U.S. Department of Energy

Energy Frontier Research Centers

One Page Overviews

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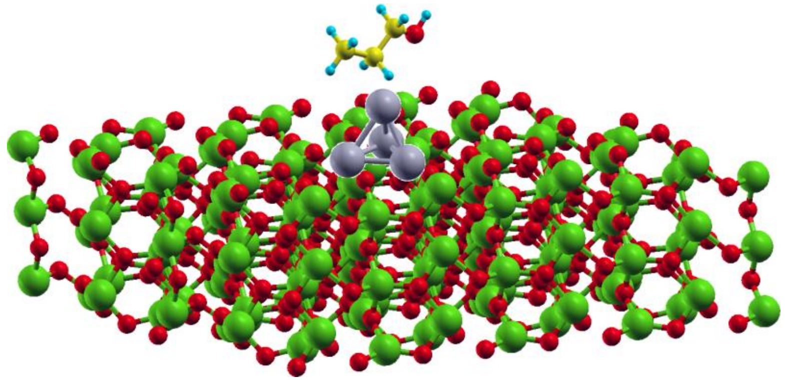
Institute for Atom-efficient Chemical Transformations
Christopher L. Marshall (Argonne National Laboratory)

Summary statement: The *Institute for Atom-efficient Chemical Transformations (IACT)* a collaboration between Argonne National Laboratory, Northwestern University, University of Wisconsin and Purdue University is focused on advancing the *science* of catalysis for the efficient conversion of energy resources into usable forms.

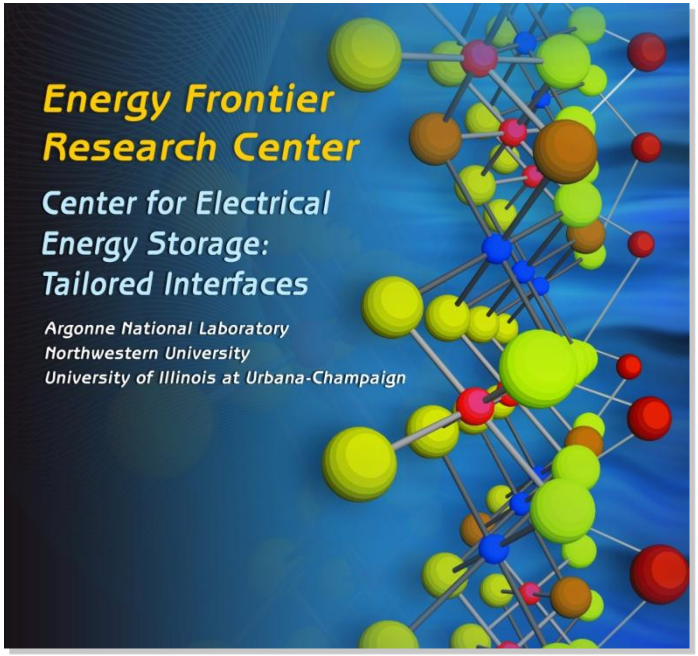


RESEARCH PLAN AND DIRECTIONS

Using a multidisciplinary approach involving integrated catalyst synthesis, advanced characterization, catalytic experimentation, and computation, IACT will address the key chemistries for the efficient removal of oxygen and hydrogen addition associated with the utilization of two primary energy resources in the United States, namely coal and biomass.

Center for Electrical Energy Storage
Michael Thackeray (Argonne National Laboratory)

The Center's overarching mission is to acquire a fundamental understanding of interfacial phenomena controlling electrochemical processes that will enable dramatic improvements in the properties and performance of electrical energy storage devices such as batteries and supercapacitors.



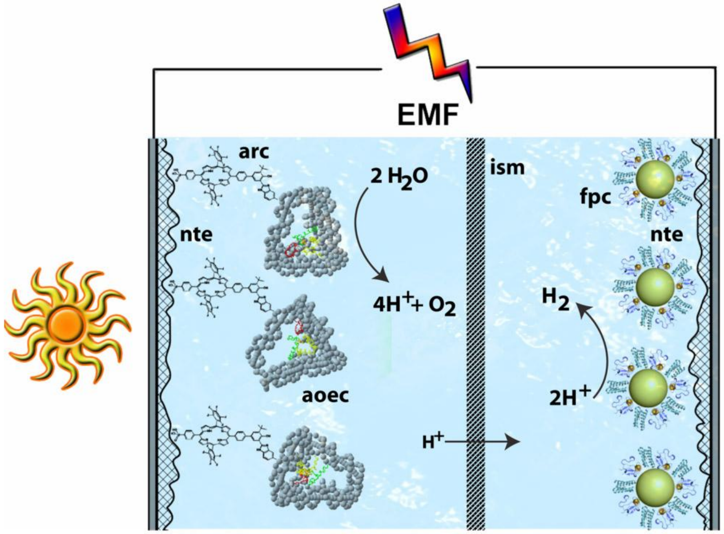
RESEARCH PLAN AND DIRECTIONS

Control of ionic and electronic transport and the stability of an electrified interface is central to the high energy and power output, lifetime, and safety of batteries and supercapacitors. Radical improvements will be sought through the synthesis and design of novel, stabilized architectures at the electrode-electrolyte interface and the characterization of electrochemical processes at the interface.

Center for Bio-Inspired Solar Fuel Production

Devens Gust (Arizona State University)

The goal of the Center is to construct a complete system for solar-powered production of fuels such as hydrogen via water splitting. Design principles will be drawn from the fundamental concepts that underlie photosynthetic energy conversion.



RESEARCH PLAN AND DIRECTIONS

The chemistry of photosynthetic reaction centers, water oxidation proteins, and hydrogen-producing enzymes will be incorporated into nanoscale artificial constructs that make hydrogen using sunlight. Success requires advances in electron transfer chemistry, synthetic enzymes, DNA as a structural material, and functional nanostructured metal oxides. Success will lead to new technologies for solar fuels.

Center for Interface Science: Solar Electric Materials (CIS:SEM)
Neal R. Armstrong (University of Arizona)

CIS:SEM will become a national resource for:

i) **understanding and controlling the interface science underlying solar energy conversion technologies based on organic and organic-inorganic hybrid materials;**

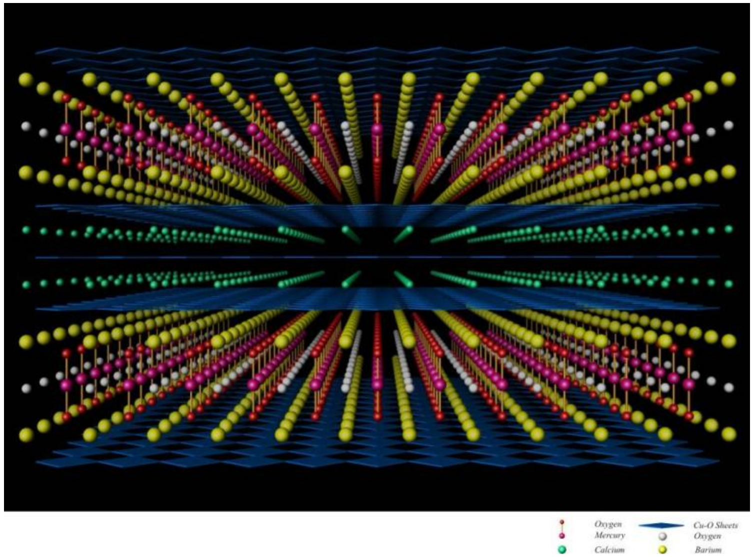
ii) **inspiring, recruiting and training future scientists and leaders in the basic science of solar electric energy conversion.**

RESEARCH PLAN AND DIRECTIONS

Characterize & control of composition and structure of interfaces between nanostructured organic semiconductors and oxides or metals. Interfaces limit the energy conversion efficiencies and scale-up of Generation III solar cells. New materials and characterization methods will enable scientific understandings that lead to future low-cost solar-electric energy conversion technologies with unprecedented performance .

Center for Emergent Superconductivity (Brookhaven National Lab.)

The objectives of CES are to explore and develop higher temperature and higher critical current superconductivity with the potential for application to a superconducting power grid.



CES RESEARCH PLAN AND DIRECTIONS

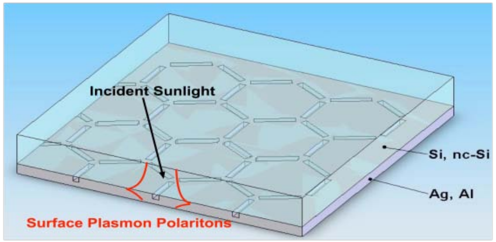
CES research will be directed towards three key areas: finding new strongly correlated superconducting materials, understanding the mechanisms leading to higher temperature superconductivity, and controlling vortex matter so as to raise the loss-less current carrying performance of these superconductors.

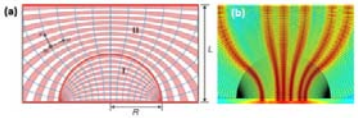
Light-Matter Interactions in Energy Conversion

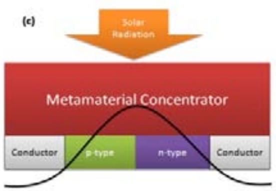
Harry A. Atwater (Caltech)

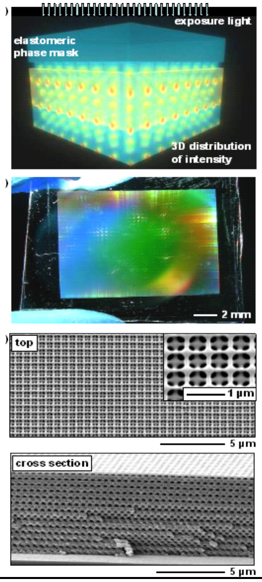
LMI EFRC: a national resource for fundamental optical principles for solar energy.

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









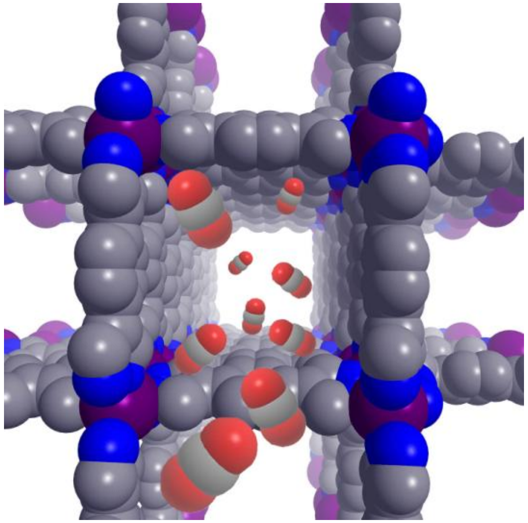
RESEARCH PLAN AND DIRECTIONS

Challenge: Establish fundamental photonic principles for light absorption, propagation and emission in complex dielectric, plasmonic and metamaterial structures. Approach: materials design for enhanced solar absorption, for cooperative up-conversion, and for enhanced spontaneous emission. Expected Outcomes: materials with greatly enhanced photovoltaic and photoelectrochemical energy conversion efficiency.

