U.S. Department of Energy

Energy Frontier Research Centers

One Page Overviews

Office of Science
8/30/2012
Revised on 10/01/2013

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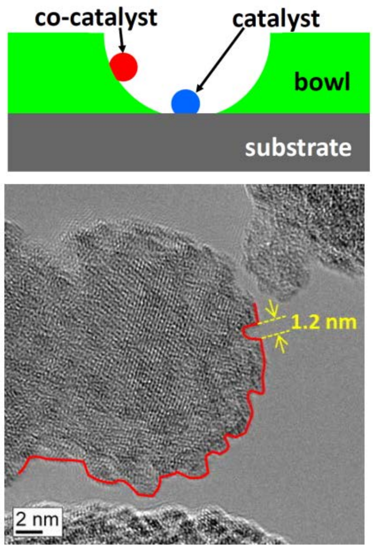
Ordered by Institution and then by Director

Institute for Atom-efficient Chemical Transformations (IACT)

Christopher L. Marshall (Argonne National Laboratory)

***Mission Statement**: IACT is addressing the key catalytic conversions that could improve the efficiency of producing fuels from biomass. This Center is focusing on advancing the science of catalysis for the efficient conversion of energy resources into usable forms. IACT's goal is to find ways to achieve control and efficiency of chemical conversions comparable to those in Nature.*

Atomically-precise metal catalysts located in nanobowl structures (at right) can be used to both isolate and stabilize nanostructured catalysts under severe bioprocessing conditions.



RESEARCH PLAN AND DIRECTIONS

- **Acquire fundamental understanding of catalytic processes for the selective removal of oxygen from biomass.**
- **Develop synthetic control of catalyst structures at the atomic and nanometer length scale. Synthesis of three-dimensional nanostructured catalysts**
- **Understand how catalyst structure evolves in a reactive environment**

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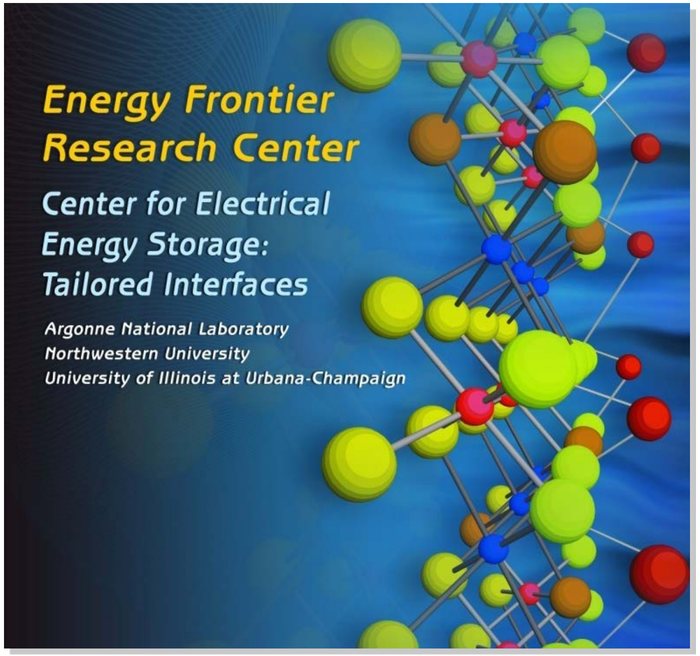
Center for Electrical Energy Storage
Michael Thackeray (Argonne National Laboratory)

***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.

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Center for Bio-Inspired Solar Fuel Production
Devens Gust (Arizona State University)

The goal of BISfuel is to construct a complete artificial photosynthetic system for solar-powered production of fuels such as hydrogen via water splitting. Design principles are drawn from the fundamental concepts that underlie photosynthesis – the natural energy conversion process responsible for fossil fuels such as coal, oil and natural gas.

RESEARCH PLAN AND DIRECTIONS

The chemistry of natural photosynthetic reaction centers, water oxidation proteins, and hydrogen-producing enzymes is being incorporated into nanoscale artificial constructs that oxidize water and make hydrogen and oxygen using sunlight. Hydrogen is vital for production of liquid fuels such as gasoline, and can be employed for making renewable fuels from carbon dioxide, or as an energy source on its own.

