict such cluster catalysts for conversions of natural gas into methanol and oligomers, with new quantum and classical simulation techniques.

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

EFRC mission: To investigate the mechanisms and structural basis controlling **electron bifurcation, electron-ion coupling, and redox catalysis** in model enzymes; this detailed understanding of how biological systems control and exploit electron flow will be used to develop modular biochemical conversions for the production of hydrocarbon and hydrogen biofuels.



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

RESEARCH PLAN

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

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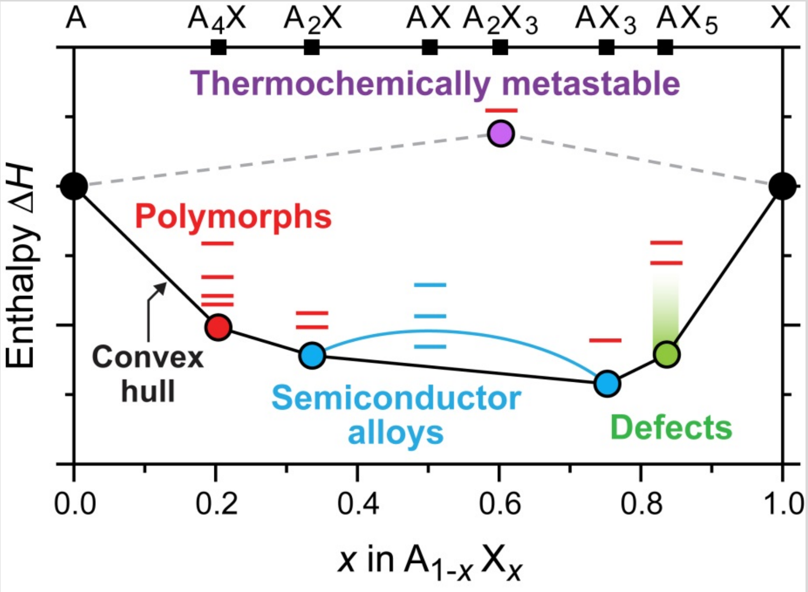
U.S. DEPARTMENT OF ENERGY | Office of Science | BETCy | NREL

Center for Next Generation of Materials by 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 searching, 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.