Center for Gas Separations Relevant to Clean Energy Technologies

Berend Smit (UC Berkeley)

The aim of this EFRC is to develop new strategies and materials that allow for *energy efficient* selective *capture* or *separation* of CO_2 from gas mixtures based on molecule-specific chemical interactions.

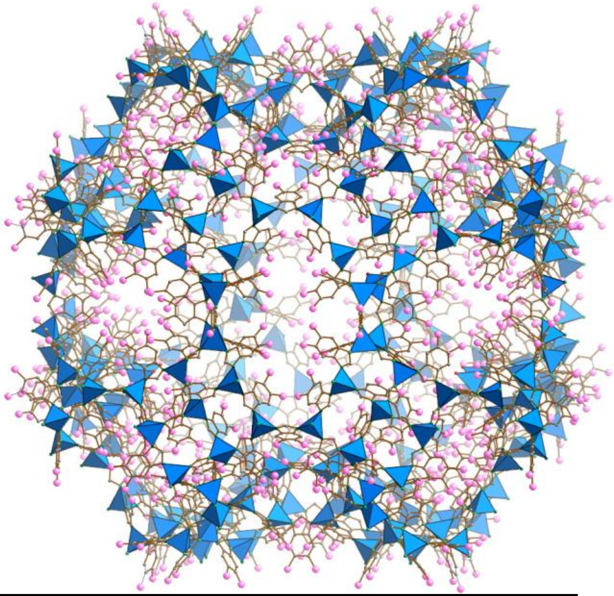


RESEARCH PLAN AND DIRECTIONS

Capture of CO_2 from gas mixtures requires the molecular control offered by nanoscience to tailor-make those materials exhibiting exactly the right adsorption and diffusion selectivity to enable an economic separation process. Characterization methods and computational tools will be developed to guide and support this quest.

Molecularly Engineered Energy Materials (MEEM)
Vidvuds Ozolins (UCLA)

Summary: **Using inexpensive custom-designed molecular building blocks, EFRC will create revolutionary new materials for highly efficient organic solar cells, next-generation electrochemical supercapacitors, and advanced systems for capturing and storing greenhouse gases.**



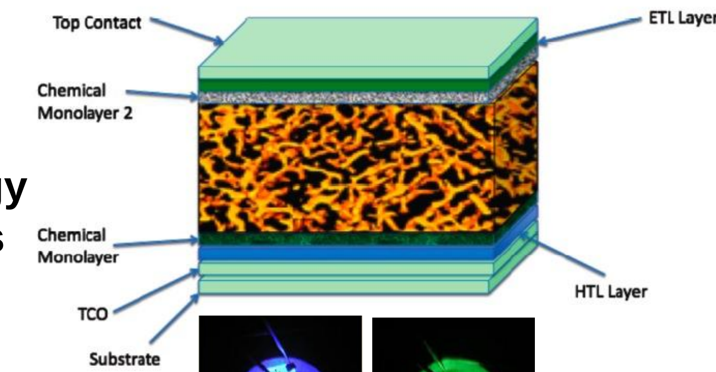
RESEARCH PLAN AND DIRECTIONS

Widespread adoption of renewable energy technologies requires significant improvements in their efficiency and cost. EFRC will create new nanoscale materials that can efficiently generate, transport and store energy and mass. Successful completion of research program will dramatically improve the performance of inexpensive organic solar cells, supercapacitors, and carbon capture systems.

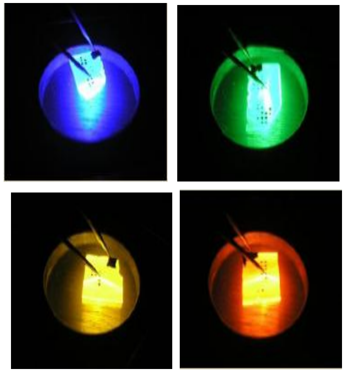
CEEM

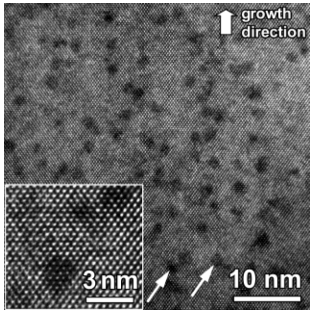
Center for Energy Efficient Materials
John Bowers (UC Santa Barbara)

A fundamental research effort to discover and develop new materials that control the interactions between light, electricity, and heat at the nanoscale, for significantly improved efficiencies in solar energy conversion, solid-state lighting, and thermoelectrics for conversion of heat into electricity.



- **New materials and methods for control of their internal nanostructure for high-efficiency, solution-processed, organic bulk heterojunction solar cells**
- **Semiconductor-based, multiple junction, thin film photovoltaics for 50% power conversion efficiency**
- **Bio-inspired, kinetically controlled, catalytic nanofabrication of heterojunction photovoltaics**
- **Semiconductor-based, nonpolar white light sources with luminous efficiencies >300 Lm/W**
- **Novel nanostructured thermoelectric materials with higher Seebeck coefficient and ZT > 2.5**





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Energy Frontier Research in Extreme Environments
Ho-kwang Mao (Carnegie Institution)

The EFree Center will allow us to expand our fundamental studies of materials under extreme environments while at the same time focus our research on solutions needed to address major energy challenges facing the nation and the world.

Discovery at high pressures

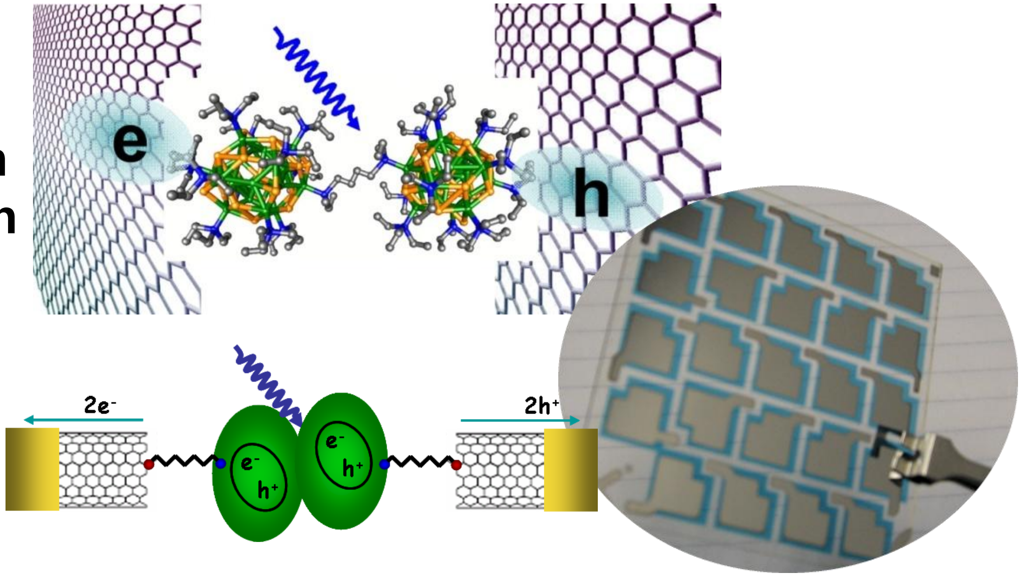
Recovery for energy application

High-pressure studies will be conducted for discoveries of novel materials with optimal properties, including fuels with exceedingly high hydrogen contents, superconductors at record high temperatures, and key components resistive to extremely harsh environments. We will design alternative routes to bring the novel materials to ambient conditions for energy applications.

Re-Defining Photovoltaic Efficiency Through Molecule Scale Control

James Yardley (Columbia University)

The Columbia EFRC will create enabling technology to re-define efficiency in nanostructured thin-film organic photovoltaic devices through fundamental understanding and through molecule-scale control of charge formation, separation, extraction, and transport.



RESEARCH PLAN AND DIRECTIONS

Fundamental understanding of photo-physical and kinetic properties on the nanoscale will allow us to design systems for efficient photovoltaic generation and separation of charges. By using new conducting materials such as graphene we can transport these charges to macroscopic electrical systems, providing basis for revolutionary low cost, high efficiency devices.

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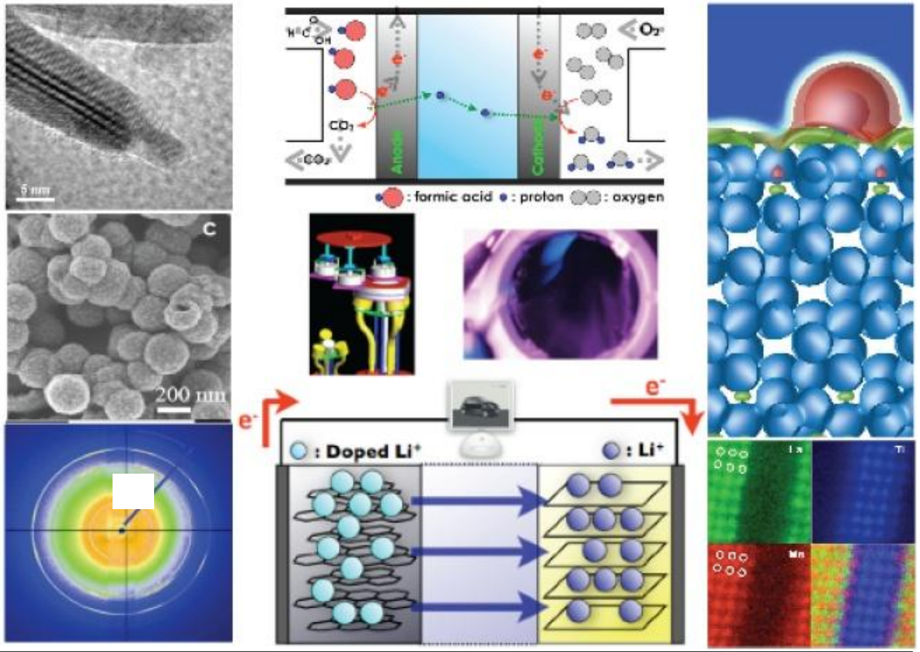
Energy Materials Center at Cornell (EMC^2)
Héctor D. Abruña (Cornell University)

Summary statement: We aim to achieve a detailed understanding, via a combination of synthesis of new materials, experimental and computational approaches, of how the nature, structure, and dynamics of nanostructured interfaces affect energy generation, conversion and storage with emphasis on fuel cells and batteries.



RESEARCH PLAN AND DIRECTIONS

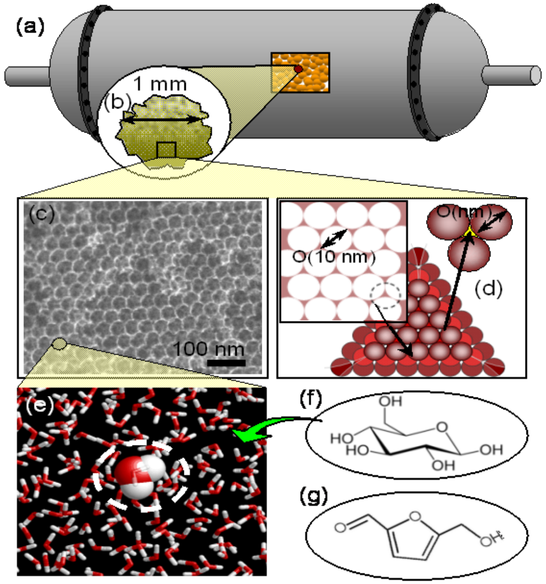
The major challenges relate to materials performance in energy generation, conversion and storage technologies especially fuel cells and batteries. To address these, we will prepare and characterize novel nanoscale materials including ordered intermetallic phases and "atomically engineered" complex oxides. These will be characterized through novel experimental tools and computational platforms.

