U.S. Department of Energy

Energy Frontier Research Centers

One Page Overviews

Office of Science
1/31/2011
Updated 07/16/2012

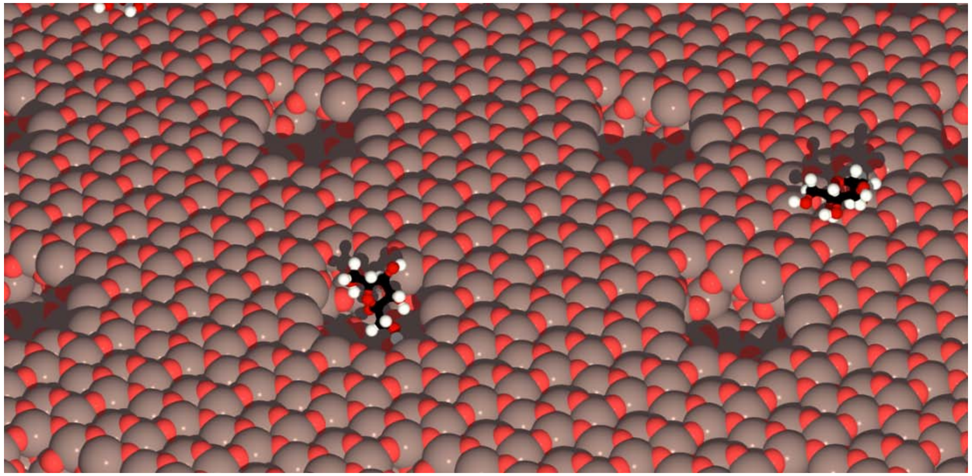
TABLE OF CONTENTS

Institute for Atom-efficient Chemical Transformations (IACT)

Christopher L. Marshall (Argonne National Lab)

U.S. DEPARTMENT OF ENERGY | Office of Science

The *Institute for Atom-efficient Chemical Transformations (IACT),* a collaboration between Argonne National Laboratory, Northwestern University, University of Wisconsin and Purdue University, focuses 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.

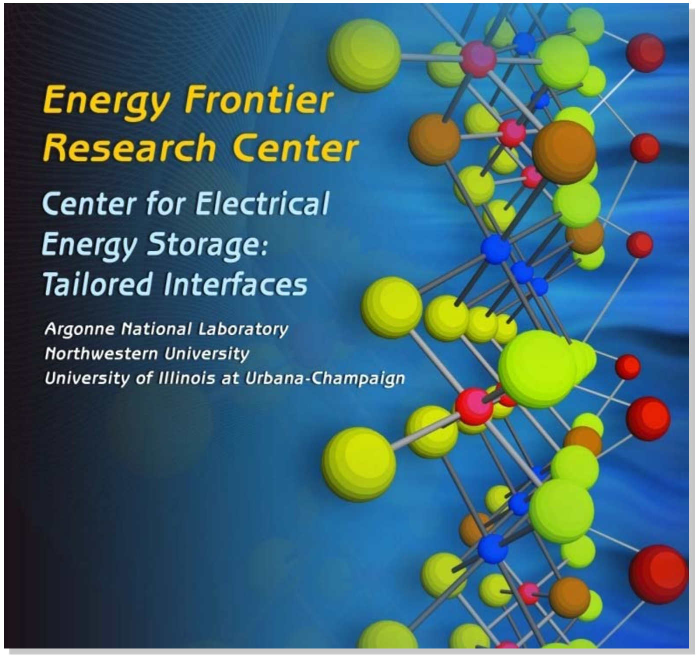
Argonne National Laboratory | Northwestern University | Brookhaven National Laboratory | The University of Wisconsin Madison | Purdue University

an Office of Basic Energy Sciences
Energy Frontier Research Center

U.S. DEPARTMENT OF ENERGY | Office of Science

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. The use-inspired research is focused predominantly on lithium batteries*.**

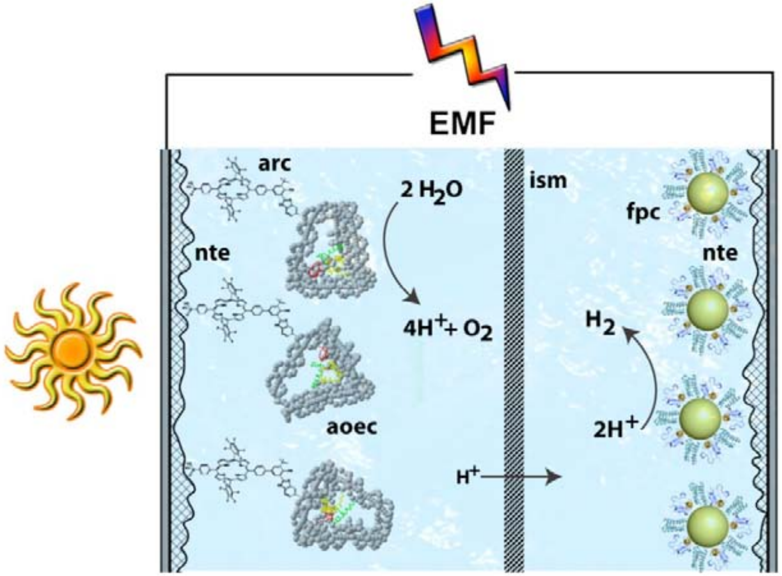


RESEARCH PLAN AND DIRECTIONS

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. Radical approaches to improvements in battery performance are being enabled through the synthesis and design of novel electrode-electrolyte architectures and characterization of electrochemical processes at the electrode-electrolyte 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 are 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 is being incorporated into nanoscale artificial constructs that oxidize water and make hydrogen using sunlight. Success requires advances in electron transfer chemistry, synthetic enzymes, DNA as a structural material, and functional nanostructured metal oxides. The research will lead to new technologies for solar fuels.

U.S. DEPARTMENT OF ENERGY | Office of Science

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

***Vision*:**
CISSEM will become a nationally and internationally recognized center of excellence for the science of interfaces in photovoltaic (PV) devices based on organic and inorganic nanostructured, hybrid materials.

(http://solarinterface.org/)

RESEARCH PLAN AND DIRECTIONS

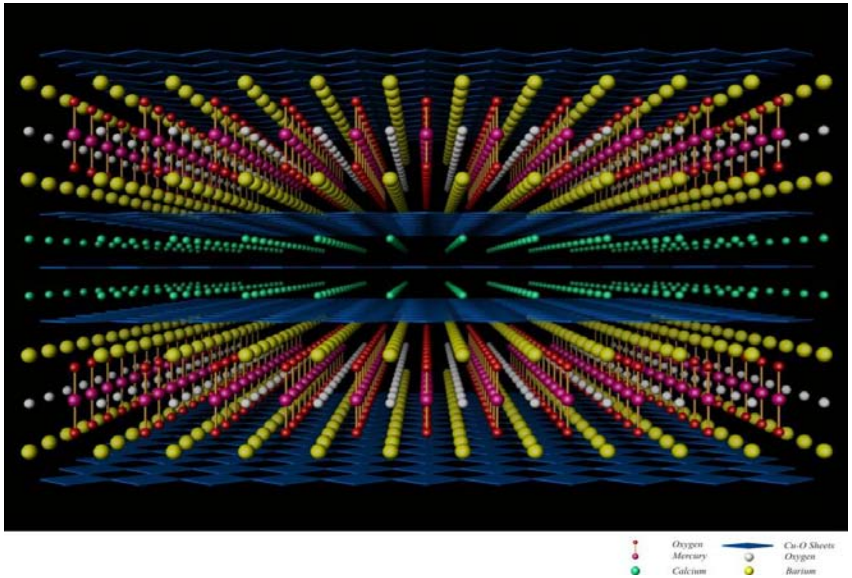
Interfacial processes at nanometer length scales in thin-film PV technologies are the thrust of our efforts, in particular at organic/oxide, organic/metal and oxide/oxide interfaces. Our research is an integrated, multi-investigator effort from five institutions to understand how interface composition and morphology can be controlled and improved in thin-film PVs.

The University of Arizona
Georgia Institute of Technology
NREL National Renewable Energy Laboratory
University of Washington
Princeton University
CIS:SEM

an Office of Basic Energy Sciences
Energy Frontier Research Center

Center for Emergent Superconductivity (J.C. Séamus Davis, 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.

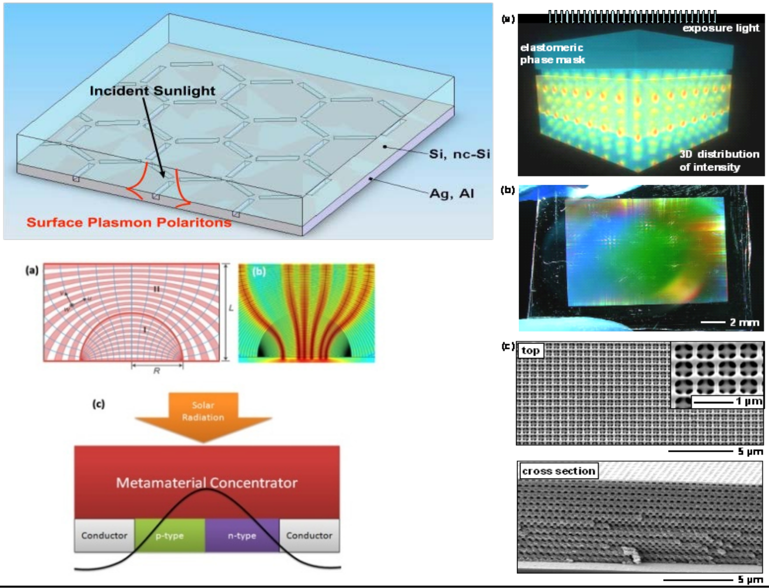


CES RESEARCH PLAN AND DIRECTIONS

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-Material 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

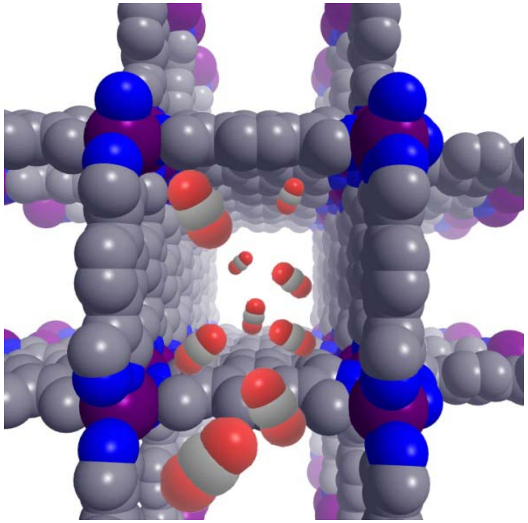
Challenge: Establish fundamental photonic principles for light absorption, propagation and emission in complex dielectric, plasmonic and metamaterial structures. Approach: materials design for enhanced solar absorption, for optical frequency conversion, and for enhanced spontaneous emission. Expected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

* Updated 5/10/2012

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.