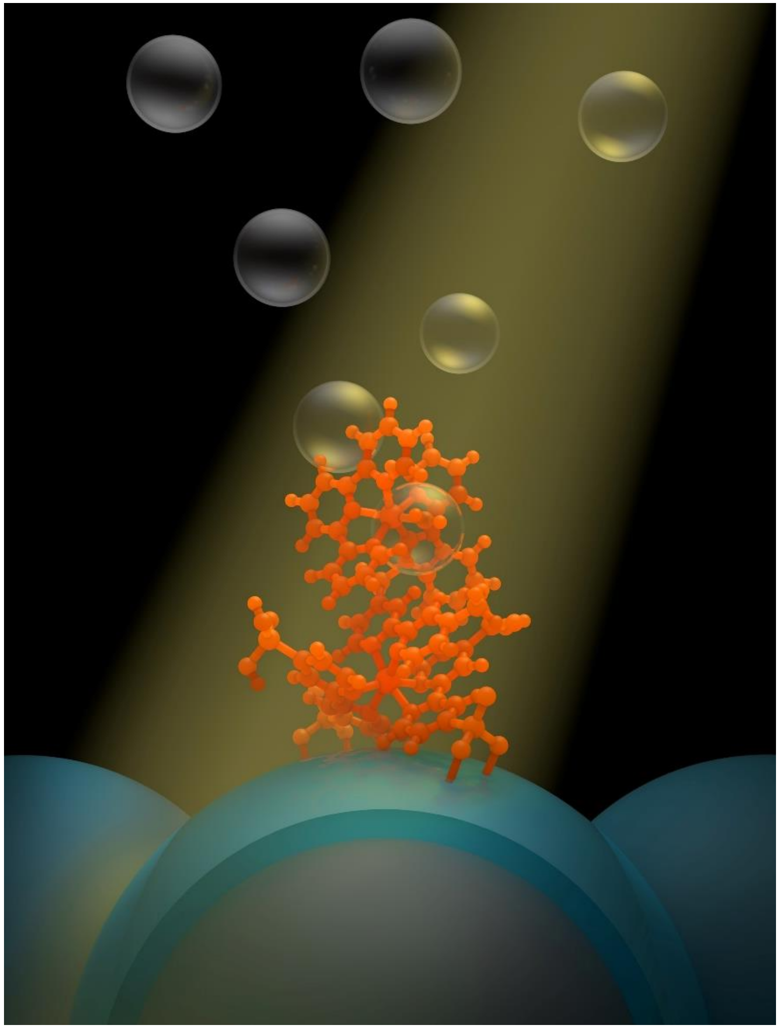
RESEARCH PLAN

- **Integrate high-throughput theory, experiment, and data mining to develop a rapid search and design methodology for *discovery of new functional materials*.**
- **Develop new tools to accelerate materials discovery incorporating *metastable semiconductors*: *polymorphs*; *defects, disorder* and *interfaces*; and *alloys*.**
- **Predict *synthesis pathways* by coupling theory and *in-situ* characterization.**

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 dye sensitized photoelectrosynthesis cells (DSPECs) for water splitting and tandem cells for the reduction of carbon dioxide to carbon-based solar fuels.**



RESEARCH PLAN

A modular approach is applied to design, test, and evaluate high efficiency DSPEC device prototypes for solar water splitting and CO_2 reduction to formate or syngas H_2:CO mixtures.

Results are being integrated from research on water oxidation, CO_2 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.

WWW.EFRC.UNC.EDU

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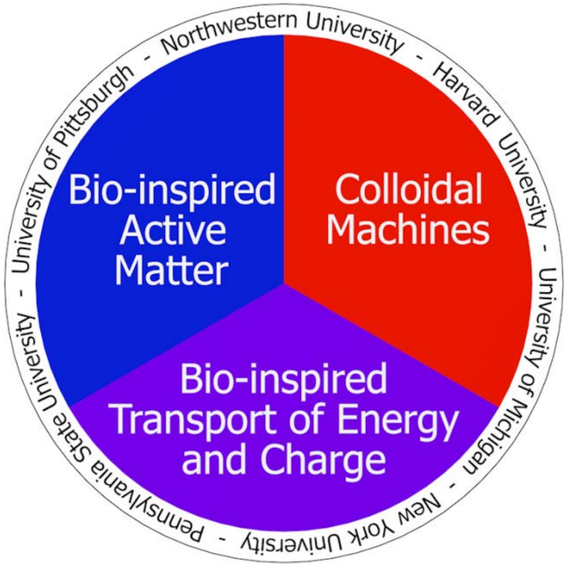
Center for Bio-inspired Energy Science (CBES)
Samuel Stupp (Northwestern University)

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).

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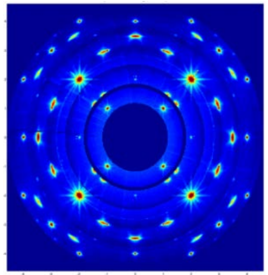
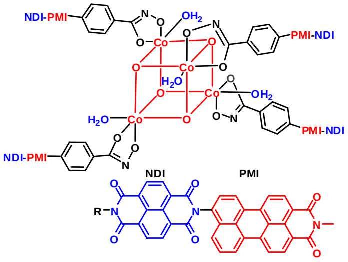
Argonne-Northwestern Solar Energy Research (ANSER) Center
Michael R. Wasielewski (Northwestern University)

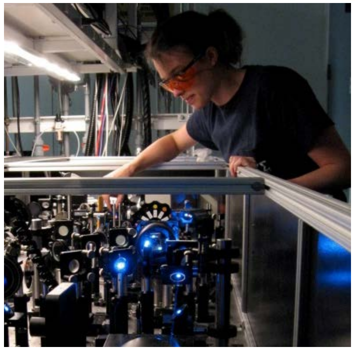
The mission of the ANSER Center is to revolutionize our understanding of molecules, materials, and methods necessary to create dramatically more efficient technologies for solar fuels and electricity production.