Cornell University

BERKELEY LAB

Catalysis Center for Energy Innovation (CCEI)
Dion Vlachos (Univ. of Delaware)

Summary statement: The central aim of the CCEI is to develop innovative heterogeneous catalytic technologies for future biorefineries and to educate the workforce needed to lead to further, sustainable economic growth of the US.



RESEARCH PLAN AND DIRECTIONS

Biomass feedstocks vary considerably with source, and their transformation entails complex, multiscale reactions and processes. The CCEI members develop novel catalytic materials and processes, based on a fundamental understanding of the underlying chemistry, to set the foundations for the operation of modern biorefineries for carbon free production of chemicals and fuels.

Center for Advanced Biofuel Systems
Richard Sayre, Director

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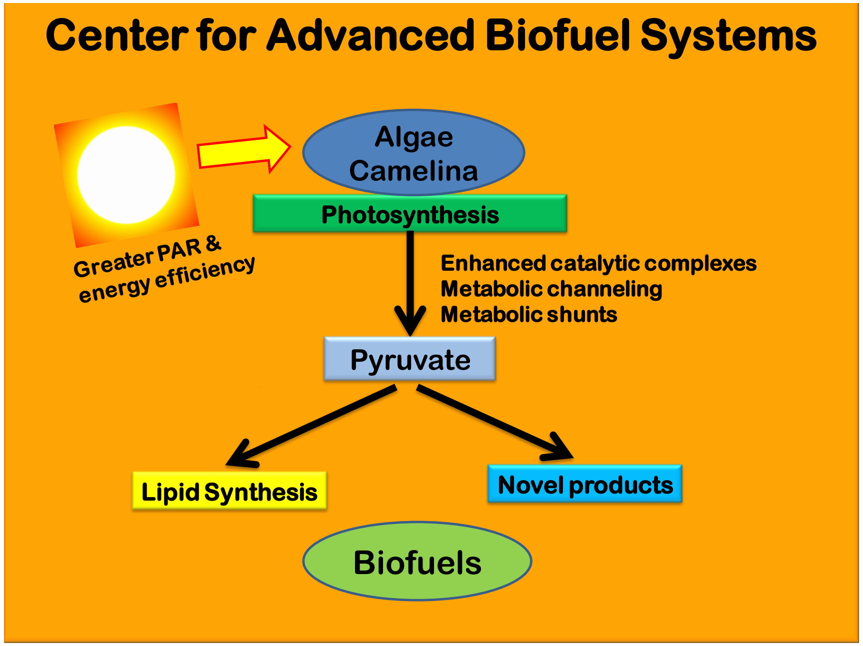
The overall objectives of the Center for Advanced Biofuel Systems are to increase the thermodynamic and kinetic efficiency of biofuel production systems using rational metabolic engineering approaches coupled with the expression of enhanced enzyme catalytic complexes.

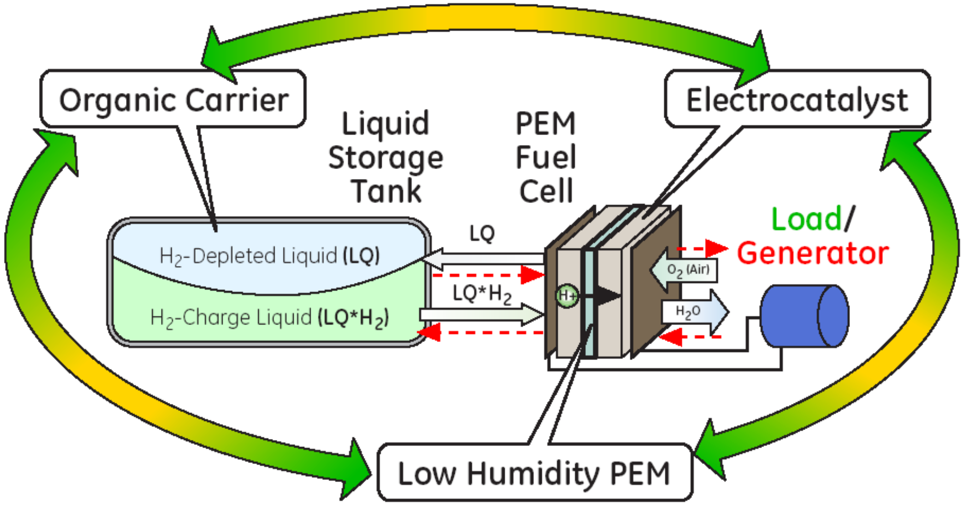


RESEARCH PLAN AND DIRECTIONS

To achieve our objectives we will; 1) employ novel protein catalysts that increase the thermodynamic and kinetic efficiencies of photosynthesis and oil biosynthesis in algae and the oil seed crop, camelina, 2) engineer metabolic networks to enhance pyruvate production and its channeling towards lipid synthesis, and 3) engineer new metabolic networks for biofuel production.

Center for Electrocatalysis, Transport Phenomena, and Materials for Innovative Energy Storage
Dr. Grigorii Soloveichik (GE Global Research)

Electrocatalysis, transport phenomena and membrane materials research aimed to three novel components of an entirely new high-density energy storage system combining the best properties of a fuel cell and a flow battery: organic carriers, electro(de)hydrogenation catalysts, and compatible PEM



RESEARCH PLAN AND DIRECTIONS

Challenges: - Effective electrocatalysts for (de)hydrogenation of organic carriers
- Transport of protons and electrons
- Compatibility of cell components

Approaches: combination of modeling, synthetic chemistry and electrochemistry

Unique aspects: using PEM fuel cell with organic carriers instead hydrogen gas

Potential outcome: high-density mobile and stationary energy storage systems

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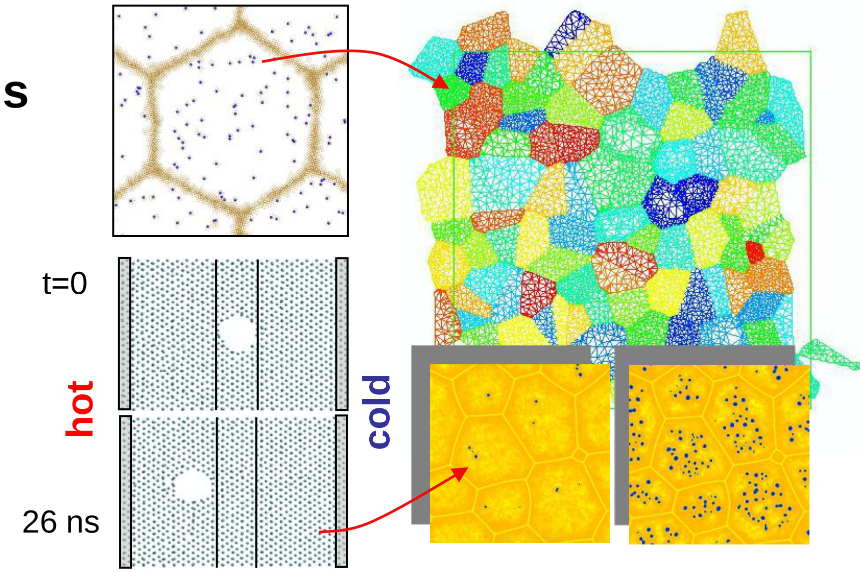
Center for Materials Science of Nuclear Fuel
Dieter Wolf (Idaho National Laboratory)

Summary: **The central theme of the Center is *'Microstructure Science under Irradiation'*, i.e., the determination of how concurrent microstructure formation and evolution under irradiation control the thermo-mechanical behavior of UO_2 as a model nuclear-fuel material.**



RESEARCH PLAN AND DIRECTIONS

Develop an *experimentally validated, multi-scale modeling approach* for micro-structure evolution under irradiation (void-, fission-gas and phase behavior, stress development, ...) and predict how these affect, e.g., thermal transport. Incorporation of microstructural processes based on atomic-level mechanisms is critical towards developing a *predictive* fuels-performance capability.

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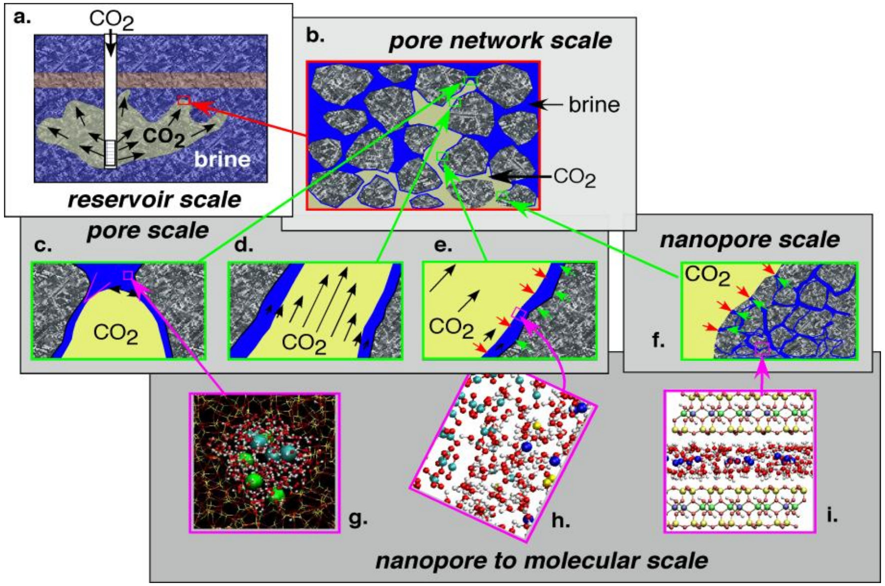
Nanoscale Controls on Geologic CO_2

Donald J. DePaolo (LBNL/ESD)

OBJECTIVES are to (1) develop molecular, nano-scale, and pore network scale approaches for controlling flow, dissolution, and precipitation in subsurface rock formations during emplacement of supercritical CO_2; and (2) achieve a new level of prediction of long-term performance



RESEARCH PLAN AND DIRECTIONS: Properties and interactions of complex fluids and minerals must be determined at elevated temperature and pressure, and effects at interfaces and in confined nano-scale pore spaces understood. Novel experimental and computational approaches, and unique DOE experimental facilities (including ALS, SNS, NERSC, Molecular Foundry) will be used.