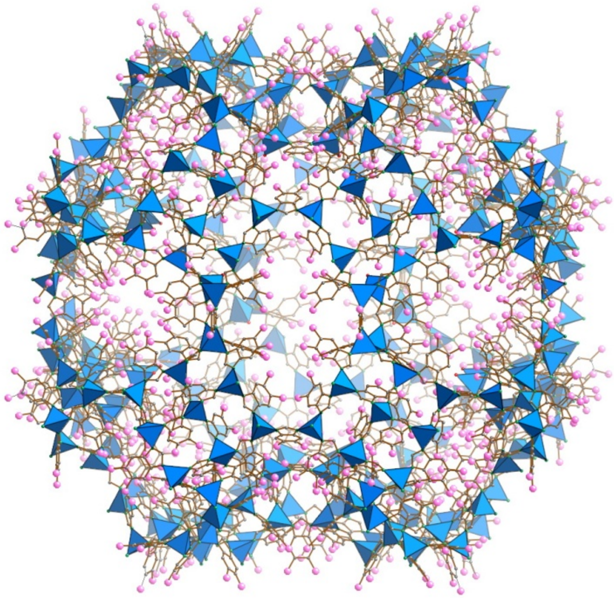
* Updated 6/1/2012

U.S. DEPARTMENT OF ENERGY | Office of Science

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

Vision statement

Using inexpensive custom-designed molecular building blocks, MEEM aims to create revolutionary new materials for highly efficient organic solar cells, next-generation supercapacitors, and efficient greenhouse gas capture systems.



RESEARCH PLAN AND DIRECTIONS

Widespread adoption of renewable energy technologies requires significant improvements in their efficiency and cost. MEEM will create new nanoscale materials that can efficiently generate, transport and store energy and mass. These materials will be used to improve the performance of organic solar cells, supercapacitors, and carbon capture systems.

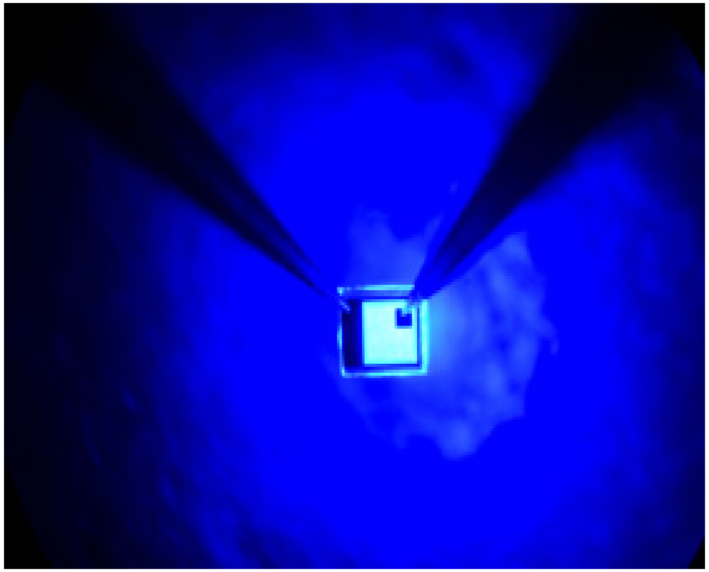
* Updated 7/16/2012

UCLA | Berkeley University of California | KU | NREL | EASTERN WASHINGTON UNIVERSITY

an Office of Basic Energy Sciences
Energy Frontier Research Center

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

A basic research program to discover and characterize new materials that control the interactions between light, electricity, and heat at the nanoscale, and to apply them to achieve higher efficiencies in photovoltaic solar cells, solid-state lighting, and thermoelectric conversion of heat into electricity.



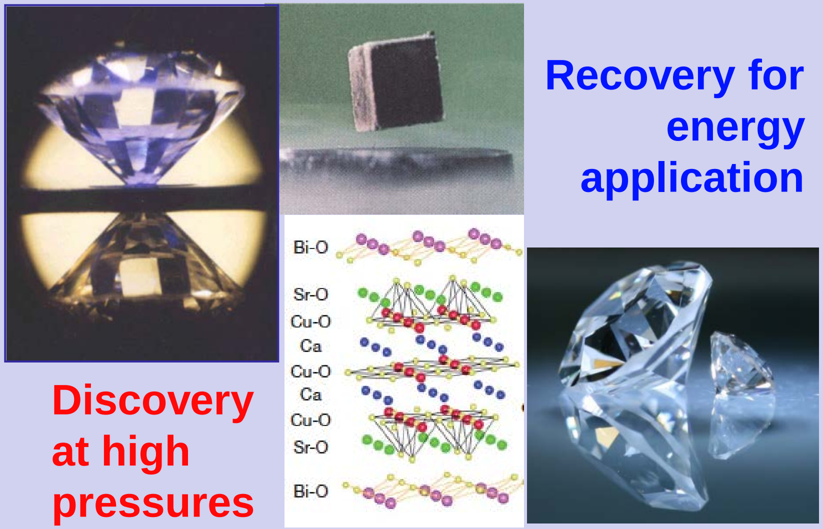
<u>Research thrusts</u>:

- **New materials and methods for control of the internal nanostructure for solution-processed, organic bulk heterojunction solar cells**
- **High efficiency semiconductor multiple-junction thin-film photovoltaics**
- **Bio-inspired, kinetically controlled, catalytic nanofabrication of heterojunction photovoltaics**
- **Semiconductor nonpolar white light sources with high luminous efficiencies**
- **Novel nanostructured thermoelectric materials for improved conversion of heat to electricity**

* Updated 5/8/2011

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

Vision: **The long-term future of the nation's energy relies upon transformative materials with extremely useful properties. The high-pressure environments represent a vast untapped frontier where the desired materials are waiting to be discovered.**



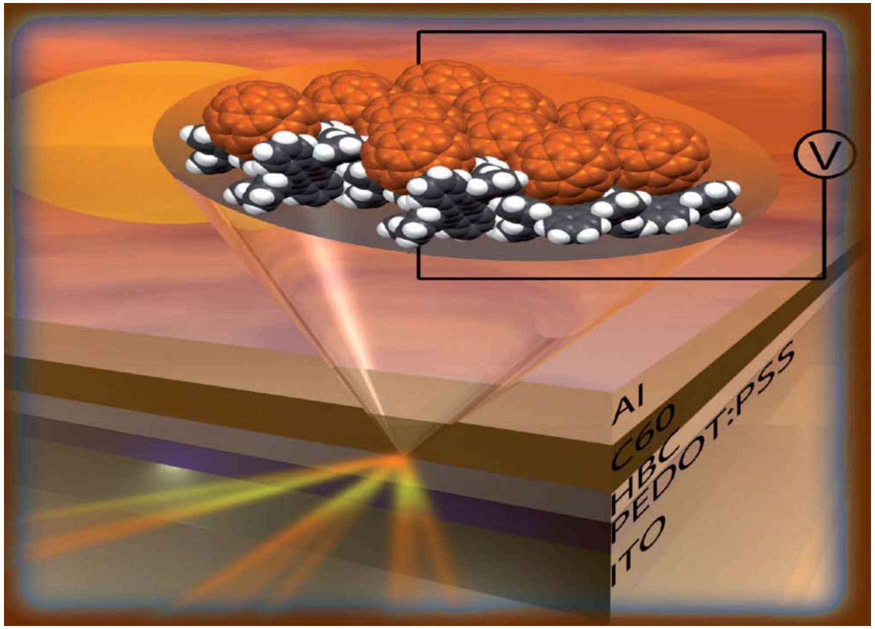
Research Plan: **High-pressure studies will be conducted for discoveries of novel materials and phenomena, including extremely efficient and clean fuels, record-high temperature superconductors, key components resistive to extremely harsh environments, etc. We will design alternative routes to bring the novel materials to ambient conditions for energy applications.**

* Updated 7/16/2012

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 and hybrid photovoltaic devices through fundamental understanding and through molecule-scale control of charge formation, separation, extraction, and transport.



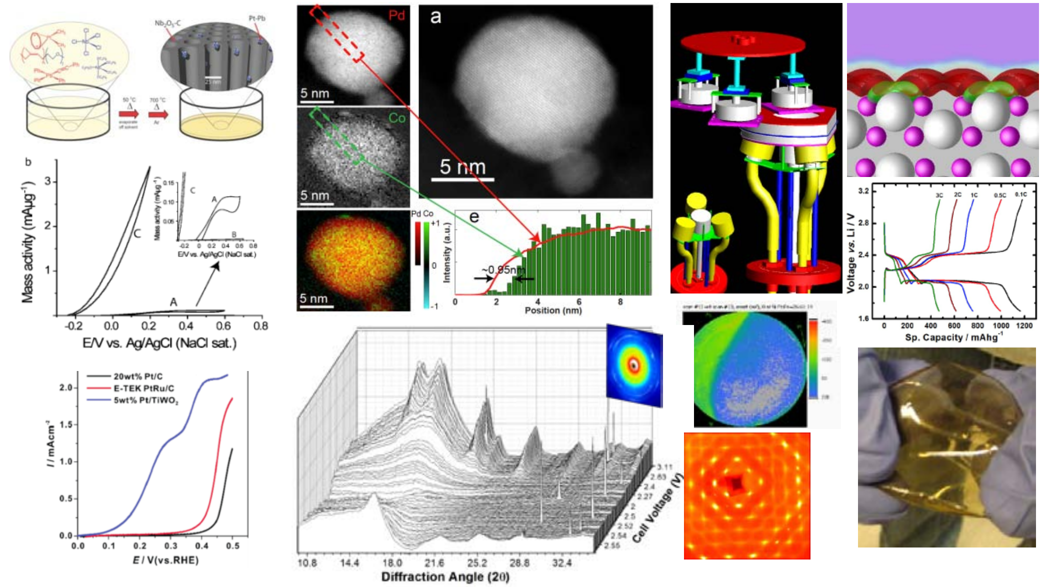
RESEARCH PLAN AND DIRECTIONS

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. New conducting materials such as graphene can transport these charges to macroscopic electrical systems, providing basis for revolutionary low cost, high efficiency devices.

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.