http://www.AnserCenter.org

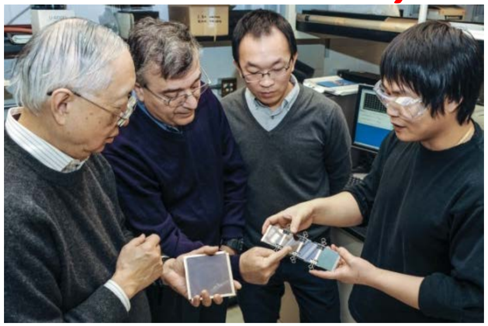
Solar Fuels

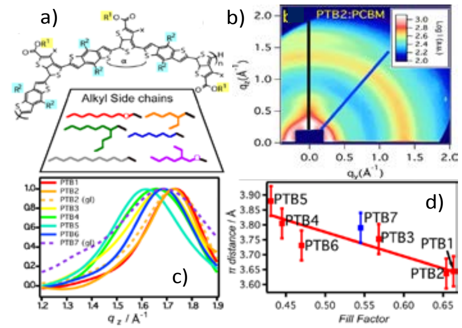






Solar Electricity





RESEARCH PLAN

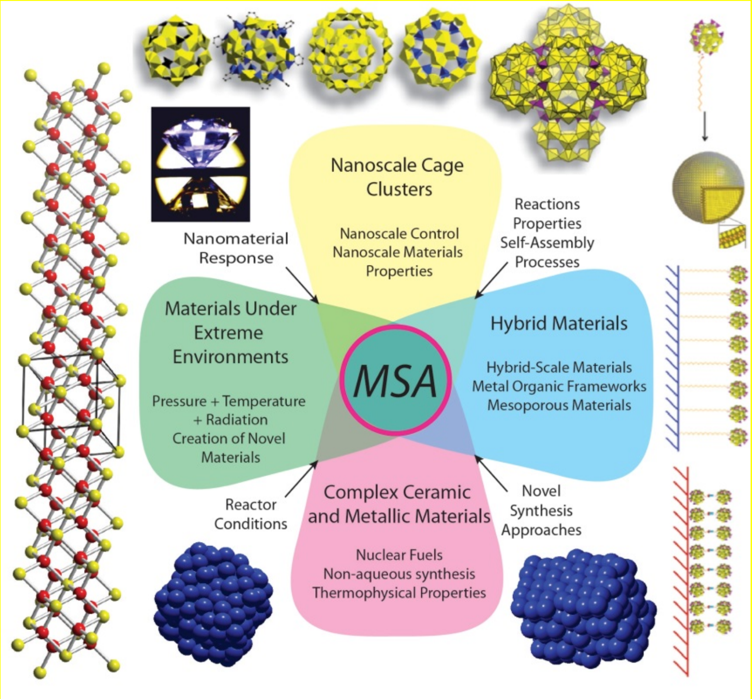
Develop a fundamental understanding of how to:

- **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.**

Materials Science of Actinides (MSA)
Peter C. Burns (University of Notre Dame)

The MSA EFRC seeks to understand and control, at the nanoscale, materials that contain actinides (radioactive heavy elements such as uranium and plutonium) to lay the scientific foundation for advanced nuclear energy systems.