Berkeley Lab | Oak Ridge National Laboratory (Managed by UT-Battelle for the Department of Energy) | UC Davis Peter A. Rock Thermochemistry Laboratory

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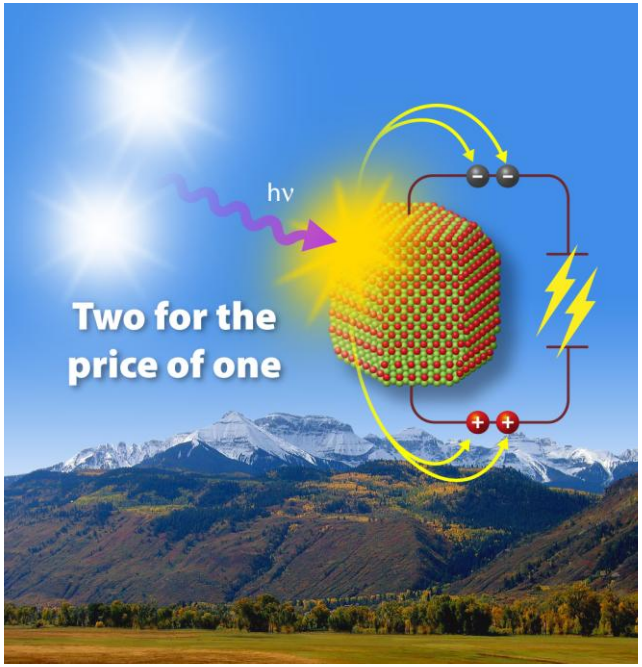
Center for Advanced Solar Photophysics
Victor I. Klimov (Los Alamos National Laboratory)

The goal of this center is to explore and exploit the unique physics of nanostructured materials to boost the efficiency of solar energy conversion through novel light-matter interactions, controlled excited-state dynamics, and engineered carrier-carrier coupling.



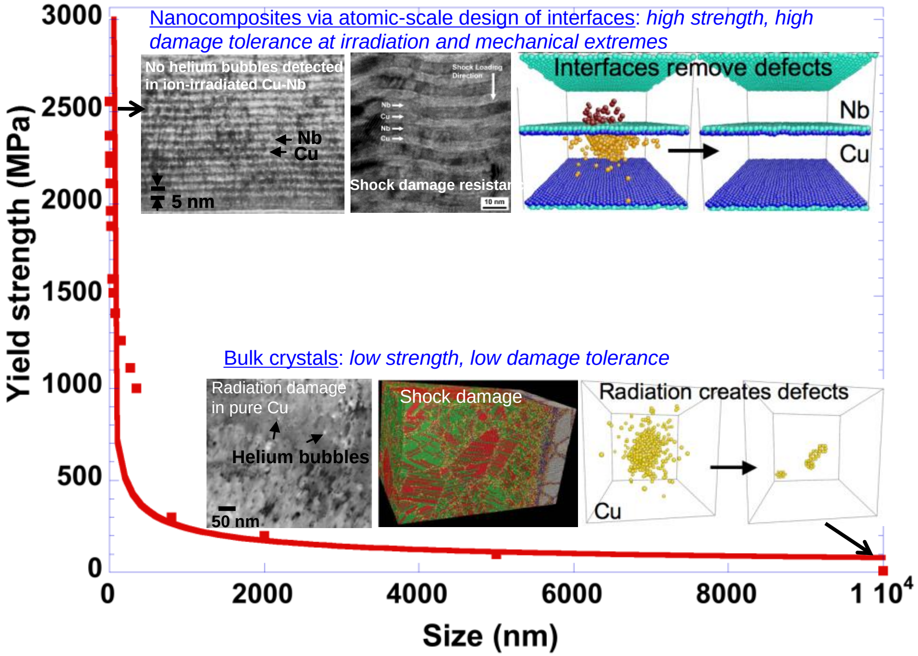
RESEARCH PLAN AND DIRECTIONS

The major challenge is to reach or exceed thermodynamic efficiency limits via approaches such as band-structure engineering, carrier multiplication, plasmonic and photonic effects, and defect-tolerant excitonic transport. The potential outcome of this work is low-cost, high-efficiency photovoltaics based on nanostructures fabricated via scalable chemical methods.

Materials at Irradiation and Mechanical Extremes
Michael Nastasi (Los Alamos Nat. Lab.)

***Summary statement*:**

The purpose of this EFRC is to understand, at the atomic scale, the behavior of materials subjected to extreme radiation doses and mechanical stress in order to synthesize new materials that can tolerate such conditions.



The EFRC will develop a fundamental understanding of how atomic structure and energetics of interfaces contribute to defect and damage evolution in materials, and use this information to design nanostructured materials with tailored response at irradiation and mechanical extremes with potential applications in next generation of nuclear power reactors, transportation, energy and defense.

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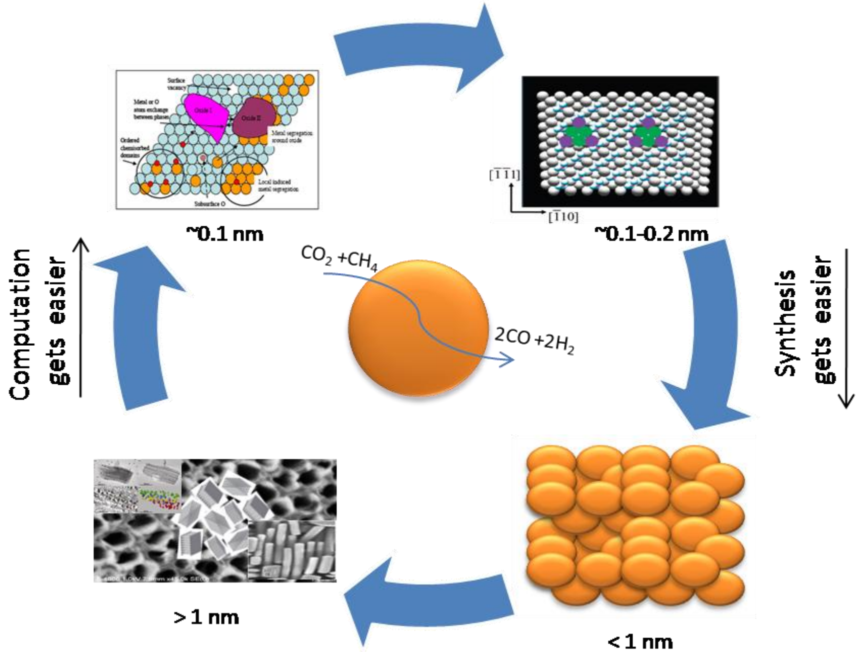
“Theoretical investigations guiding experimental research on surfaces”

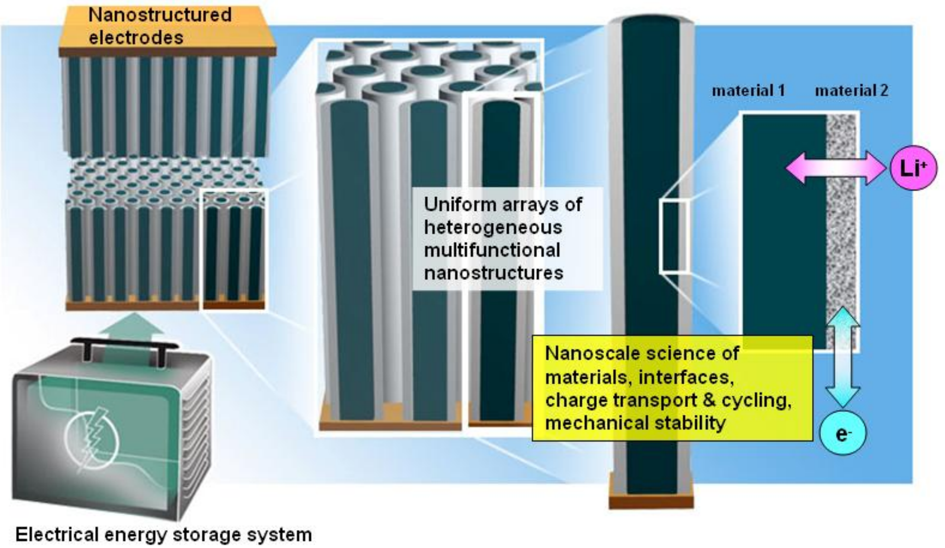


RESEARCH PLAN AND DIRECTIONS

To develop next-generation computational and synthesis/characterization tools to engineer solid catalysts for energy-related conversion processes.

The EFRC will pursue multifunctional nanostructures as the basis for a next generation of high performance electrical energy storage to:

- power **electric vehicles** over long distances and recharge quickly, and
- capture, hold, and deliver energy from **renewable sources**.



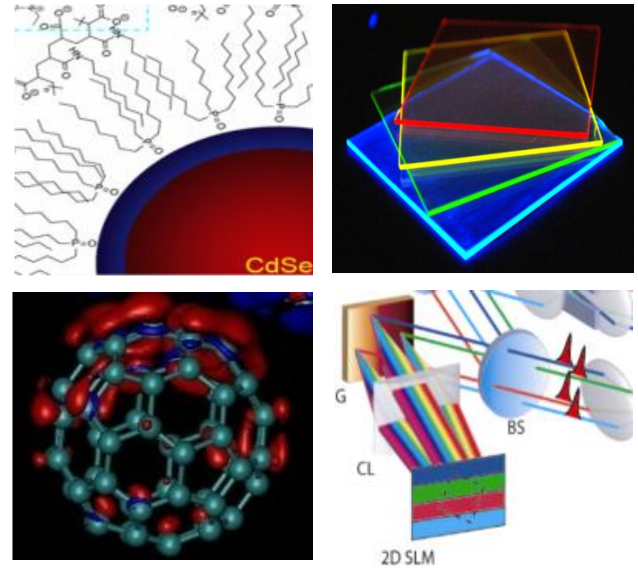
EFRC features:

- Metal oxide and silicon nanowires to hold and cycle charge
- Carbon-nanowire composite nanostructures for faster charge transport and structural stability during charge cycling
- Fundamental understanding of nanostructure synthesis, properties, and electrochemical behavior, supported by novel instruments and theory
- Uniform, predictable structures for scientific analysis and as prototypes of massive arrays in future technology

Center for Excitonics
Marc Baldo (MIT)

Electronics vs Excitonics

Excitons are characteristic of low-cost materials for solar cells and solid state lighting. We seek to supersede traditional electronics with devices that use excitons to mediate the flow of energy.