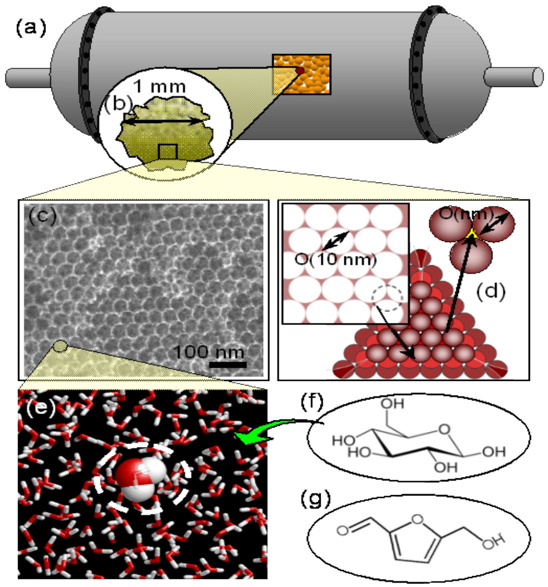
RESEARCH PLAN AND DIRECTIONS

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.

an Office of Basic Energy Sciences
Energy Frontier Research Center

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

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

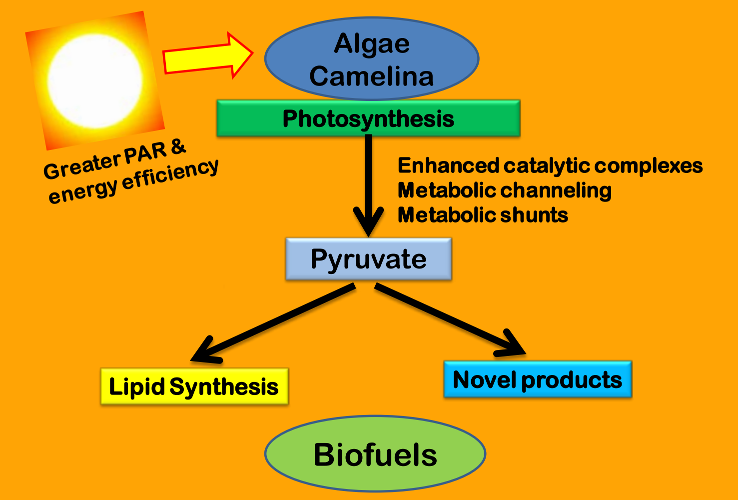
Biomass feedstocks vary considerably with source, and their transformation entails complex, multiscale reactions and processes. The CCEI members develop novel catalytic materials and processes, based on a fundamental understanding of the underlying chemistry, to set the foundations for the operation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

* Updated 7/16/2012

Center for Advanced Biofuel Systems
Jan Jaworski (Donald Danforth Plant Science Center)

The 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.

Center for Advanced Biofuel Systems



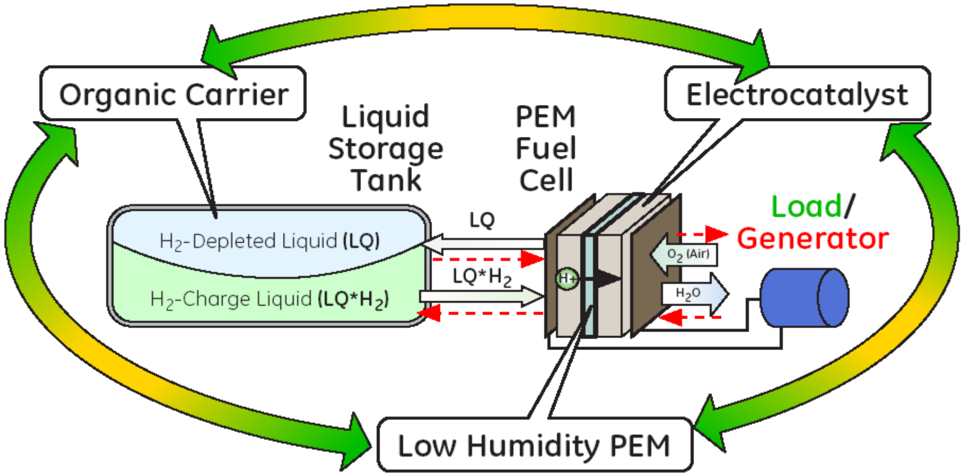
RESEARCH PLAN AND DIRECTIONS

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 flux and channeling towards lipid synthesis, and 3) engineer novel metabolic networks for biofuel production.

Center for Electrocatalysis, Transport Phenomena, and Materials for Innovative Energy Storage

Dr. Grigorii Soloveichik (GE Global Research)

The EFRC will develop the fundamental understanding of electrocatalysis, transport phenomena and membrane materials for an entirely new high-density energy storage system that combines the best properties of a fuel cell and a flow battery



RESEARCH PLAN AND DIRECTIONS

Main focus: - Effective (de)hydrogenation electrocatalysts

- Energy dense reversible organic carriers
- Water-free proton exchange membranes, transport of protons and electron
- Compatibility of cell components

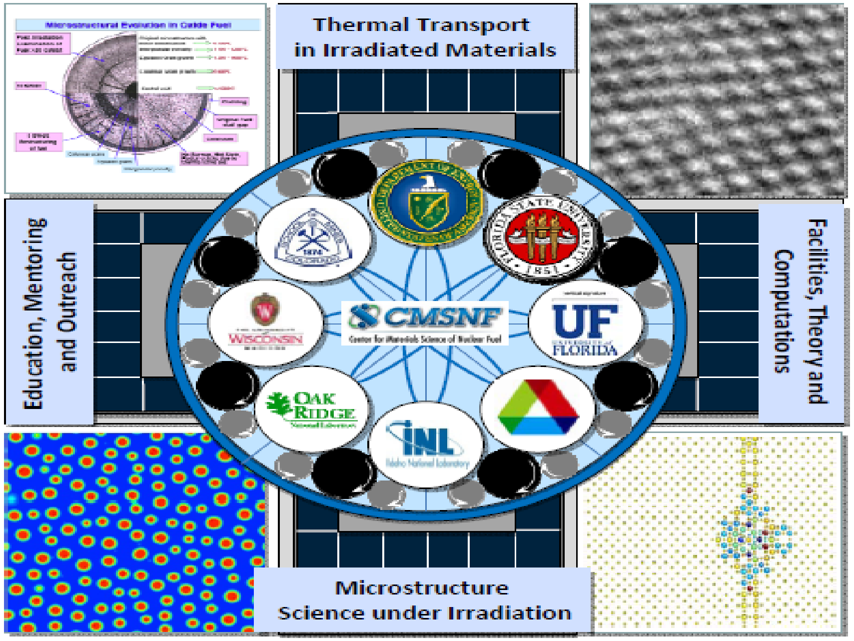
Approaches: Combination of modeling, synthetic chemistry and electrochemistry

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

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

EFRC Center for Materials Science of Nuclear Fuel
Todd Allen (Idaho National Laboratory)

***Vision Statement*: The Center for Materials Science of Nuclear Fuel will achieve a first-principles based understanding of the *impact of complex defect structures on thermal transport in irradiated nuclear fuels*, with UO_2 as a model fuel system.**



RESEARCH PLAN AND DIRECTIONS

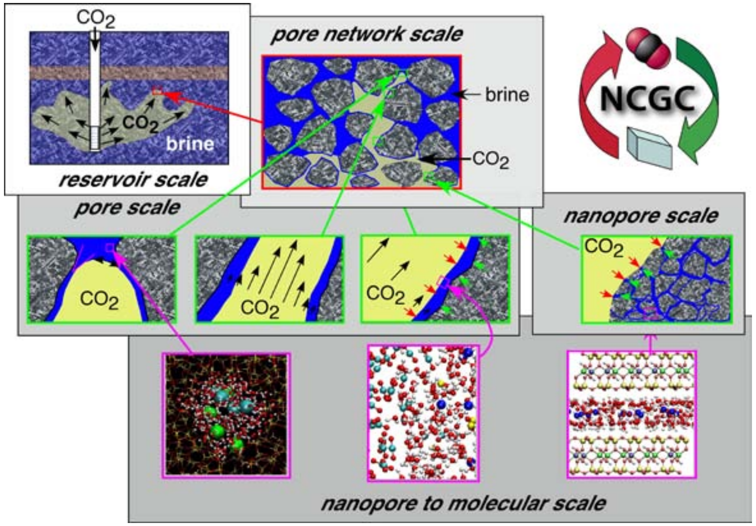
***Our research integrates the physics of thermal transport with the science of microstructure evolution in irradiated materials*; the center's research includes modeling and measurement of thermal transport in oxide fuels with different levels of impurities, lattice disorder and irradiation-induced microstructure, as well as a theoretical and experimental investigation of the evolution of disorder, stoichiometry and microstructure in nuclear fuel under irradiation.**

* Updated 12/20/2011

Center for Nanoscale Control of Geologic CO_2 (NCGC)

Donald J. DePaolo (LBNL/ESD)

VISION: **The NCGC Center's objectives are to 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 achieve a new level of prediction of long-term performance to enhance storage security and efficiency**