http://msa-efrc.com



RESEARCH PLAN

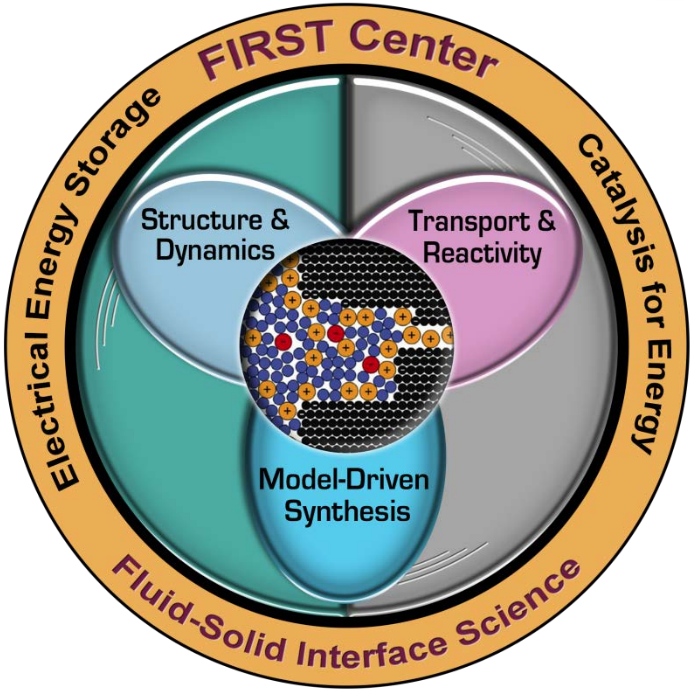
This EFRC blends experimental and computational approaches to study highly complex actinide materials (such as materials for fuels, waste forms, or separations), with an emphasis on the nanoscale. The behaviors and properties of such materials in extreme environments of radiation and pressure is a major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

Fluid Interface Reactions, Structures and Transport (FIRST)
David J. Wesolowski (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 will integrate 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.

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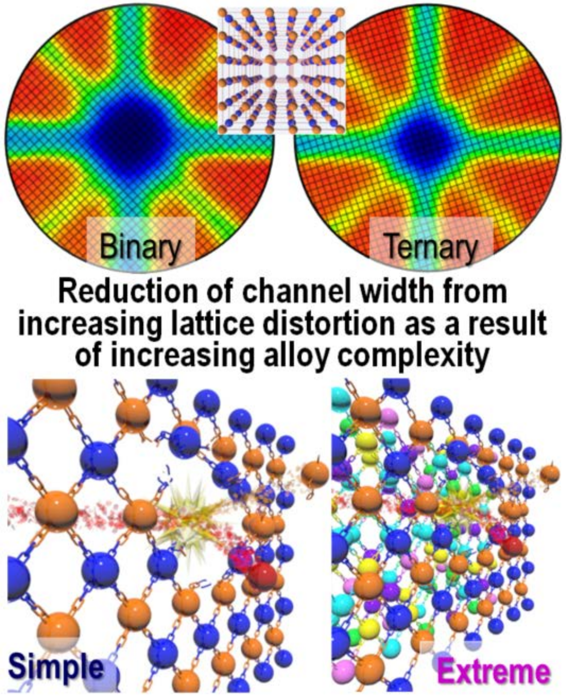
Energy Dissipation to Defect Evolution (EDDE)
Yanwen Zhang (Oak Ridge National Laboratory)

EFRC Mission: To develop a fundamental understanding of energy dissipation mechanisms through electrons, phonons and magnons, and ultimately control defect evolution in a radiation environment; and to yield new design principles for radiation–tolerant structural alloys for nuclear energy applications.

http://edde.ornl.gov/



RESEARCH PLAN

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

Approach: Understand the mechanisms of energy dissipation and how they are influenced by alloy complexity.