RESEARCH PLAN AND DIRECTIONS

We address the two grand challenges in excitonics:

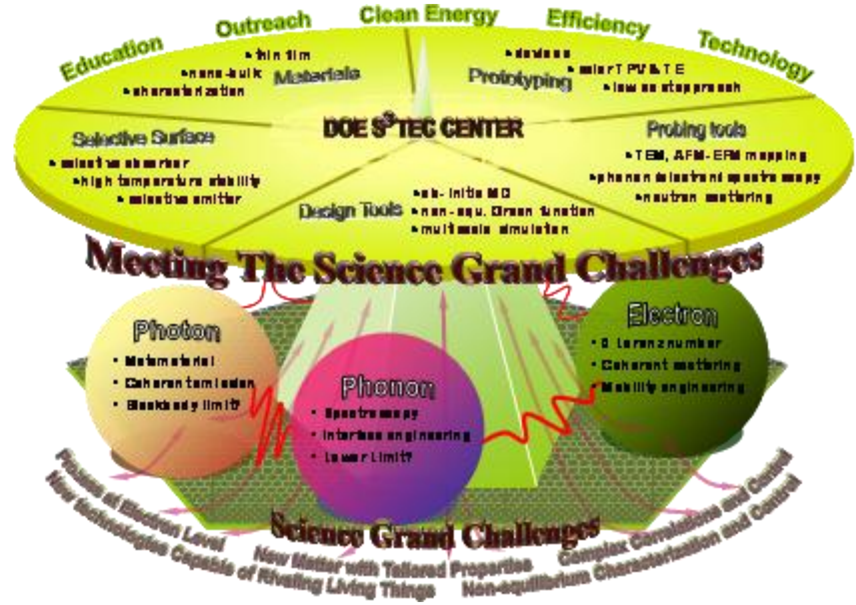
(1) Understand, control and exploit exciton transport

(2) Understand and exploit the energy conversion processes between excitons, electrons, and photons.

Our advances will be applied to low-cost solar cells and solid state lighting.

Solid-State Solar Thermal Energy Conversion Center (S^{3}TEC)
Gang Chen (MIT)

S^{3}TEC Center aims at developing transformational solid-state energy technologies to convert solar energy into electricity via heat, by advancing fundamental science of energy carrier coupling and transport, designing new materials, and inventing cost-effective manufacturing processes, and training energy workforce.



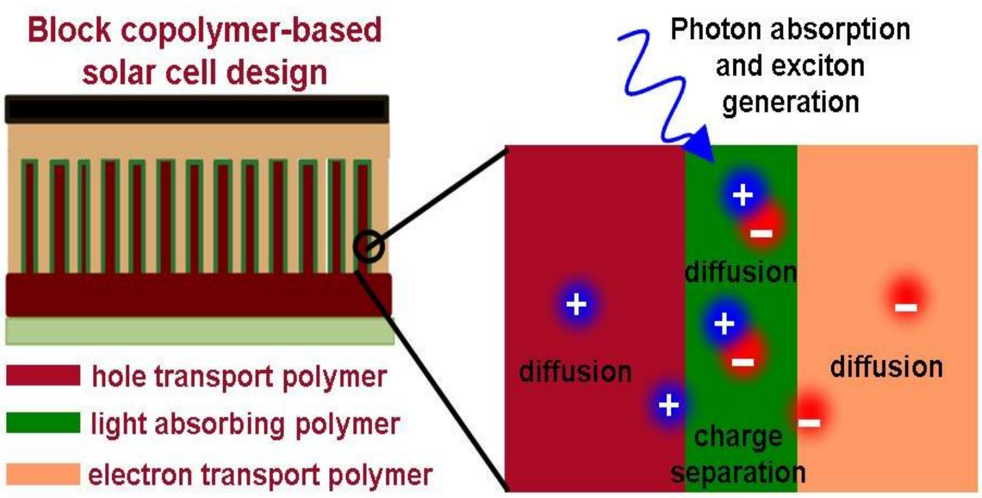
RESEARCH PLAN AND DIRECTIONS

(1) Engineering electron and phonon transport in nanostructures to achieve high performance thermoelectric materials, (2) controlling photon absorption and emission for materials working at high temperatures, and (3) device prototyping to demonstrate the high efficiency and low cost potential of the solar thermoelectric and solar thermophotovoltaic energy conversion technologies.

Polymer-Based Materials for Harvesting Solar Energy

T. P. Russell, P. Lahti (U. Massachusetts)

Summary statement: Maximize the collection and conversion efficiency of a broad frequency range of the solar spectrum using the guided self-assembly of polymer-based materials so as to optimize the design and fabrication of inexpensive devices.



RESEARCH PLAN AND DIRECTIONS

Organic-based devices, while relatively inexpensive and easy to fabricate, have low efficiencies. They are also plagued by low long-term stability problems. We face the challenge of producing affordable, efficient and robust photovoltaic devices.

University of Pittsburgh | UMASS LOWELL | Oak Ridge National Laboratory — Managed by UT-Battelle for the Department of Energy | NREL National Renewable Energy Laboratory — Innovation for Our Energy Future | KONARKA | PennState

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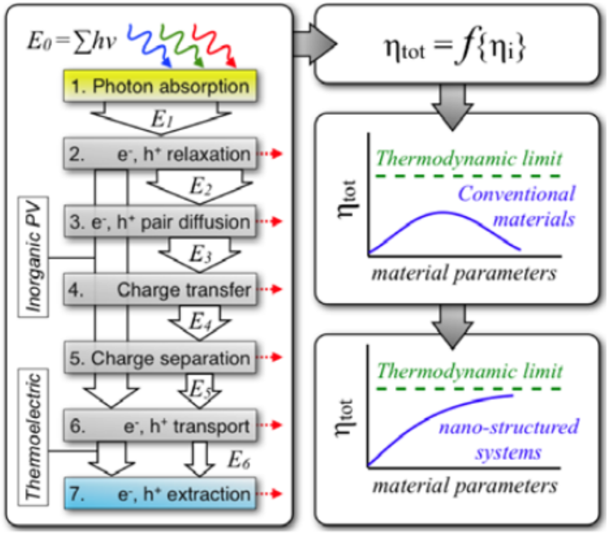
CENTER FOR SOLAR AND THERMAL ENERGY CONVERSION (CSTEC)

Peter F. Green (University of Michigan)

Summary statement: The goal of the center is to develop the science necessary to elucidate and mitigate energy loss processes in low dimensional, and/or complex nanostructured, organic, inorganic, and hybrid materials for high efficiency photovoltaic (PV) and thermoelectric (TE) energy conversion.

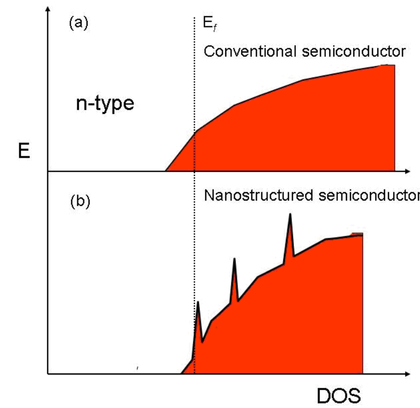


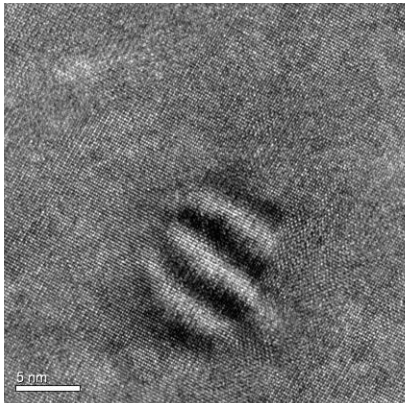
RESEARCH PLAN AND DIRECTIONS

The research will involve cross-cutting efforts in theory, computation, materials synthesis and physical property measurements, including the use of ultrafast optical spectroscopy techniques. It will lead to a fundamental understanding of the dynamics and interactions of charge carriers and phonons, which is essential to control and to "tailor" the conversion efficiencies of low dimensional, and/or complex nanostructured, organic, inorganic, and hybrid materials for TE and PV applications.

Revolutionary Materials for Energy Conversion
Donald T. Morelli (Michigan State University)

The Center for Revolutionary Materials for Energy Conversion will focus on the fundamental science of thermoelectricity. It will combine experimental, theoretical, and computational approaches to synthesize, characterize, and understand the nature of the thermoelectric energy conversion process.





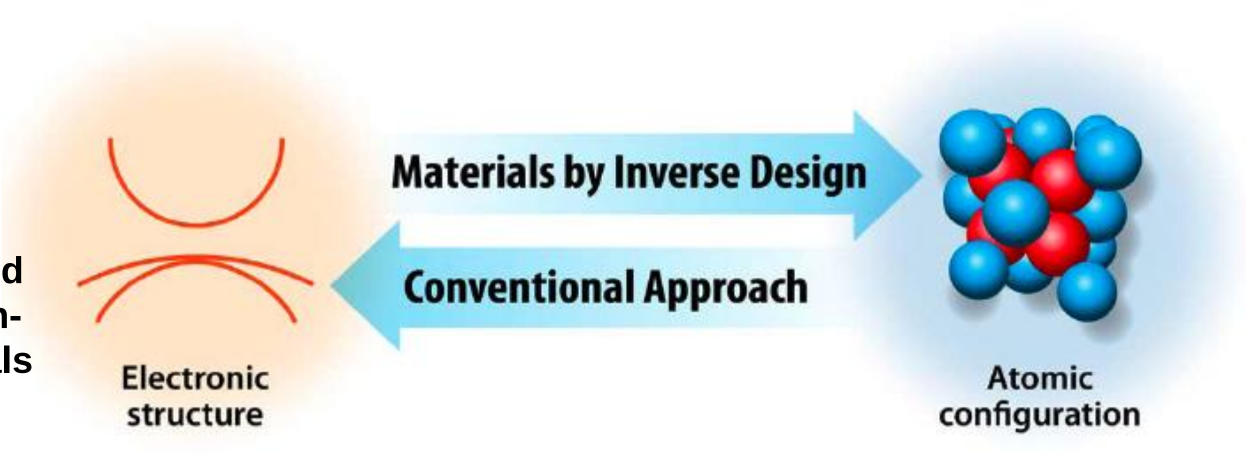
RESEARCH PLAN AND DIRECTIONS

- **Challenges:** create "contraindicated" properties in solids
- **Approaches:** synthesis of novel structures, compounds, and alloys; computational and theoretical investigations
- **Uniqueness:** nanoscience, self-assembly of nanostructures, laser-enhanced tomography of nanostructure, first-principles calculations
- **Outcomes:** deeper understanding of thermoelectric energy conversion

Center for Inverse Design
Alex Zunger (NREL)

Summary statement:

We will focus on material discovery via an "Inverse Band Structure" (IBS) methodology to theoretically identify promising structures and compositions and then apply a combination of high-throughput and targeted materials synthesis to experimentally converge on the optimum properties.

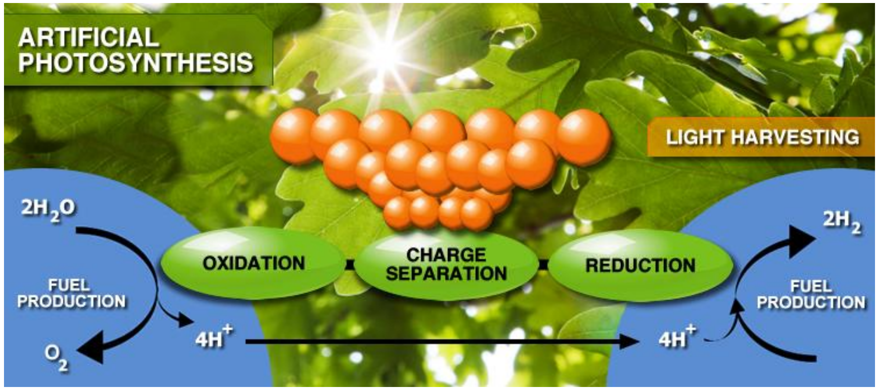


RESEARCH PLAN AND DIRECTIONS

Rather than use the conventional approach "given the structure, find the electronic properties" this center will address the Materials by Inverse design :" given the desired property ,find the structure" .Target properties include new semiconductor absorbers , transparent conductors and nanostructures for energy sustainability .Predictions will be iteratively examined by various synthetic approaches including high -throughput parallel materials science .