ASU Arizona State University | BISfuel

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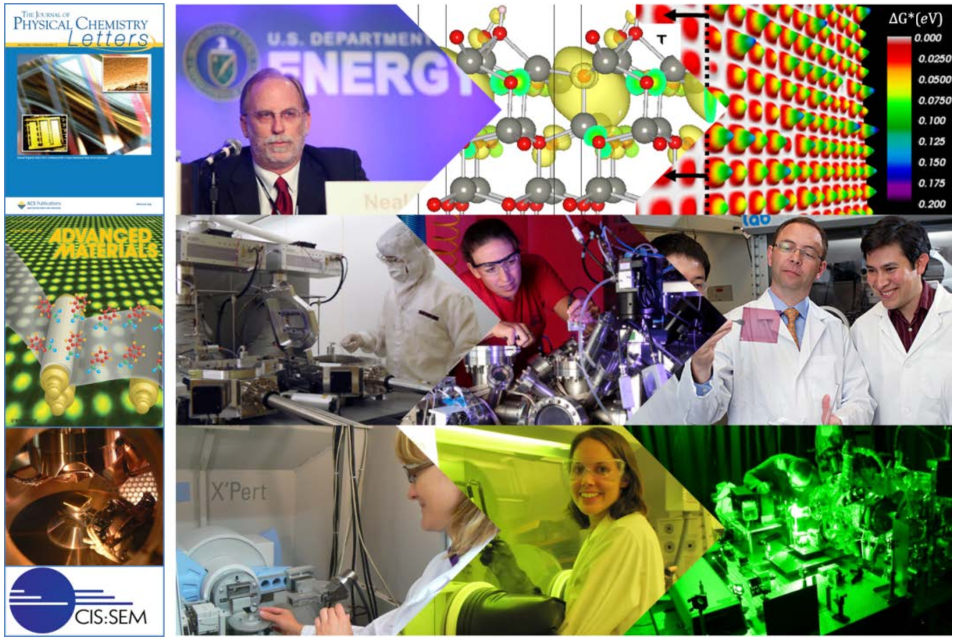
Center for Interface Science: Solar Electric Materials (CISSEM)

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://www.solarinterface.org/



RESEARCH PLAN AND DIRECTIONS

CISSEM is focused on creating an understanding of the electronic properties of interfaces between molecular semiconductors and electrical contact or interlayer materials that lead to efficient charge harvesting and improved thin-film PV performance. We are an integrated, multi-investigator effort combining five institutions.

The University of Arizona | Georgia Tech | NREL National Renewable Energy Laboratory | Princeton University | University of Washington | CIS:SEM

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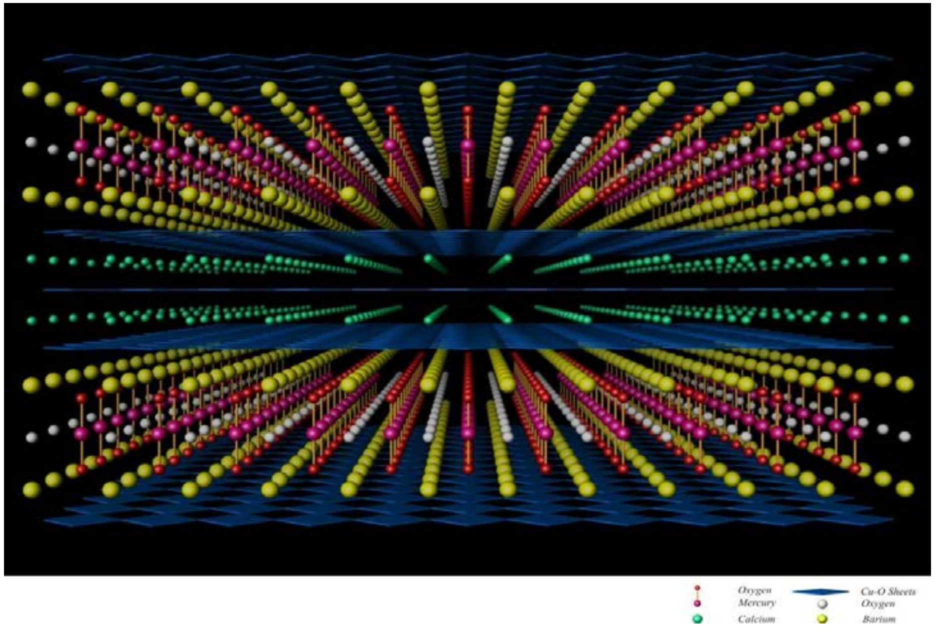
Center for Emergent Superconductivity (CES)
J.C. Séamus Davis (Brookhaven National Lab)