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

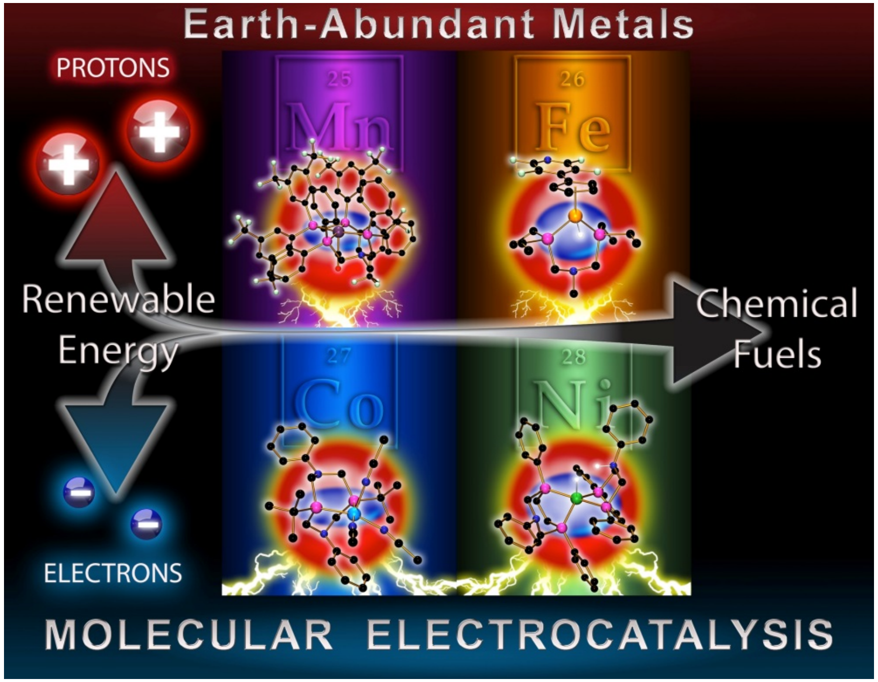
Revised 08/31/2015

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

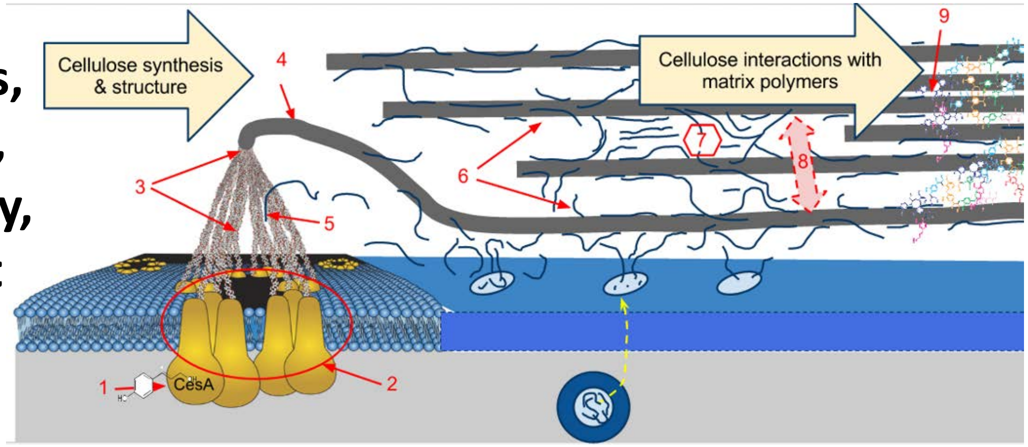


RESEARCH PLAN

Catalysts enable the conversion of electricity obtained from carbon-neutral, sustainable energy sources (such as solar and wind) into chemical bonds in fuels, such as the H-H bond of hydrogen. CME's research addresses how proton relays regulate the movement of protons and electrons to enhance the rate and efficiency of electrocatalysts.

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.