Solar Fuels and Next Generation Photovoltaics
Thomas J. Meyer (UNC-CH)

Summary statement: Research in Solar Fuels and Photovoltaics will integrate light absorption and electron transfer driven catalysis in structurally controlled molecular assemblies and composite materials to create efficient devices for solar energy conversion through artificial photosynthesis.

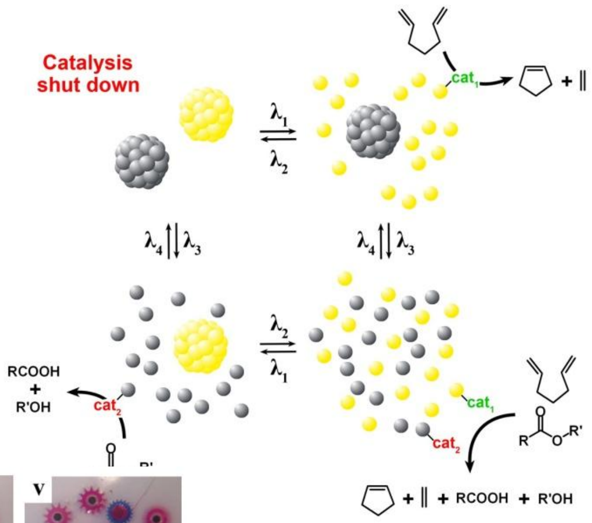


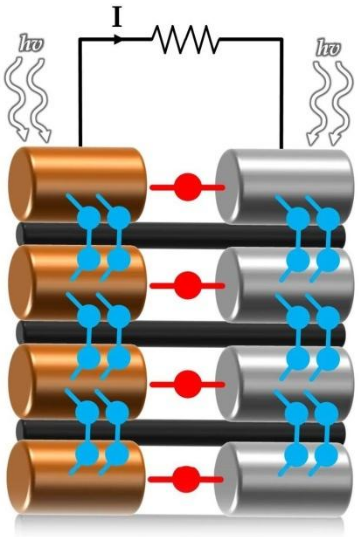
RESEARCH PLAN AND DIRECTIONS

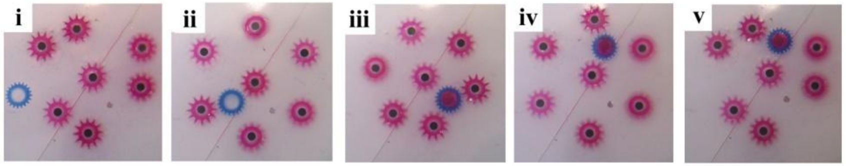
We will combine the best features of academic and translational research to study light/matter interactions and chemical processes for the efficient collection, transfer, and conversion of solar energy into chemical fuels.

Non-equilibrium Energy Research Center
Bartosz A. Grzybowski (Northwestern)

To understand self-organization far from equilibrium and to use this knowledge to synthesize adaptive, reconfigurable materials for energy storage and transduction.







The practical goal of this research is to synthesize metastable materials that can adapt to changing environmental conditions and can harness and/or transduce maximal amounts of useful energy. These materials will be formed by non-equilibrium self-assembly and will comprise "programmable" nanoscopic components.

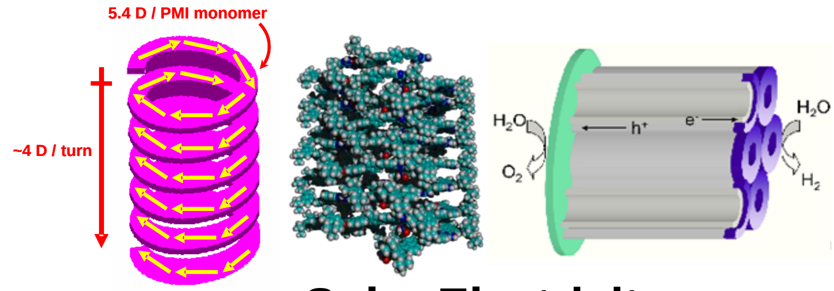
Argonne-Northwestern Solar Energy Research (ANSER) Center

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.

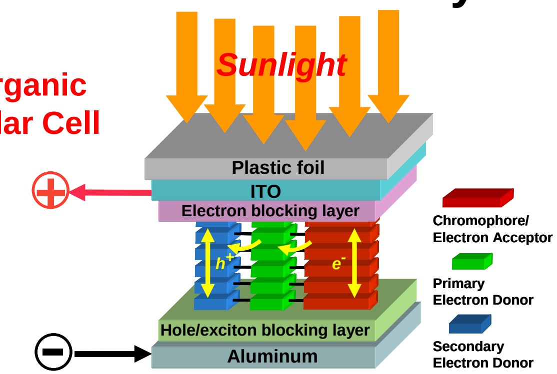
Solar Fuels

Artificial Photosynthetic Systems

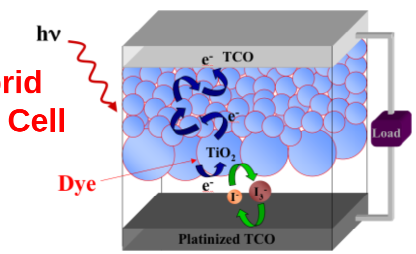


Solar Electricity

Organic Solar Cell



Hybrid Solar Cell



RESEARCH PLAN AND DIRECTIONS

- Discover the basic science necessary to produce bio-inspired artificial photosynthetic systems to generate hydrogen fuel from water.
- Discover new materials, understand materials interfaces and develop new architectures for efficient organic and hybrid solar cells.
- Harnessing solar energy will produce abundant, renewable, carbon-neutral fuels and electricity to satisfy US energy needs.

NORTHWESTERN UNIVERSITY

Argonne NATIONAL LABORATORY

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

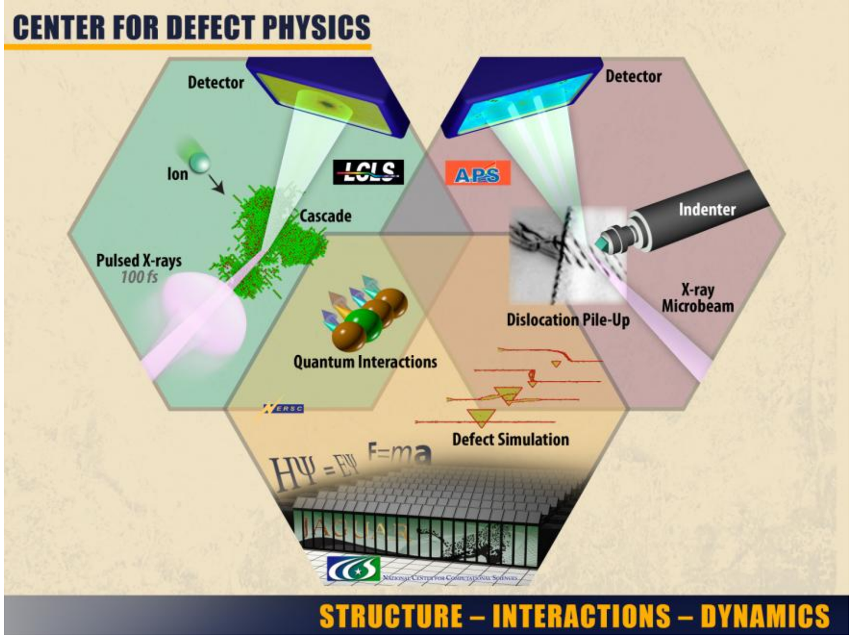
The Materials Science of Actinides EFRC seeks to understand and control, at the nanoscale, materials that contain actinides (radioactive heavy elements such as uranium and plutonium) to lay the scientific foundation for advanced nuclear energy systems.

RESEARCH PLAN AND DIRECTIONS

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 behavior and properties of such materials in extreme environments of radiation and pressure is a major focus of this research.

Center for Defect Physics

G. Malcolm Stocks (ORNL)



Our goal is to provide a fundamental understanding of materials' defects, defect interactions, and defect dynamics, thereby enabling atomistic control and manipulation of defects and the charting of new pathways to the development of improved materials – materials with ultra-high strength, toughness, and radiation resistance.

We deploy first-of-their-kind measurements and *ab initio* quantum calculations of the structure, interactions, and dynamics of defects in structural materials. The Center focuses on three interrelated thrust areas:

- ***Fundamental Physics of Defect Formation and Evolution during Irradiation***
- ***Fundamental Physics of Defect Interactions during Deformation***
- ***Quantum Theory of Defects and their Interactions***

Oak Ridge National Laboratory — Managed by UT-Battelle for the Department of Energy

The University of Tennessee Knoxville

Berkeley

Lawrence Livermore National Laboratory — Science in the National Interest

The Ohio State University

Carnegie Mellon

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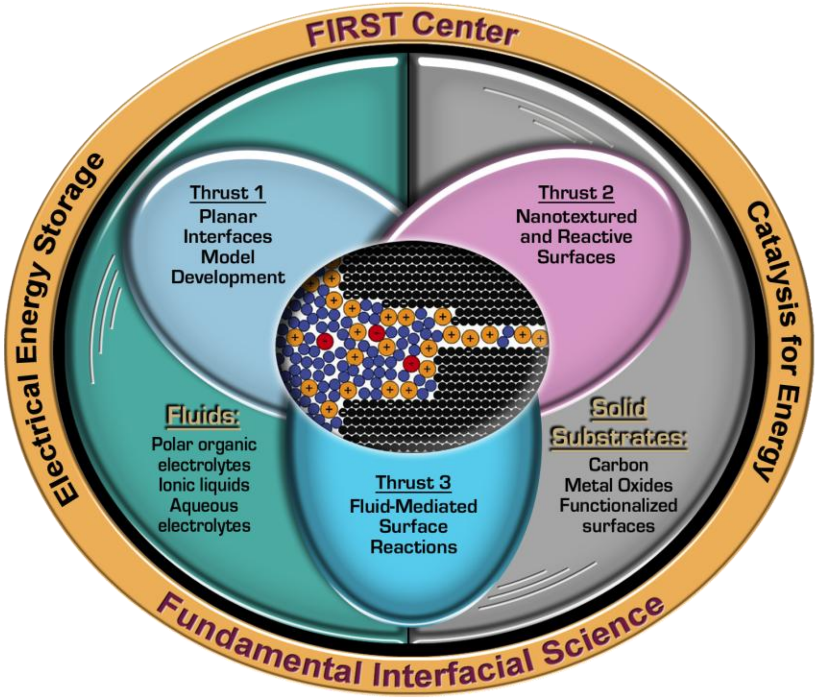
Fluid Interface Reactions, Structures and Transport (FIRST) Center
David J. Wesolowski (Oak Ridge National Lab)

The goal of the FIRST Center is to develop quantitative and predictive models of the unique nanoscale environment at the interface between fluids and solids in order to achieve transformative advances in electrical energy storage and catalysis for energy applications.