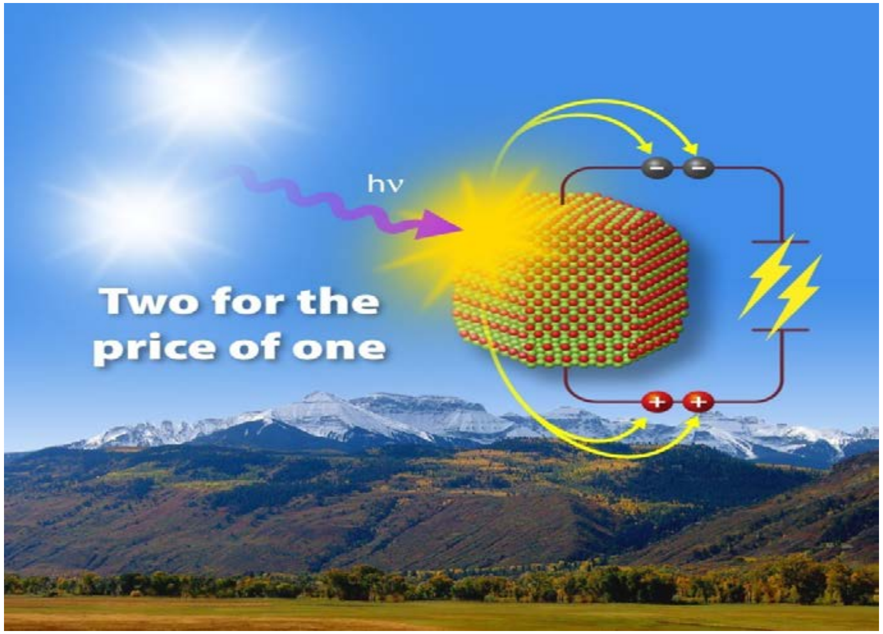
***RESEARCH DIRECTION*:** **Properties and interactions of complex fluids and minerals must be determined at elevated temperature and pressure, and effects at interfaces and in confined nano-scale pore spaces understood. Novel experimental and computational approaches, and unique DOE experimental facilities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

an Office of Basic Energy Sciences

Energy Frontier Research Center

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

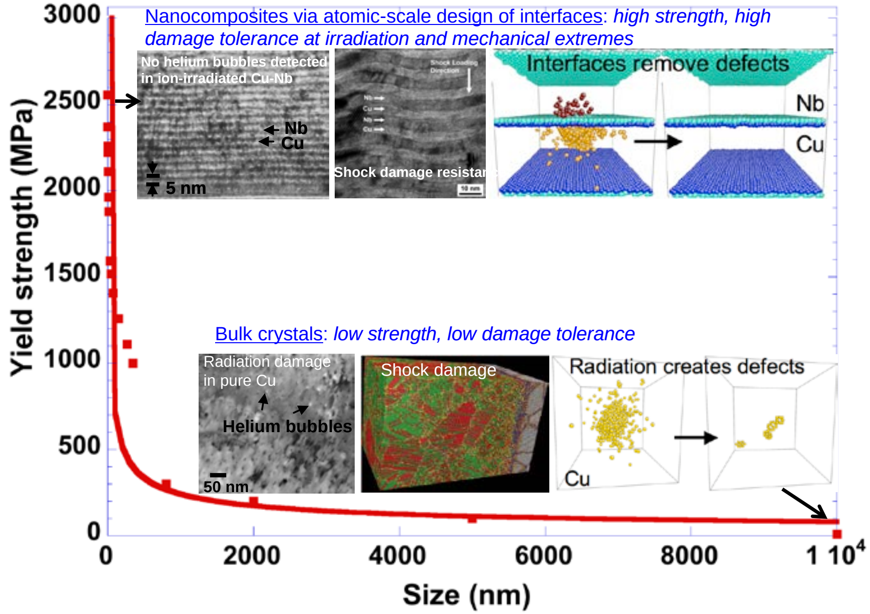
The major challenge is to reach or exceed thermodynamic efficiency limits via approaches such as band-structure engineering, carrier multiplication, plasmonic and photonic effects, and defect-tolerant excitonic transport. The potential outcome of this work is low-cost, high-efficiency photovoltaics based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

* Updated 7/16/2012

Center for Materials at Irradiation and Mechanical Extremes (CMIME)

Amit Misra (Los Alamos National Lab)

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.



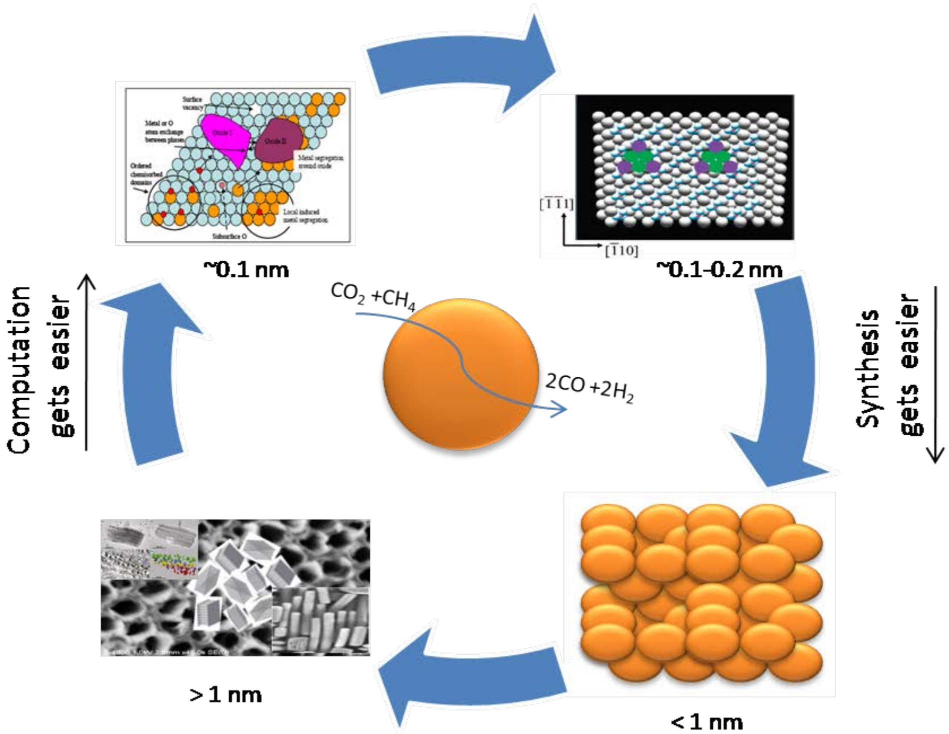
RESEARCH PLAN AND DIRECTIONS

CMIME is developing a fundamental understanding of how atomic structure and energetics of interfaces contribute to defect and damage evolution in materials, and will 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.

* Updated 12/20/2011

Center for Atomic-level Catalyst Design
James J. Spivey (Louisiana State University)

"Theoretical investigations guiding experiments on reactive surfaces"



RESEARCH PLAN AND DIRECTIONS

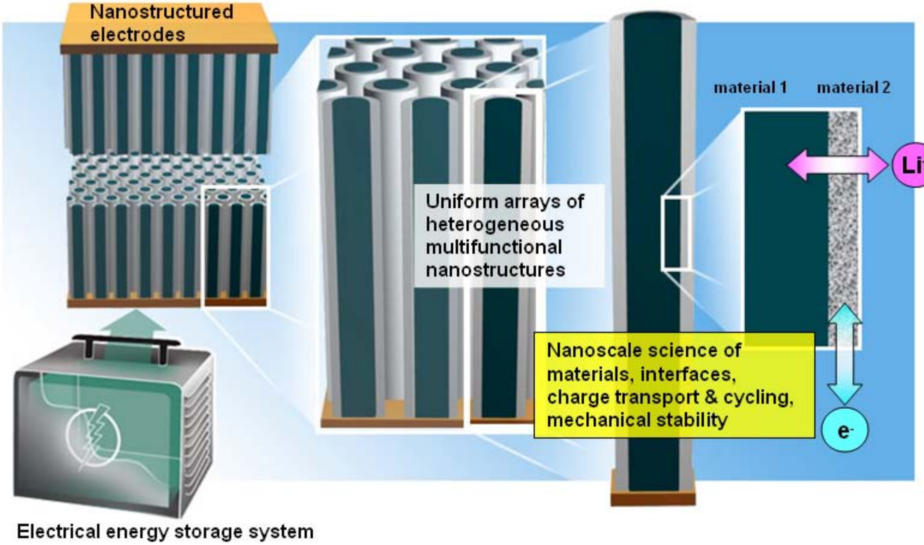
To develop next-generation computational and synthesis/characterization tools to design and prepare solid catalysts for energy-related conversion processes.

* Updated 4/24/2012

Nanostructures for Electrical Energy Storage (NEES)
Gary W. Rubloff, University of Maryland

NEES investigates nanostructures to provide the scientific foundation for batteries and supercapacitors with dramatically higher power and energy density to **power electric vehicles** and **store energy from renewable resources**.

www.efrc.umd.edu

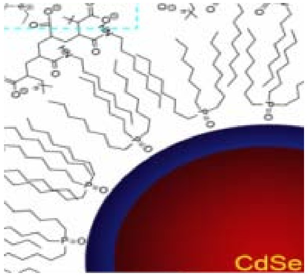


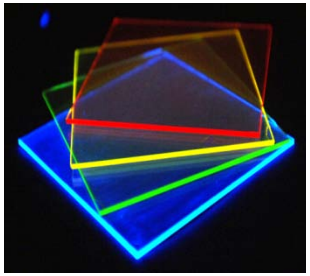
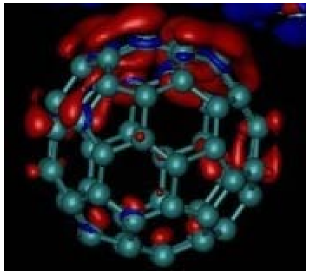
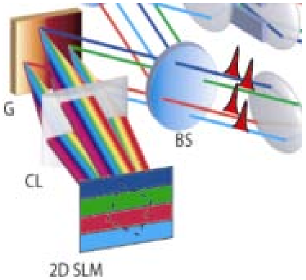
The Center…

- ***synthesizes nanosized structures*** **including carbon nanotubes, silicon nanowires, or thin layers of oxide materials to make composites that are mechanically strong and conduct high densities of ions and electrons.**
- ***designs new instruments*** **to measure properties of materials at the nanoscale inside electrochemical devices**
- ***develops new experimental and computational models*** **to clarify the mechanisms at work inside nanostructures for batteries.**

an Office of Basic Energy Sciences
Energy Frontier Research Center

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.

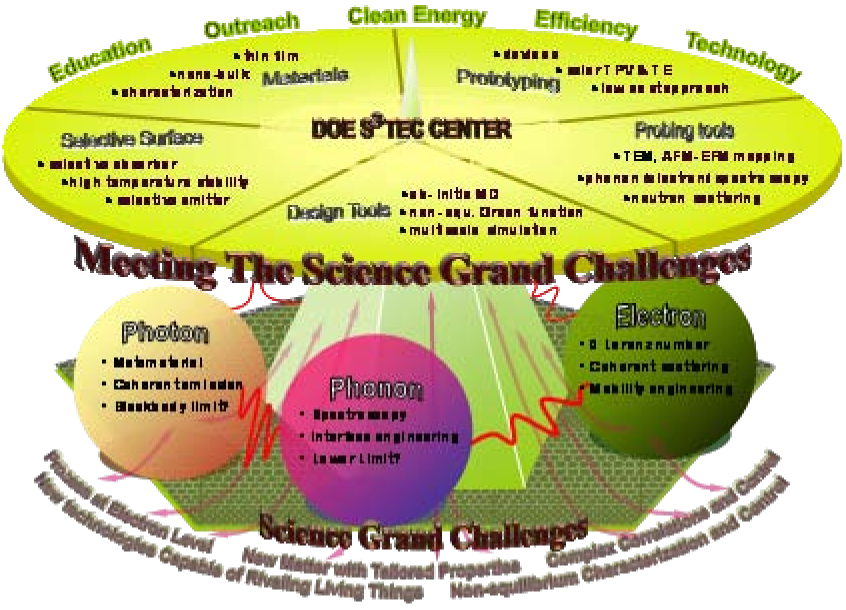
Our advances will be applied to low-cost solar cells and solid state lighting.