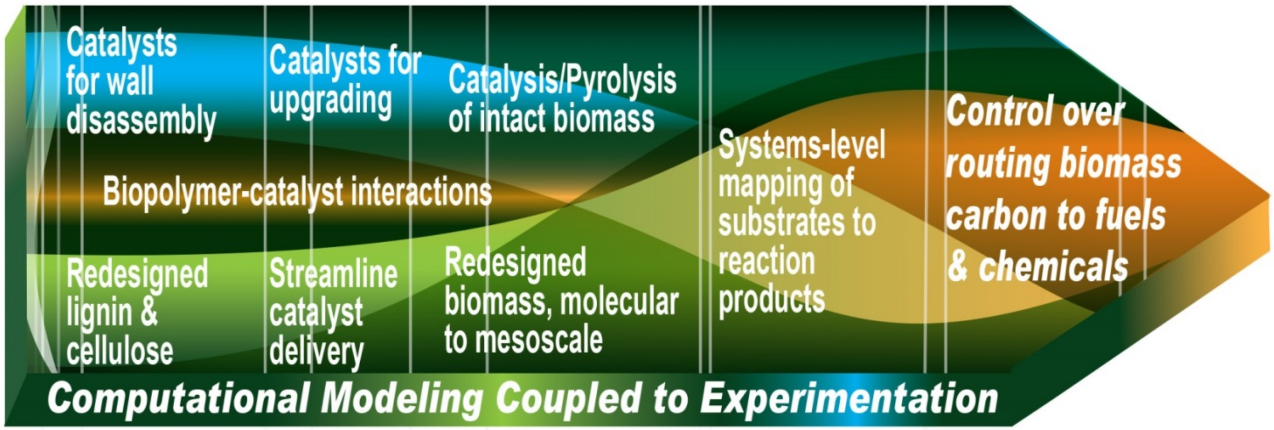
www.lignocellulose.org

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.

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://C3bio.org

RESEARCH PLAN

C3Bio will develop 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 will modify cell wall composition and catalytically transform intact biomass to specify both the structures within, and the reaction products from, lignocellulosic biomass.

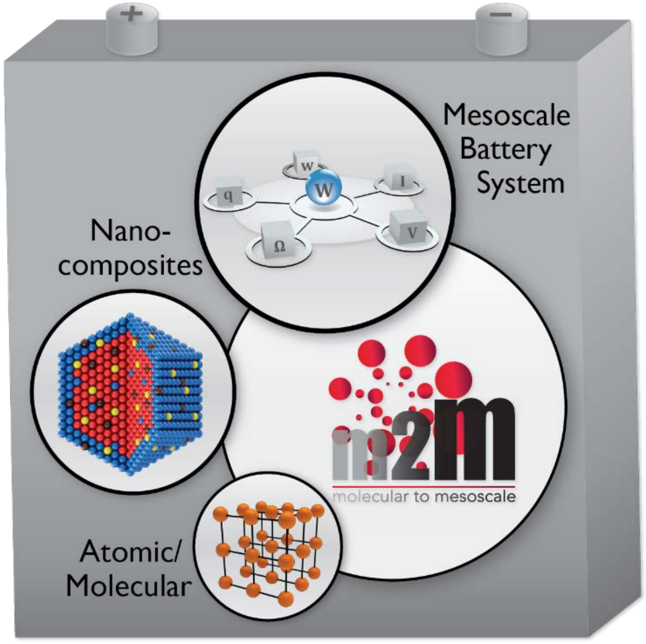
Revised 08/31/2015

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.

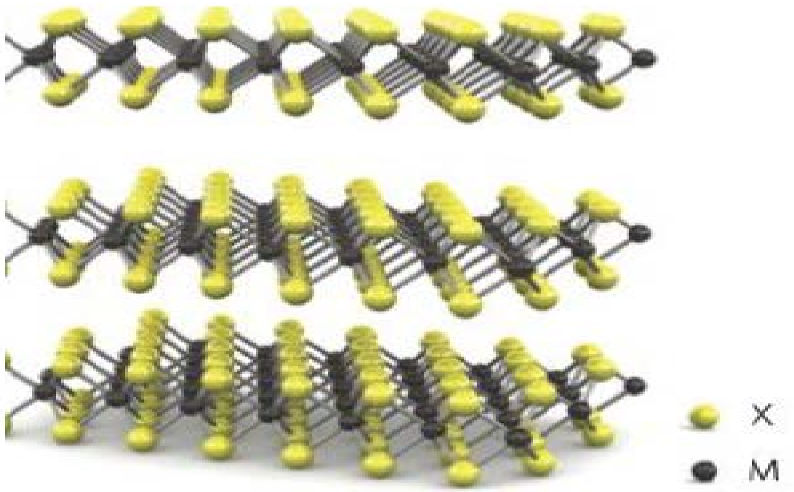
Revised 08/31/2015

Center for the Computational Design of Functional Layered Materials (CCDM)
John P. Perdew (Temple University)

EFRC mission statement

To design new or defect-engineered functional layered materials on the computer, for applications such as solar cells, batteries, and catalysts to generate hydrogen fuel or to convert carbon dioxide to methanol.