RESEARCH PLAN AND DIRECTIONS

Our multidisciplinary team will integrate advanced neutron and X-ray scattering, spectroscopies, experiments, syntheses and multiscale molecular modeling to provide a predictive capability for controlling and designing new interfacial systems for 21st century energy needs.

Oak Ridge National Laboratory · Vanderbilt University · Argonne National Laboratory · Drexel University · University of Virginia · Northwestern University

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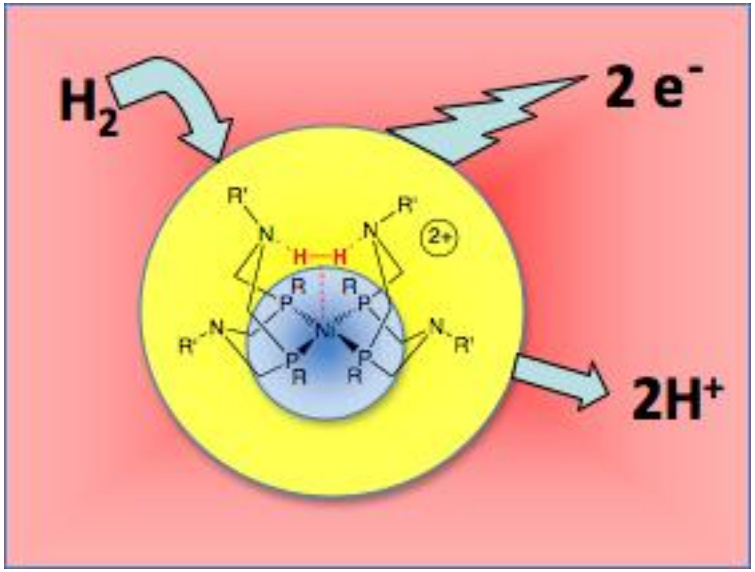
Energy Frontier Research Center

Center for Molecular Electrocatalysis
R. Morris Bullock, Director
(Pacific Northwest National Laboratory)

Our goal is to achieve transformational changes in our ability to design molecular electrocatalysts that efficiently convert electrical energy into chemical bonds in fuels, or the reverse, converting chemical energy to electrical energy.



RESEARCH PLAN AND DIRECTIONS

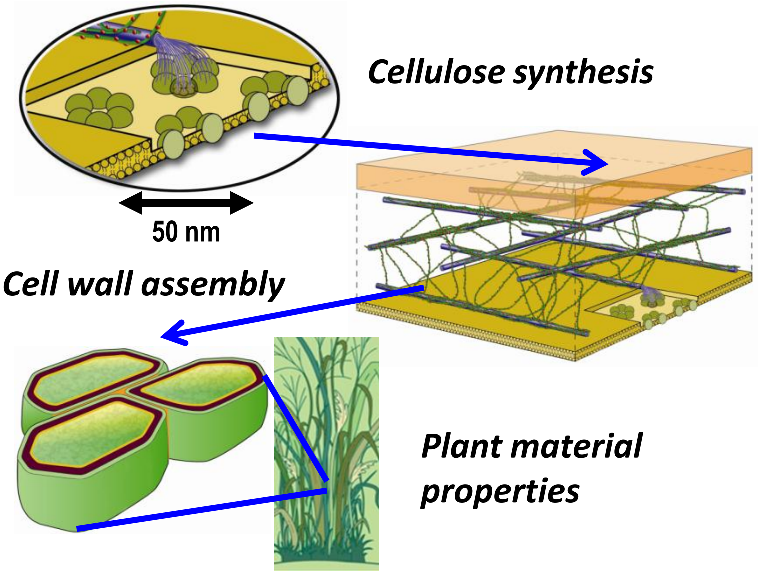
A secure energy future will require catalysts for the oxidation of hydrogen, reduction of oxygen, and reduction of nitrogen. These reactions involve movement of multiple protons and electrons. Our research will address how proton relays can regulate the movement of protons and electrons to enhance the rates of electrocatalysts.

U.S. DEPARTMENT OF ENERGY

Center for Lignocellulose Structure and Formation

Daniel Cosgrove (Penn State University)

Lignocellulose is the major structural material in plants and a vast source of renewable biomaterials and bioenergy. CLSF studies the physical structure of lignocellulose at the nano scale and the physicochemical rules by which plants create this most versatile of materials.



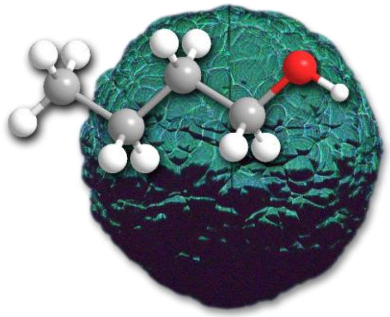
RESEARCH PLAN AND DIRECTIONS

With a unique mix of molecular biologists, chemists, physicists, engineers and modelers, CLSF will tackle key questions of lignocellulose structure and formation. This is a key step towards unlocking the energy-rich biomaterial for the next generation of sustainable biofuels and for creating new cellulosic biomaterials with diverse economic applications.

Combustion Energy Frontier Research Center

Chung K. Law (Princeton University)

Summary statement: The Combustion-EFRC is focused on the science underlying the combustion and fuel chemistry of non-petroleum-based fuels, especially renewable biofuels, and their development for and optimal use in advanced engines for transportation applications.



RESEARCH PLAN AND DIRECTIONS

- **Challenge:** The combustion characteristics of non-petroleum-based fuels, especially renewable biofuels, in advanced engines are largely unknown.
- **Approaches:** Multidisciplinary study involving quantum chemistry, chemical kinetics, and fluid dynamics relevant to understanding fuel/engine optimization of performance and emissions
- **Unique aspects:** Multi-scale investigation ranging from electronic structure to nanoscale particulate formation to turbulent flame control and emission minimization
- **Outcomes:** Predictive modeling capability to optimize the combustion of renewable transportation fuels in advanced engines

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

Maureen McCann (Purdue University)

Summary statement: C3Bio aims to develop transformational technologies for the direct conversion of plant lignocellulosic biomass to biofuels and other biobased products, currently derived from oil, by the use of new chemical catalysts and thermal treatments.

RESEARCH PLAN AND DIRECTIONS

We will maximize the energy and carbon efficiencies of advanced biofuels production by the design of both thermal and chemical conversion processes and the biomass itself. Impacts are to *more than double* the carbon captured into fuel molecules and *expand* the product range to alkanes and other energy-rich fuels.

EFRC for Solid-State Lighting (SSL) Science
Jerry A. Simmons & Mike Coltrin
(Sandia National Labs)

U.S. DEPARTMENT OF ENERGY

Goal: Improve the energy-efficiency in the way we light our homes and offices, which currently accounts for 20% of the nation's electrical energy use. Solid-State Lighting (SSL) has the potential to cut that energy consumption in half – or even more.

Research plan: Investigate conversion of electricity to light using radically new designs, such as luminescent nanowires, quantum dots, and hybrid architectures; study energy conversion processes in structures whose sizes are even smaller than the wavelength of light; understand and eliminate defects in SSL semiconductor materials that presently limit the energy efficiency.

Sandia National Laboratories · Rensselaer Polytechnic Institute · The University of New Mexico · Northwestern University · UMass · Los Alamos National Laboratory · Philips · California Institute of Technology

Heterogeneous Functional Materials Center
Ken Reifsnider (University of South Carolina)

The aim of this EFRC is to establish foundations of understanding and control science that enable the prescriptive design and ordered synthesis of the local compositions, interfaces, and morphology of heterogeneous material systems for specific functional behavior and system performance.

RESEARCH PLAN AND DIRECTIONS

The greatest challenge to the creation of nano-synthesis concepts and processes that control nano-structural configurations and interfaces of active phases is to understand "what the picture should look like." We will use science to bridge the gap between multi-scale analysis and nano-synthesis methodologies to create new functional materials.

University of South Carolina Department of Mechanical Engineering · NanoTech Nanoscience + Nanotechnology @ Georgia Tech · SRNL · The University of Utah · University of Connecticut · RIT · Pacific Northwest National Laboratory · Princeton University · UCSB California Nanosystems Institute

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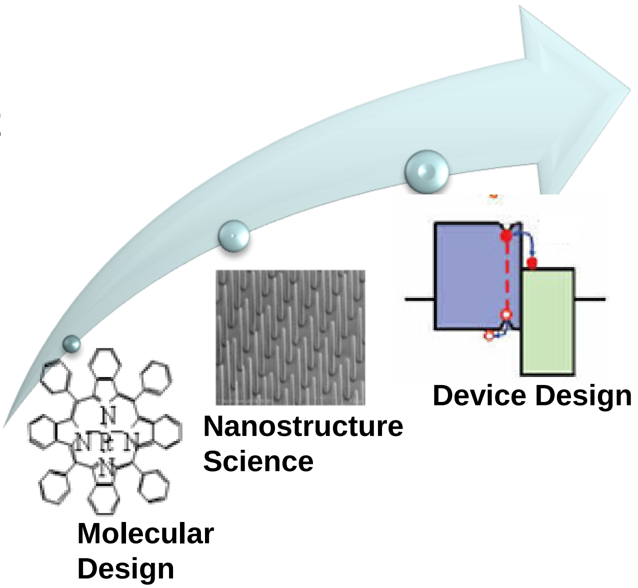
Energy Frontier Research Center

Emerging Materials for Solar Energy Conversion and Solid State Lighting

P. Daniel Dapkus (USC)

The goal of our center is to create low cost, high efficiency solar cells and light emitting diodes (LEDs). Our world renown team will use semiconductor nanotechnology and organic molecular design to produce innovative new materials, coupling with novel device designs will provide key understanding of the fundamental issues controlling performance.