U.S. DEPARTMENT OF ENERGY | Office of Science

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

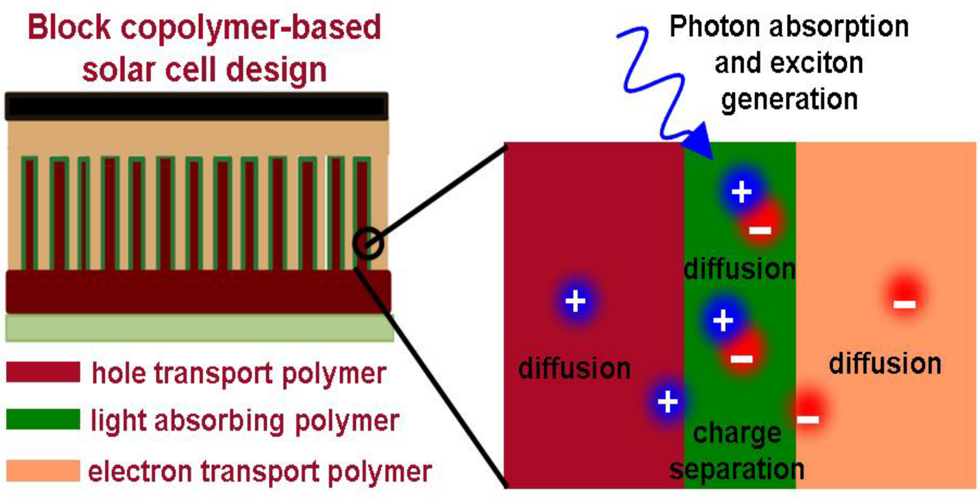
(1) Engineering electron and phonon transport in nanostructures to achieve high performance thermoelectric materials, (2) controlling photon absorption and emission for materials working at high temperatures, and (3) device prototyping to demonstrate the high efficiency and low cost potential of the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

an Office of Basic Energy Sciences
Energy Frontier Research Center

Polymer-Based Materials for Harvesting Solar Energy

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

Summary statement: Our goal is to maximize collection and conversion efficiency of a broad frequency range of the solar spectrum using directed self-assembly of polymer-based materials, to uncover basic physical principles that will allow design and fabrication of more effective and inexpensive photovoltaic devices.



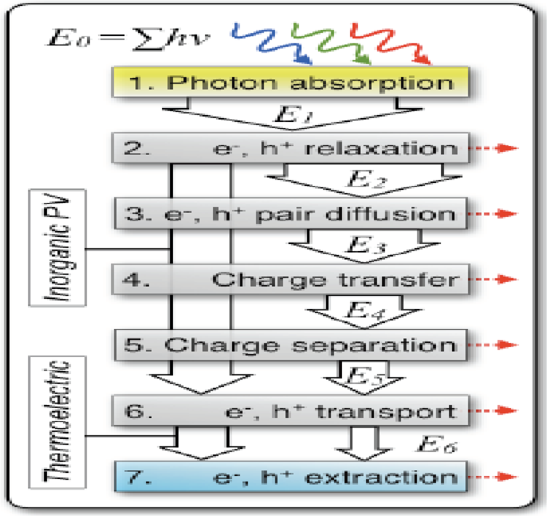
RESEARCH PLAN AND DIRECTIONS

Organic-based photovoltaics are relatively inexpensive and easy to fabricate, but have low efficiencies and do not last as long as is desirable. The Center's interdisciplinary research teams seek to maximize conversion of light to electrical charges, and to find and optimize the actual pathways of charge movement in organic-based devices. Such basic research discoveries are crucial to yield more economically viable organic photovoltaics.

CENTER FOR SOLAR AND THERMAL ENERGY CONVERSION

Peter F. Green (University of Michigan)

Researchers in the center for thermal and solar energy conversion (CSTEC) investigate fundamental processes that govern the efficiency of solar and thermal energy conversion in nanostructured, complex, and low-dimensional inorganic, hybrid, and organic materials



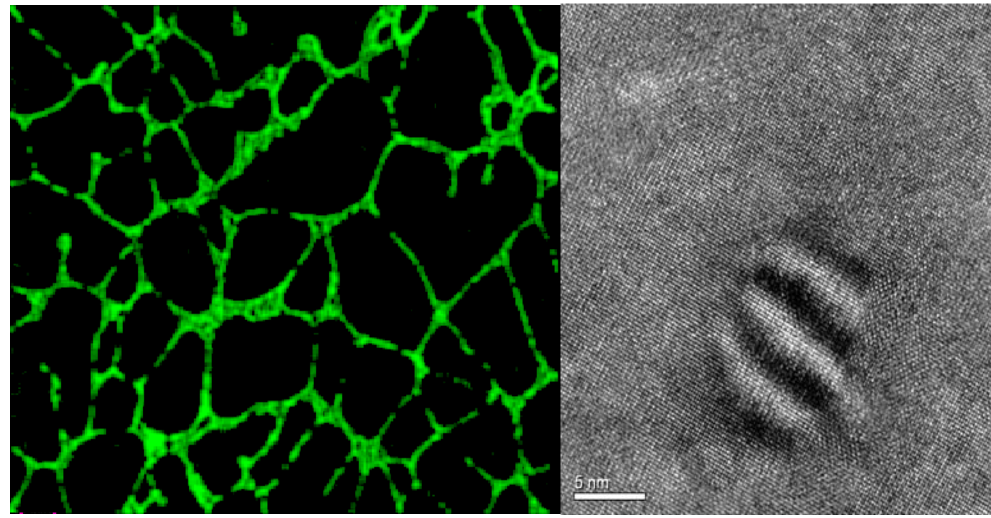
RESEARCH PLAN AND DIRECTIONS

Research is conducted in three areas:
(1) Inorganic PV investigations of site-controlled nanostructured materials: absorption phenomena and carrier transport; **(2) Thermoelectric** properties of single molecular junctions, quantum dots, wires, thin films and bulk skutterudites; **(3) Organic and Hybrid PV materials:** Absorption phenomena, molecular design (caged molecules, self-aligning polythiophene derivative molecules), nanoscale characterization, devices

U.S. DEPARTMENT OF ENERGY | Office of Science

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

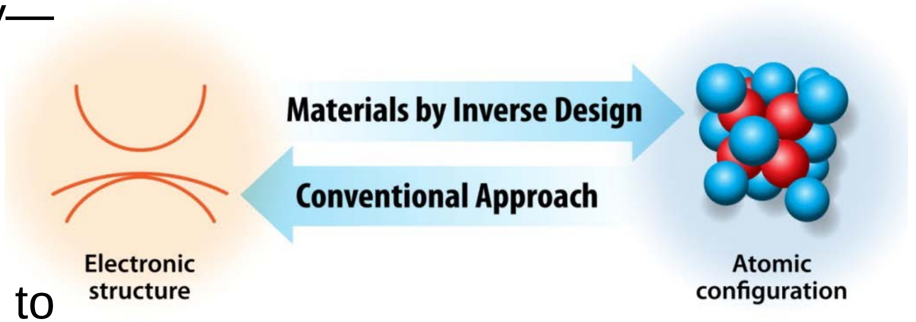
The Center for Revolutionary Materials for Solid State Energy Conversion will focus on the fundamental science of thermoelectricity. It will combine experimental, theoretical, and computational approaches to synthesize, characterize, and understand the nature of the thermo-electric energy conversion 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**
Outcomes:	**Deeper understanding of thermoelectric energy conversion**

Center for Inverse Design
Bill Tumas (NREL)

VISION: Revolutionary materials discovery—leading to better and even entirely new materials—by first (i) articulating needed material target properties, then (ii) using "Inverse Band Structure" quantum-mechanical methods and design principles to identify the structure having such properties, and (iii) using combinatorial and targeted materials synthesis to realize such new materials experimentally.



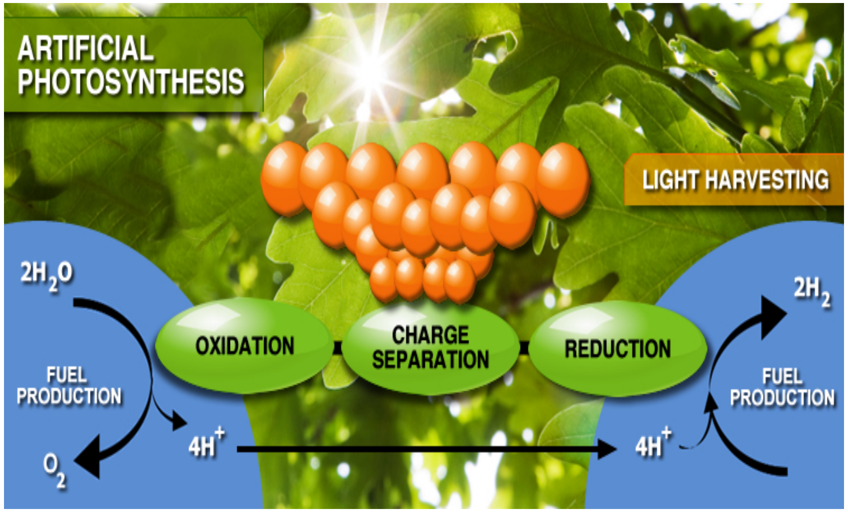
RESEARCH PLAN AND DIRECTIONS

We address the Materials by Inverse Design: Grand Challenge ("Given the desired property, find the structure and composition"), rather than using the conventional approach ("Given the structure, find the electronic properties"). Target properties include new semiconductor absorbers, transparent conductors, and nanostructures for energy sustainability. We will study predictions iteratively by various synthetic approaches (e.g., high-throughput parallel materials science).

Center for Solar Fuels
Thomas J. Meyer (UNC Chapel Hill)

UNC EFRC VISION

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.