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



Wang et al., *Nature Nanotechnology* **7**,699 (2012)

RESEARCH PLAN

The Center aims to design new or defect-engineered layered materials for clean-energy technologies, such as solar cells, batteries, and catalysts to split water for hydrogen fuel. Computational methods for many-electron systems will be improved and applied to this materials-by-design problem. Promising materials will be synthesized and characterized experimentally.

Revised 08/31/2015

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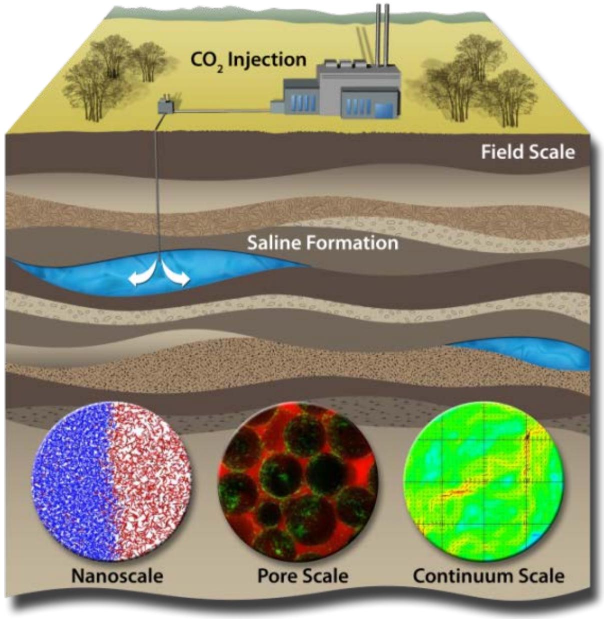
Center for Frontiers of Subsurface Energy Security
Larry W. Lake (University of Texas at Austin)

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.

http://www.utefrc.org/

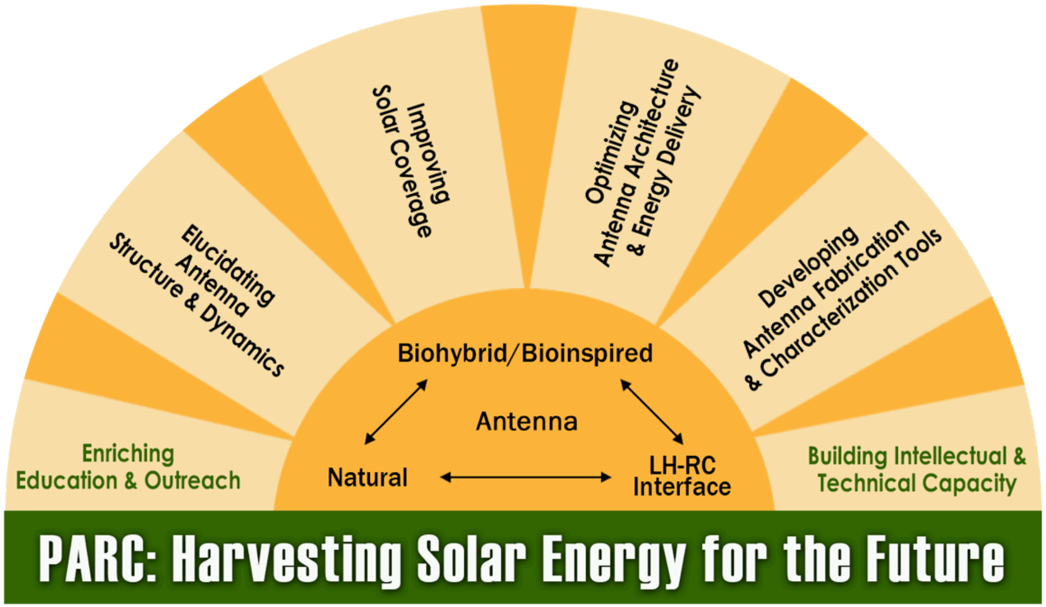


RESEARCH PLAN

CFSES will pursue scientific advances to understand chemical-mechanical coupling between supercritical CO_2 and clay minerals, understand and predict modes and fluxes of reactive CO_2 migration, and design, develop and apply novel materials that will alter fluid-assisted perturbations in heterogeneous geomaterials.

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/

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

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