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.



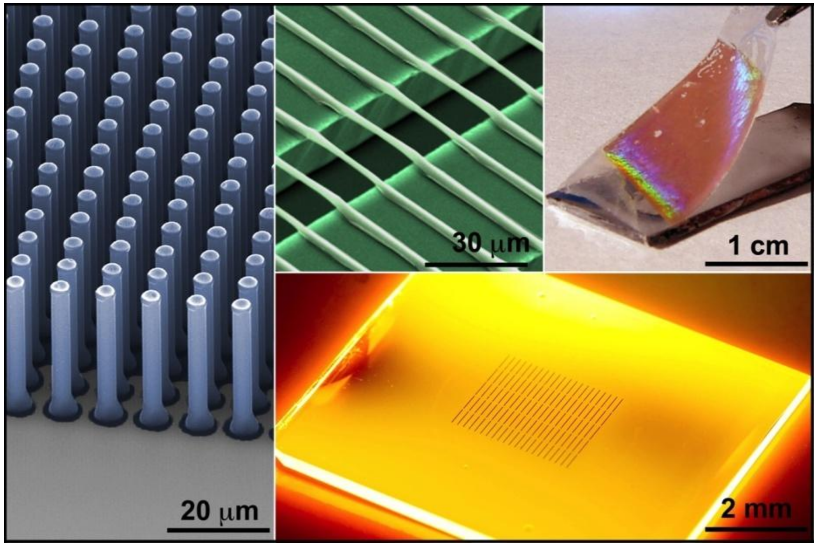
CES RESEARCH PLAN AND DIRECTIONS

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 and design for solar energy conversion.

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.



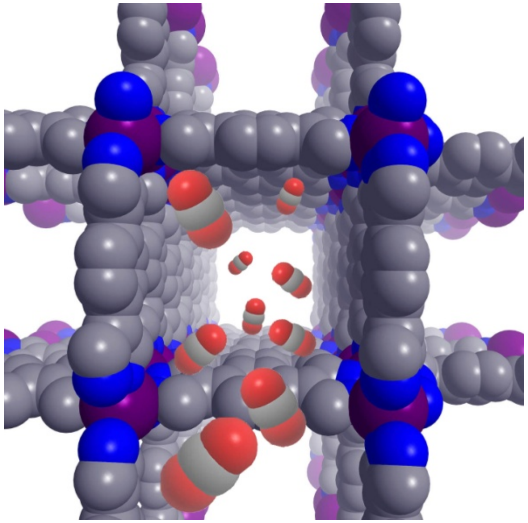
RESEARCH PLAN AND DIRECTIONS

Challenge: Establish fundamental photonic principles for light absorption, propagation and emission in complex dielectric, plasmonic and metamaterial structures. Approach: Design and synthesize complex materials for increased solar absorption, optical frequency conversion, and spontaneous emission enhancement. Outcome: Photonic principles that have enabled record photovoltaic 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)