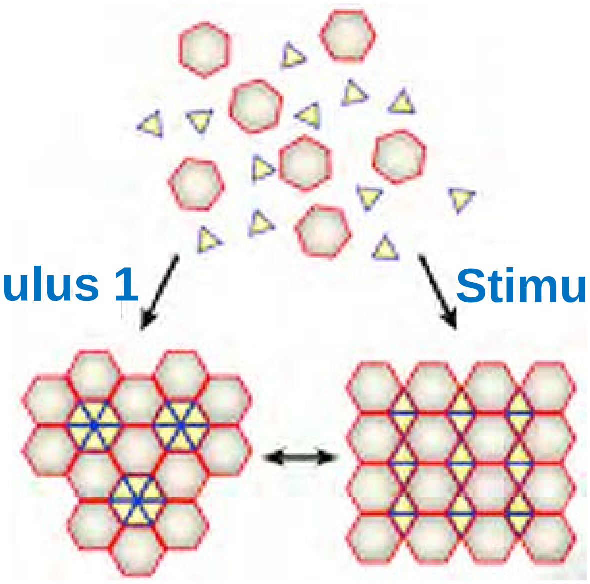
RESEARCH PLAN AND DIRECTIONS

Research in Solar Fuels 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.

* Updated 02/15/2012

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

The goal of NERC is to synthesize and characterize fundamentally new classes of materials under conditions <u>far-from-equilibrium</u> that are relevant to solar energy conversion, catalysis, and storage of electricity and hydrogen. These "<u>adaptive</u>" materials, while structurally robust, are able to change and optimize their own performance in response to <u>external stimuli</u>.



RESEARCH PLAN AND DIRECTIONS

By combining theory with cutting edge nanotechnology and/or self-assembly, materials that operate and/or maintain themselves away from thermodynamic equilibrium will be created with the purpose of shifting from "<u>static</u>," equilibrium structures to "<u>dynamic</u>," multi-purpose materials.

Argonne-Northwestern Solar Energy Research (ANSER) Center

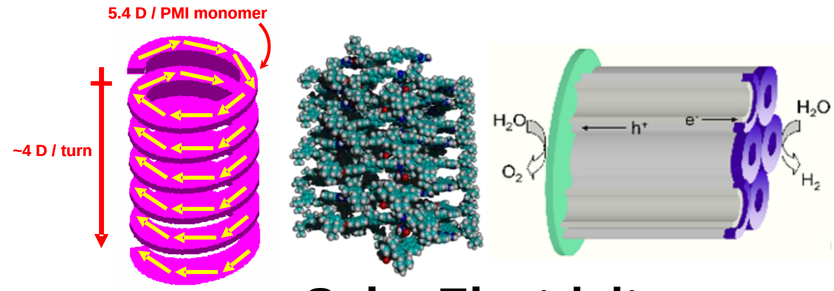
Michael R. Wasielewski (Northwestern University)

U.S. DEPARTMENT OF ENERGY | Office of Science

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.

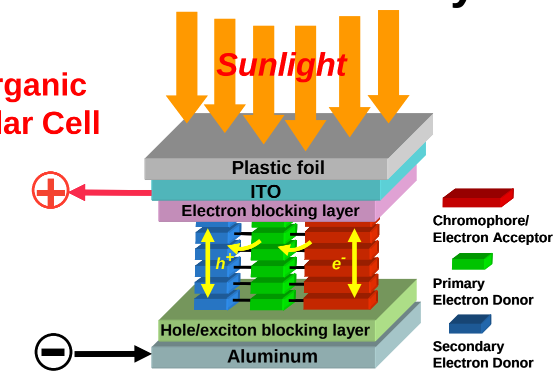
Solar Fuels

Artificial Photosynthetic Systems

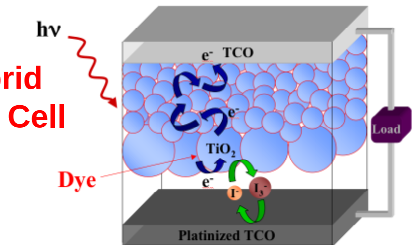


Solar Electricity

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.

Yale University | ILLINOIS University of Illinois at Urbana-Champaign | Northwestern University | Argonne-Northwestern ANSER Solar Energy Research Center | Argonne National Laboratory | The University of Chicago

an Office of Basic Energy Sciences Energy Frontier Research Center

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

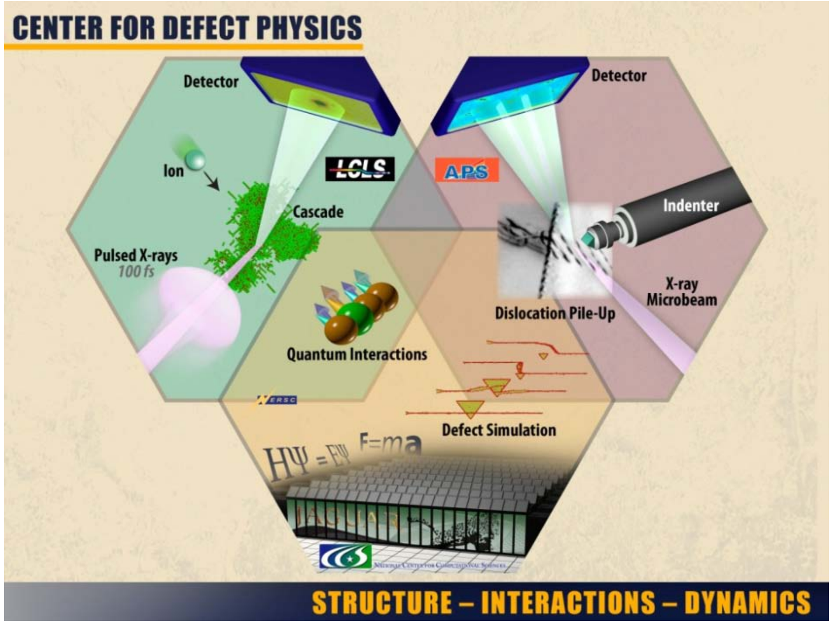
This EFRC blends experimental and computational approaches to study highly complex actinide materials (such as materials for fuels, waste forms, or separations), with an emphasis on the nanoscale. The behavior and properties of such materials in extreme environments of radiation and pressure is a major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

* Updated 6/1/2012

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; The Ames Laboratory — Creating Materials & Energy Solutions — U.S. Department of Energy; The Ohio State University; Lawrence Livermore National Laboratory; Carnegie Mellon

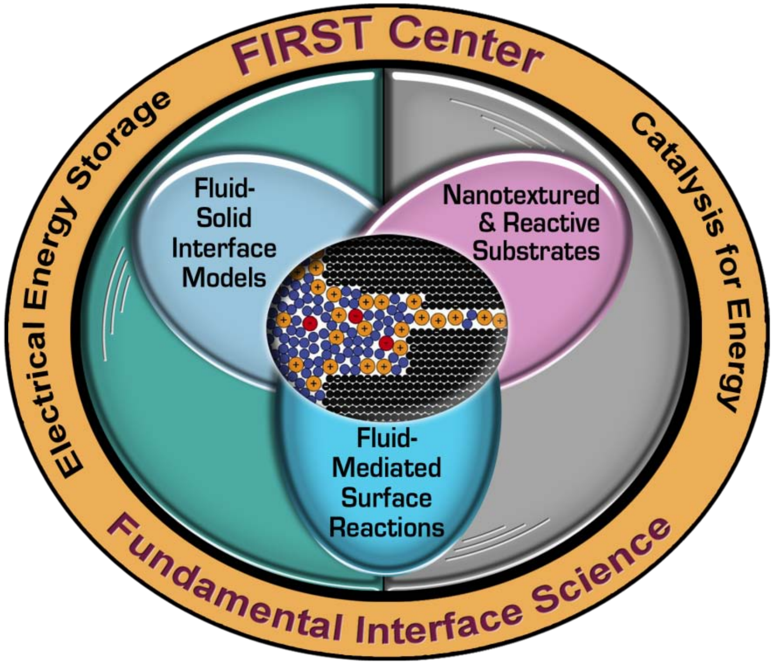
an Office of Basic Energy Sciences
Energy Frontier Research Center

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

U.S. DEPARTMENT OF ENERGY | Office of Science

FIRST Center Vision and Goal

To develop quantitative and predictive models of the unique nanoscale environment at fluid-solid interfaces to enable transformative advances in electrical energy storage and heterogeneous catalysis.



RESEARCH PLAN AND DIRECTIONS

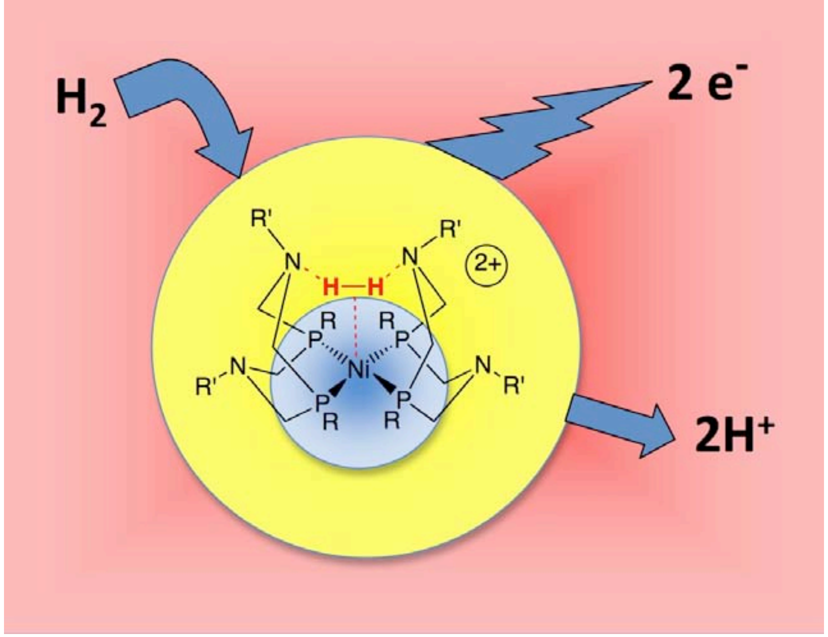
Our multidisciplinary team integrates advanced materials synthesis, neutron and X-ray scattering, various spectroscopies, macroscopic experiments, and multiscale molecular modeling to provide a predictive capability for controlling and designing new interfacial systems for 21st century energy needs.

Oak Ridge National Laboratory · Vanderbilt University · Argonne National Laboratory · Suffolk University · Drexel University · Penn State · Georgia State University · Northwestern University · University of Virginia

an Office of Basic Energy Sciences
Energy Frontier Research Center

Center for Molecular Electrocatalysis
R. Morris Bullock
(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.