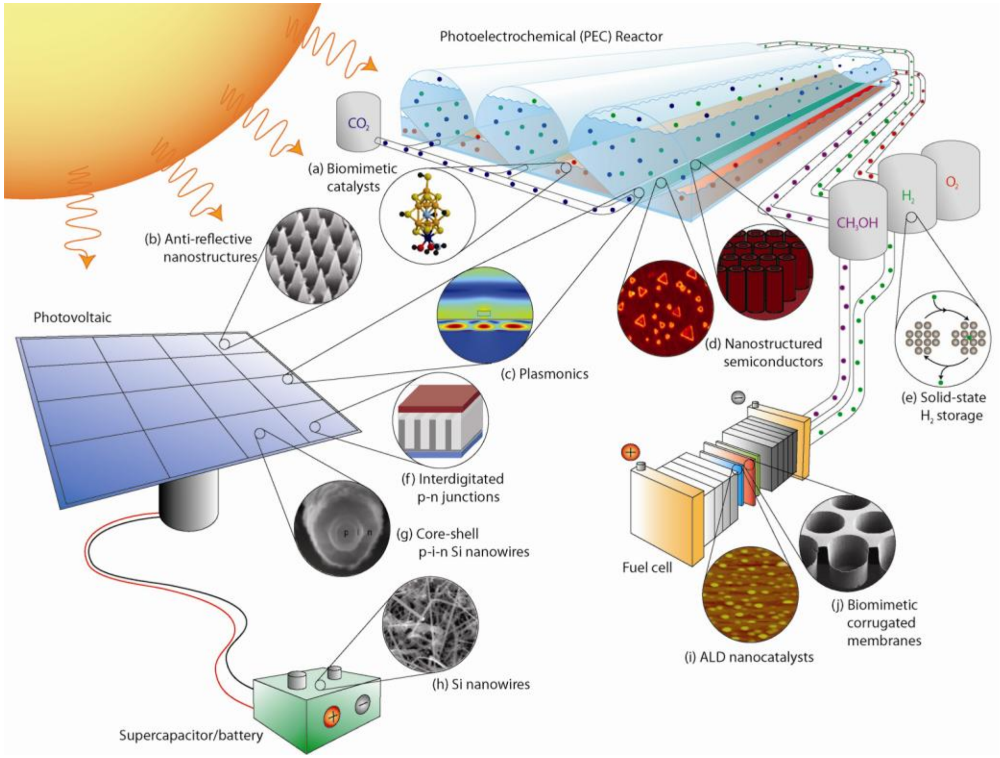


RESEARCH PLAN AND DIRECTIONS

- **Increase efficiency and reduce cost of solar cells and LEDs by 10X to create technologies that are cost competitive with the incumbents.**
- **Develop new understanding of semiconductor nanoscience, organic molecule design, and device design to enable a new generation of low cost, efficient device designs.**

Center on Nanostructuring for Efficient Energy Conversion (CNEEC)
Stacey Bent and Fritz Prinz (Stanford)

CNEEC seeks to understand and solve cross-cutting fundamental problems at the nanoscale to improve materials properties such as light absorption, charge transport, and catalytic activity. These efforts are aimed at efficient energy conversion and storage in advanced devices such as photovoltaics, fuel cells, and batteries.



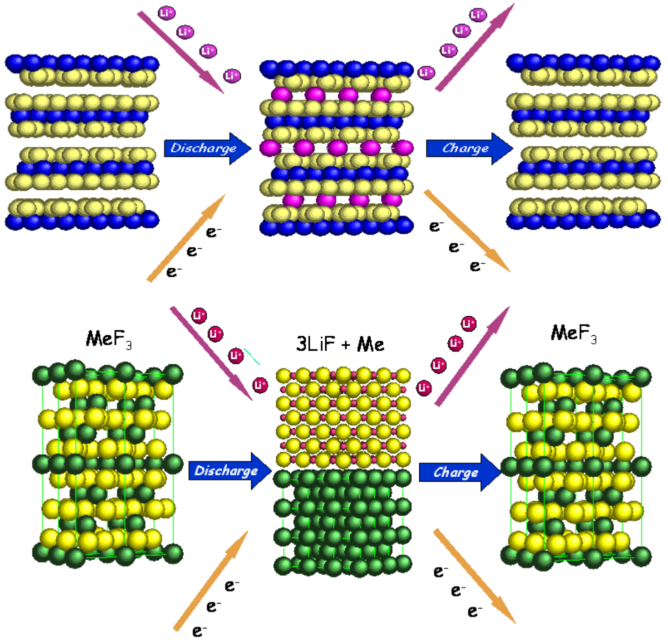
RESEARCH PLAN AND DIRECTIONS

We will use nanostructuring to tune thermodynamics, enhance kinetics, manage photonics, and accelerate charge transport in materials, each of which will be used to improve performance and efficiency in energy conversion devices.

Northeastern Center for Chemical Energy Storage (NECCES)

Clare P. Grey, Director (Stony Brook University)

Summary statement: A fundamental understanding of how key electrode reactions occur, and how they can be controlled will be developed, so as to identify critical structural and physical properties that are vital to improving battery performance; this information will be used to optimize and design new electrode materials.



RESEARCH PLAN AND DIRECTIONS

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

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Energy Frontier Research Center

Understanding Charge Separation and Transfer at Interfaces in Energy Materials

Paul F. Barbara (Univ. of Texas-Austin)

U.S. DEPARTMENT OF ENERGY

This EFRC will elucidate how the useful properties of materials for solar cells and batteries can be dramatically improved by controlling their molecular shape and arrangement.

Each light burst is a single molecule in a model solar cell.

RESEARCH PLAN AND DIRECTIONS

We will use newly developed sub-ensemble techniques (including single-molecule spectroscopy and imaging) coupled with theoretical methods to answer key outstanding questions on charge separation and transfer for solar cell and battery materials.

Expected outcomes: **new R&D tools, new high-performance materials and the education of a new generation of energy researchers**

THE UNIVERSITY OF TEXAS AT AUSTIN

Sandia National Laboratories

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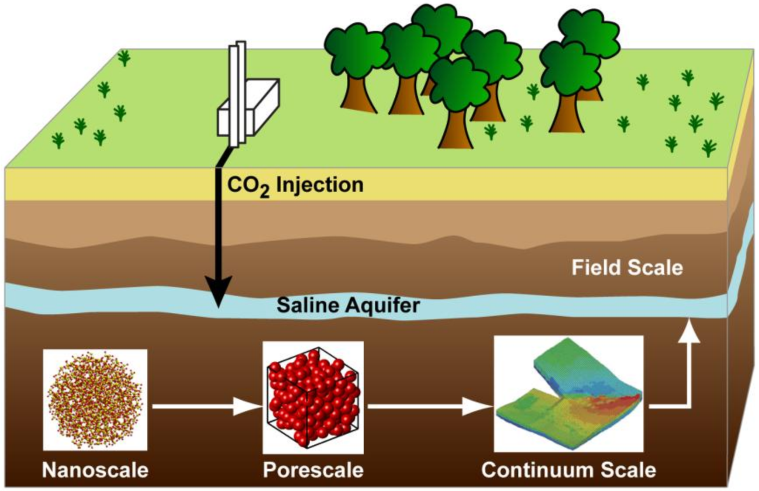
Energy Frontier Research Center

Center for Frontiers of Subsurface Energy Security

Gary. A. Pope (The University of Texas)

Summary statement: Our goal is scientific understanding of subsurface physical, chemical and biological processes from very small to very large scale so that we can predict the behavior of CO_2 and other byproducts of energy production that may need to be stored in the subsurface.

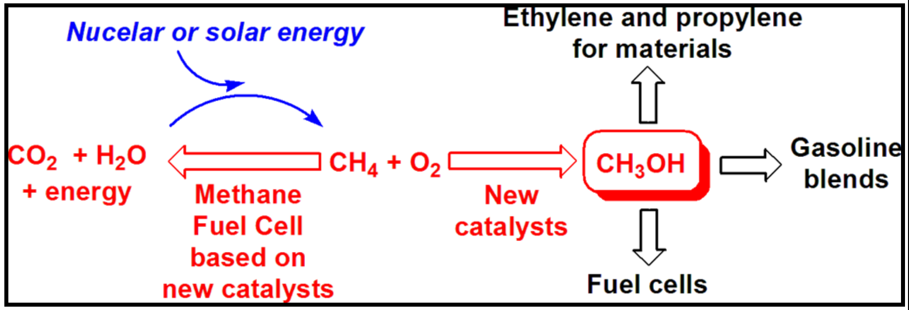


RESEARCH PLAN AND DIRECTIONS

- **Challenges and approaches: Integrate and expand our knowledge of subsurface phenomena across scientific disciplines using both experimental and modeling approaches to better understand and quantify behavior far from equilibrium.**
- **Unique aspects: The uncertainty and complexity of fluids in geologic media from the molecular scale to the basin scale.**
- **Outcome: Better understanding of long term behavior of subsurface storage.**

Center for Catalytic Hydrocarbon Functionalization
T. Brent Gunnoe (University of Virginia)

The Center for Catalytic Hydrocarbon Functionalization brings together groups in catalysis, materials, electrochemistry, bioinorganic chemistry and quantum mechanics to develop new catalyst technologies for hydrocarbon functionalization processes that can reduce energy consumption while enhancing domestic energy resources to fuel future transportation processes.

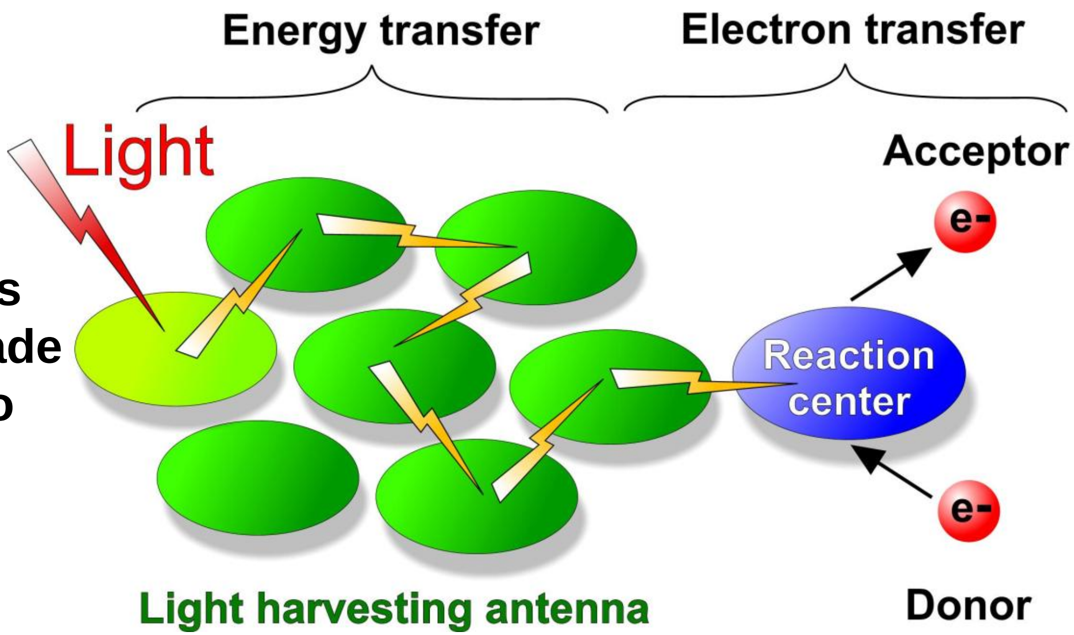


Depiction of examples of short and long term outcomes of one set of research projects in the CCHF.

Controlled hydrocarbon functionalization can lead to high impact technologies, but such catalysts require a level of molecular control beyond current means. The CCHF facilitates collaborations among the leading research groups to develop, validate, and optimize new methods to rearrange the bonds of hydrocarbons, implement enzymatic strategies into synthetic systems, and design optimal environments for catalysis.

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 man-made systems to convert sunlight into fuels.



PARC will investigate:

- **Efficiency of Natural and Genetically Modified Antenna Systems**
- **Structure and Function of Natural and Biohybrid Antenna Systems**
- **Development of Bioinspired Antenna Systems.**

INVESTIGATOR INDEX

*Directors appear in **Bold***

INSTITUTION INDEX