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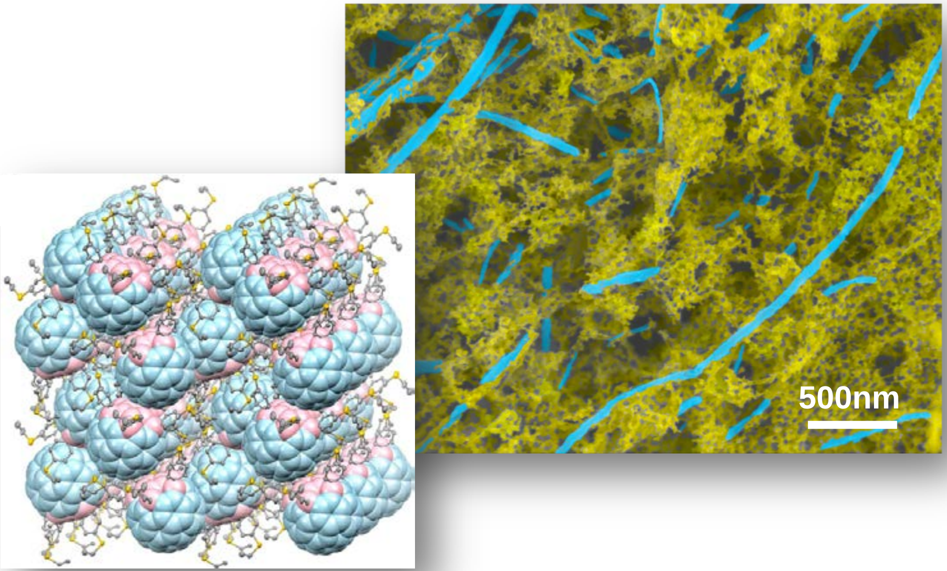
VISION STATEMENT

Using inexpensive custom-designed molecular building blocks, MEEM aims to create revolutionary new materials with self-assembled multi-scale architectures that will enable high performing energy generation and storage applications.



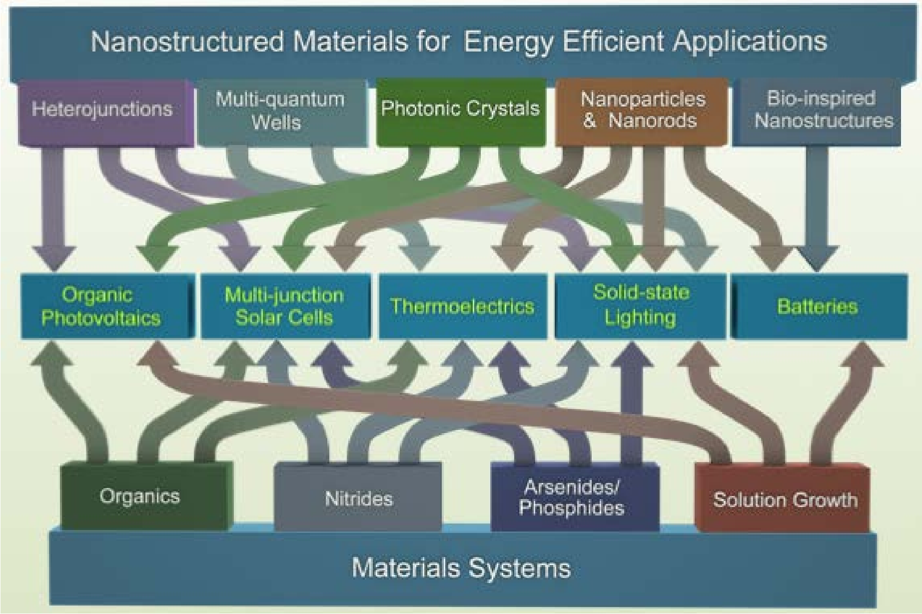
RESEARCH PLAN AND DIRECTIONS

Widespread adoption of renewable energy technologies requires significant improvements in their efficiency and cost. MEEM will conduct systematic studies of the fundamental mechanisms of carrier generation, energy conversion, as well as transport and storage of charge and mass in tunable, architectonically complex materials designed from the molecular and nanometer level. These materials will be used to significantly improve the performance of organic solar cells and supercapacitors.

UCLA · Berkeley University of California · NREL · University of Washington · KU · Eastern Washington University

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, energy storage and thermoelectric conversion of heat into electricity.