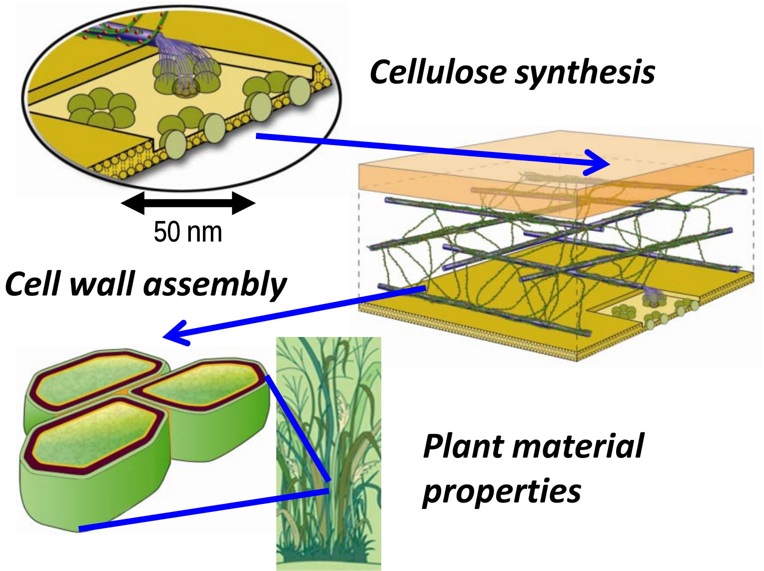


RESEARCH PLAN AND DIRECTIONS

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 regulate the movement of protons and electrons to enhance the rates of electrocatalysts.

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.



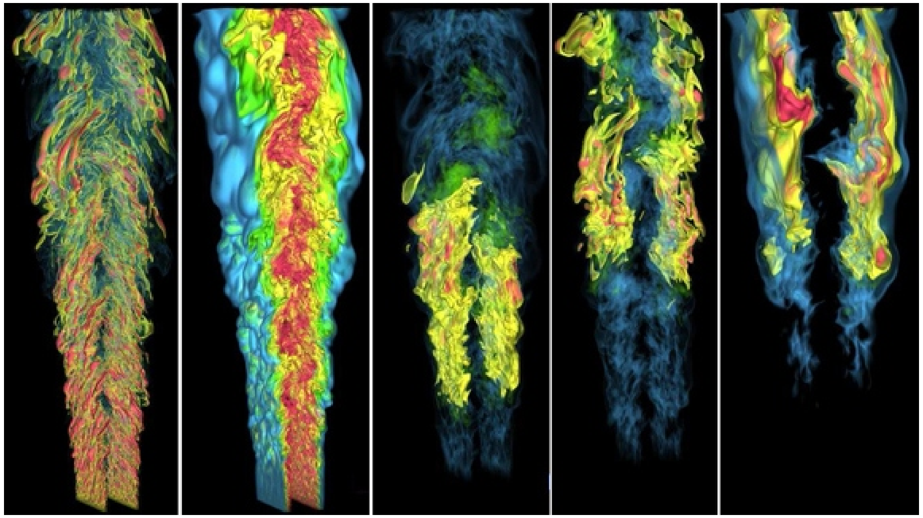
RESEARCH PLAN AND DIRECTIONS

With a unique mix of molecular biologists, chemists, physicists, engineers and modelers, CLSF is tackling key questions of lignocellulose structure and formation. This is an important 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)

Overarching Goal

The development of a validated, *predictive*, multi-scale combustion modeling capability to optimize the design and operation of evolving fuels in advanced engines for transportation applications.



RESEARCH PLAN AND DIRECTIONS

- ***Advance fundamental understanding and practice of combustion and fuel science***
- ***Create experimental validation platforms and databases for kinetics, thermochemistry, transport processes, and flame structure***
- ***Enable automated kinetic model generation and reduction***
- ***Implement validated, multi-scale, quantitative prediction methods***
- ***Establish a knowledge highway connecting the Center, academic and research institutions, and the transportation and fuel industries***
- ***Train the next generation of combustion scientists***

* Updated 07/16/2012

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

Maureen McCann (Purdue University)

U.S. DEPARTMENT OF ENERGY | Office of Science

SUMMARY STATEMENT

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

RESEARCH PLAN AND DIRECTION

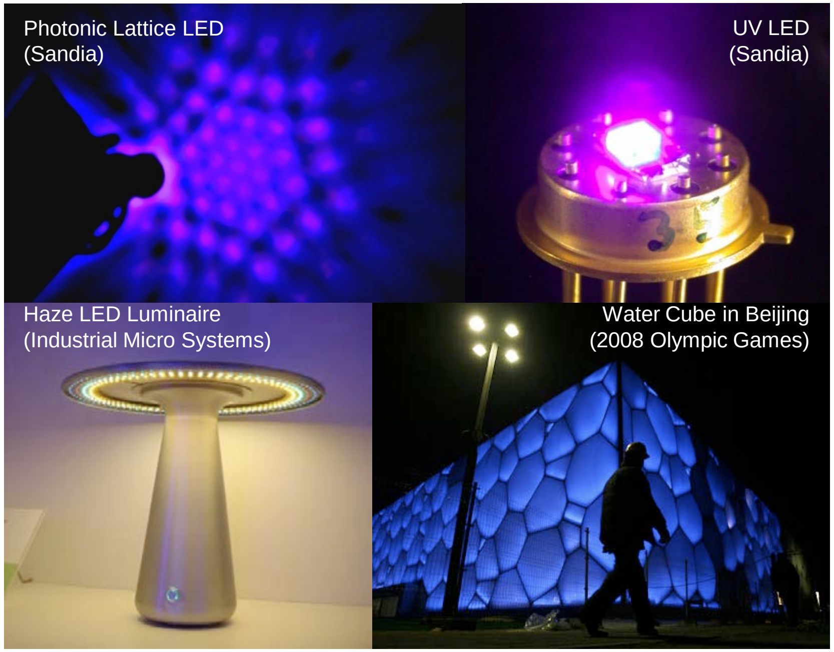
We will optimize the energy and carbon efficiencies of advanced biofuels conversion by the synergistic design of biomass and the thermal and chemical conversion processes. By applying new catalytic transformations, achieving an atomic-to-macromolecular scale understanding of the biomass:catalysts interaction, and tailoring biomass for highly efficient direct catalytic conversion, we will *more than double* the carbon captured into energy-rich advanced hydrocarbon fuels and *expand to* other high-value products.

C3Bio | Purdue University Discovery Park | UT | NREL | Northeastern University | Argonne National Laboratory

an Office of Basic Energy Sciences Energy Frontier Research Center

EFRC for Solid-State Lighting Science (SSLS)
Michael E. Coltrin (Sandia National Labs)

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.**

* Updated 02/15/2012

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

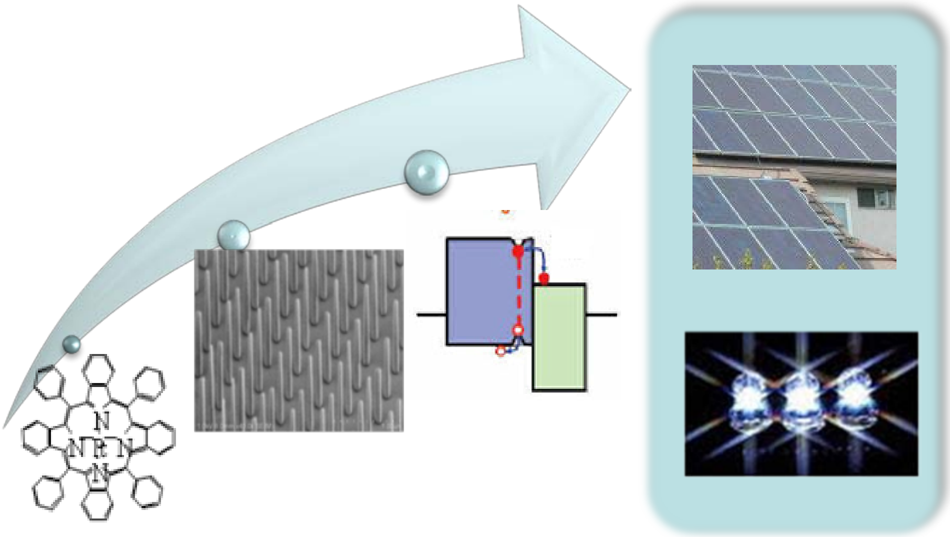
The aim of this EFRC is to establish foundations of understanding and control science that enable the prescriptive design and ordered synthesis of the local compositions, interfaces, and morphology of heterogeneous material systems for specific functional behavior and system performance.

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.

Center for Energy Nanoscience (CEN)
P. Daniel (Dan) Dapkus (USC)

The Center for Energy Nanoscience will explore organic and nano - structure materials for low cost, high efficiency solar cells and light emitting diodes (LEDs). CEN's scientists will create innovative new materials and novel device designs that follow from an understanding of the fundamental properties of these materials that control performance.



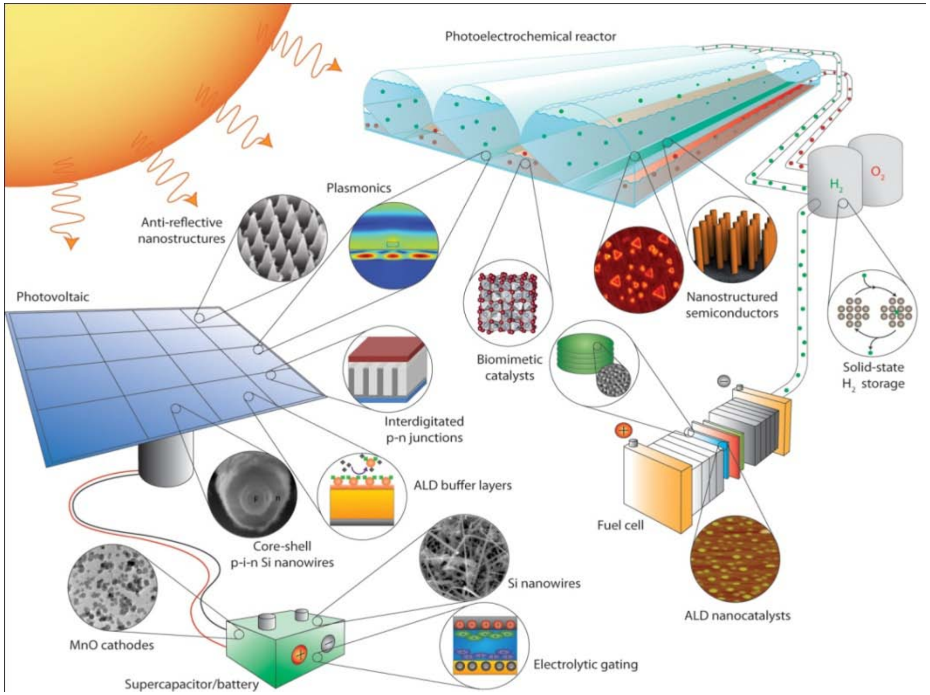
RESEARCH PLAN AND DIRECTIONS

- **Increase efficiency and reduce cost of solar cells and LEDs to create technologies that are cost competitive with the incumbents.**
- **Develop new knowledge in semiconductor nanoscience, organic molecule design, and device design to transform the science and technology of low cost, efficient device designs.**

Center on Nanostructuring for Efficient Energy Conversion (CNEEC)

Stacey Bent and Fritz Prinz (Stanford)

CNEEC seeks to understand how nanostructuring can enhance efficiency of energy conversion, 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 systems.