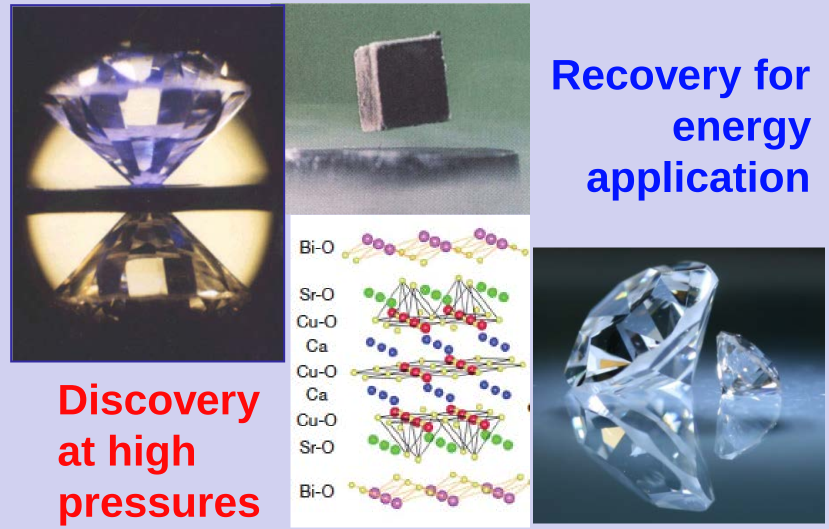


Research thrusts:

- **Conjugated polymer and small molecule semiconductor blends for organic solar cells.**
- **High efficiency semiconductor multi-junction thin-film solar cells.**
- **Nanofabrication of electrodes for high energy durable lithium ion batteries.**
- **Innovative materials and devices for LEDs with high luminous efficiency.**
- **Novel nanostructured thermoelectric materials for improved conversion of heat to electricity.**

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.**

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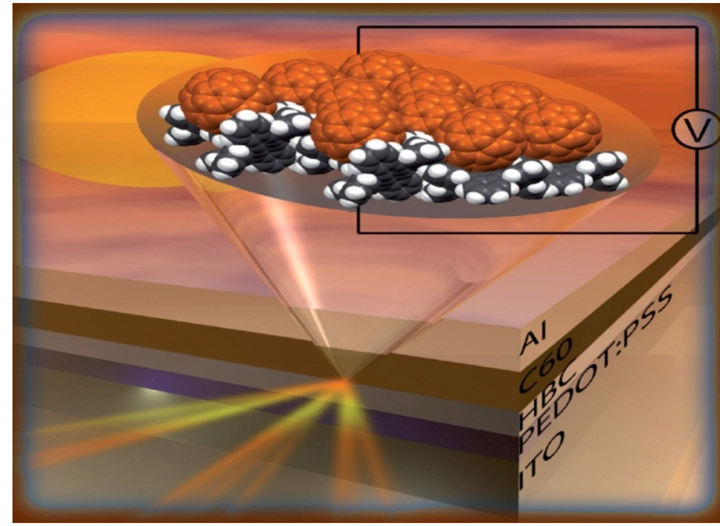
Re-Defining Photovoltaic Efficiency Through Molecule Scale Control

James Yardley (Columbia University)

The Columbia EFRC is creating 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 allow us to design systems for efficient photovoltaic generation and separation of charges. New materials including new molecular quantum dots and two-dimensional molecular sheets that can function as conductors (graphene), insulators (boron nitride), or semiconductors (molybdenum sulfide) allow nanoscale control of charge creation, separation, and extraction to provide a basis for revolutionary low cost, high efficiency devices.