.

RESEARCH PLAN AND DIRECTIONS

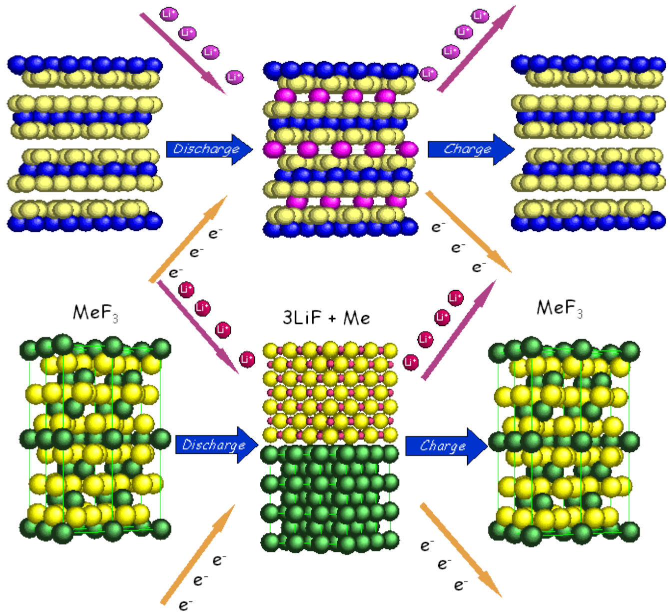
We use nanostructuring to tune thermodynamic potentials, enhance kinetics, manage photonics, and accelerate charge transport in materials, each of which contributes to improved efficiency and performance in energy conversion.

U.S. DEPARTMENT OF ENERGY | Office of Science

Northeastern Center for Chemical Energy Storage (NECCES)

M. Stanley Whittingham (Stony Brook University)

Summary statement: A fundamental understanding of how key electrode reactions occur, and how they can be controlled is being 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.

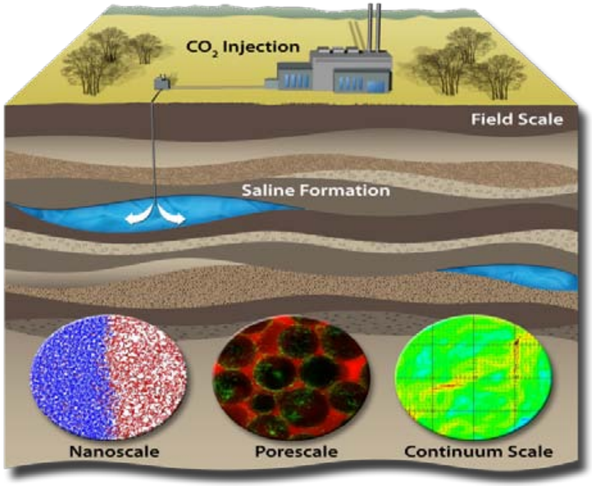


RESEARCH PLAN AND DIRECTIONS

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.

Center for Frontiers of Subsurface Energy Security
Gary A. Pope (The University of Texas)

The Center for Frontiers of Subsurface Energy Security (CFSES) is pursuing scientific understanding of multiscale, multiphysics processes to successfully predict the behavior of CO_2 and other byproducts of energy production 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.

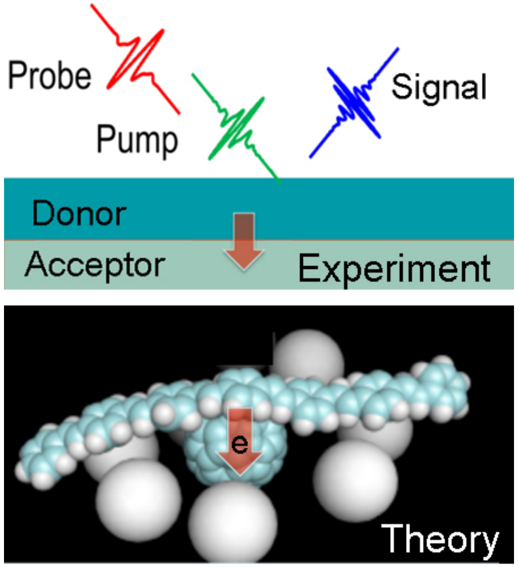
Unique aspects: The uncertainty and complexity of fluids in geologic media from the molecular scale to the basin scale.

Outcome: Better understanding of long term behavior of subsurface storage.

Understanding Charge Separation and Transfer at Interfaces in Energy Materials

Peter J. Rossky (Univ. of Texas-Austin)

This EFRC aims to elucidate the critical interfacial charge separation/ transfer processes that underpin the function of highly promising molecular materials for organic photovoltaic (OPV) and electrical-energy-storage (EES) applications.



RESEARCH PLAN AND DIRECTIONS

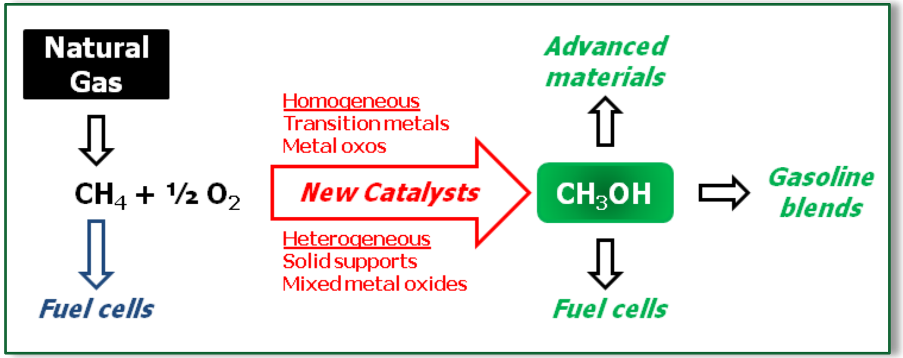
We will use newly developed experimental techniques (including interface-specific laser spectroscopy and in situ optical microscopy) coupled with advanced theoretical methods (e.g., nonadiabatic electron dynamics) to answer key outstanding questions on charge separation and transfer for solar cells and battery materials.

* Updated 6/1/2012

Center for Catalytic Hydrocarbon Functionalization (CCHF)

T. Brent Gunnoe (University of Virginia)

The CCHF facilitates collaborations among research groups with varied expertise to *develop new methods of activating and functionalizing hydrocarbons* for the production of fuels for the future.



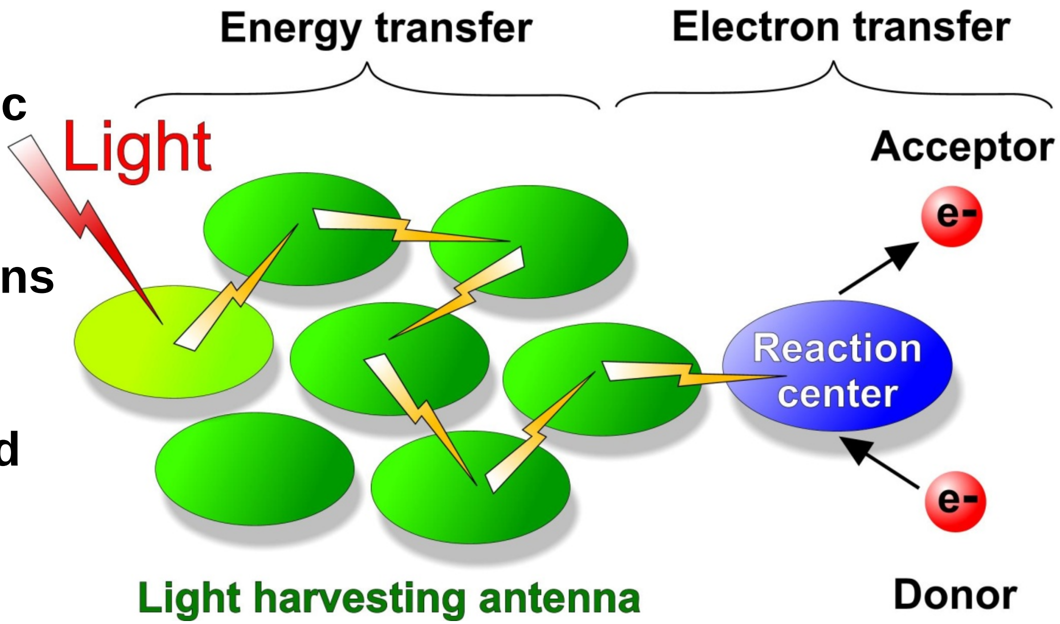
RESEARCH PLAN AND DIRECTIONS

The CCHF will design, synthesize, and test new catalysts for the selective transformation of hydrocarbons into value-added products. Multiple approaches, in conjunction with computation, are being explored including homogeneous transition metal catalysts, biomimetic metal oxo catalysts, solid supports for homogeneous catalysts, and heterogeneous catalysts. These new catalyst technologies could be applied to industrial processes for fuel production and electrochemical processes for fuel cell operation.

* Updated 7/16/2011

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

PARC aims to understand the basic scientific principles that govern solar energy collection by photosynthetic organisms and plans to use this knowledge to enhance natural antenna systems and to fabricate biohybrid and bioinspired systems for light-harvesting.



PARC will investigate:

1. **Natural Antennas to determine and manipulate the antenna size and composition to maximize photosynthetic efficiency.**
2. **Biohybrid Antennas to design proof-of-principle biohybrid architectures for energy collection and storage.**
3. **Bioinspired Antennas for fabrication of micron-scale arrays for efficient solar light harvesting, energy transfer and trapping.**

* Updated 6/1/2012

GRAND CHALLENGES INDEX

BASIC RESEARCH NEEDS INDEX

TOPICAL INDEX

EXPERIMENTAL AND THEORETICAL METHODS INDEX