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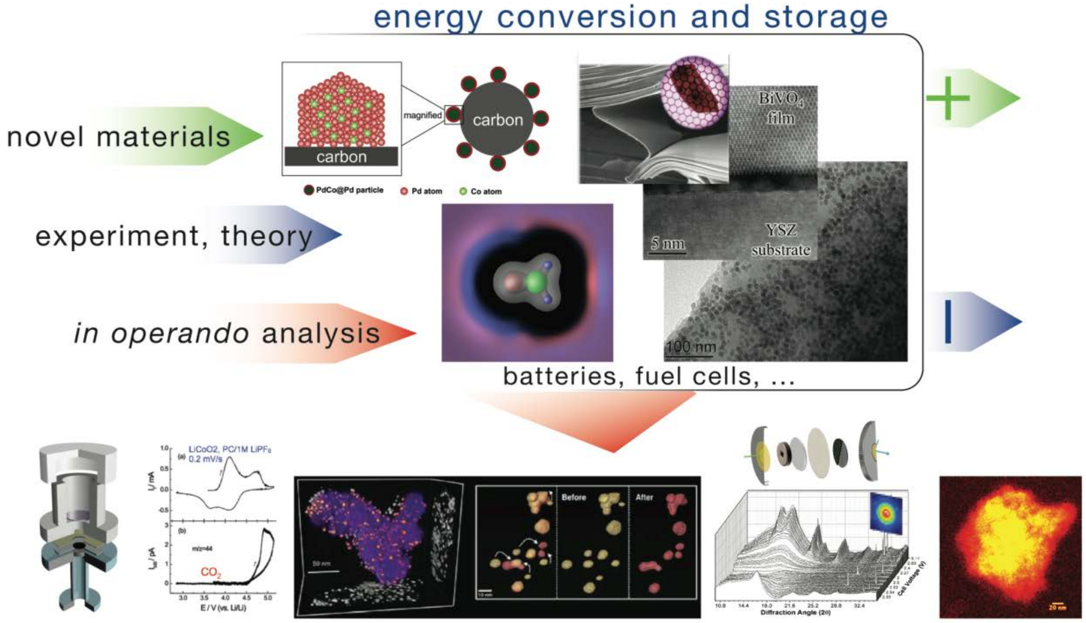
Energy Materials Center at Cornell (emc^2)
Héctor D. Abruña (Cornell University)

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 | emc^2 Energy Materials Center at Cornell

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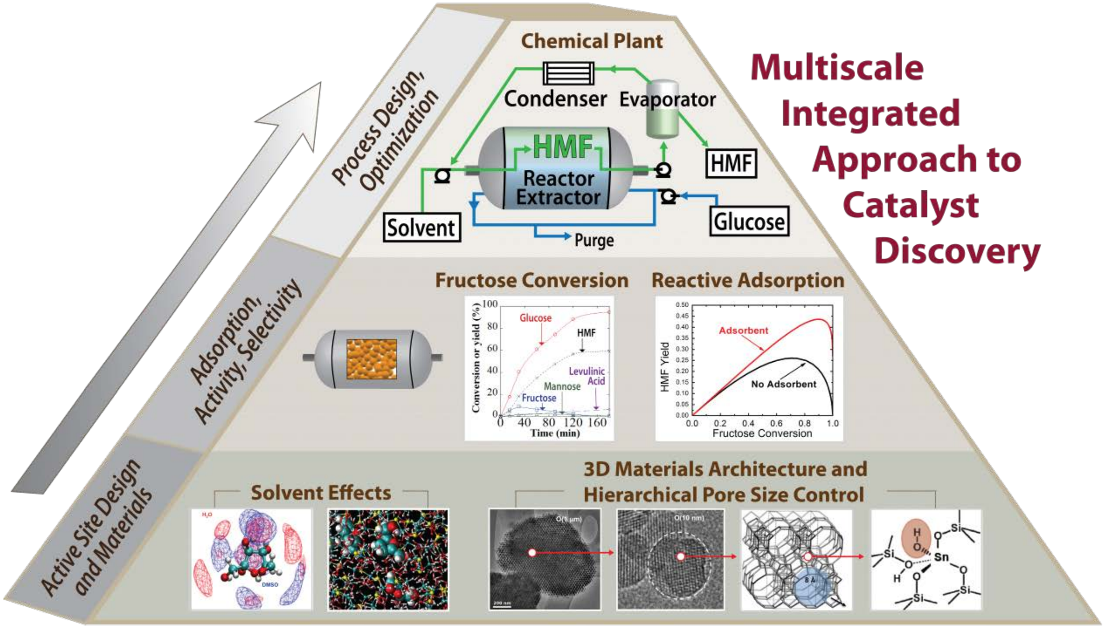
Catalysis Center for Energy Innovation (CCEI)
Dion Vlachos (University of Delaware)

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



RESEARCH PLAN AND DIRECTIONS

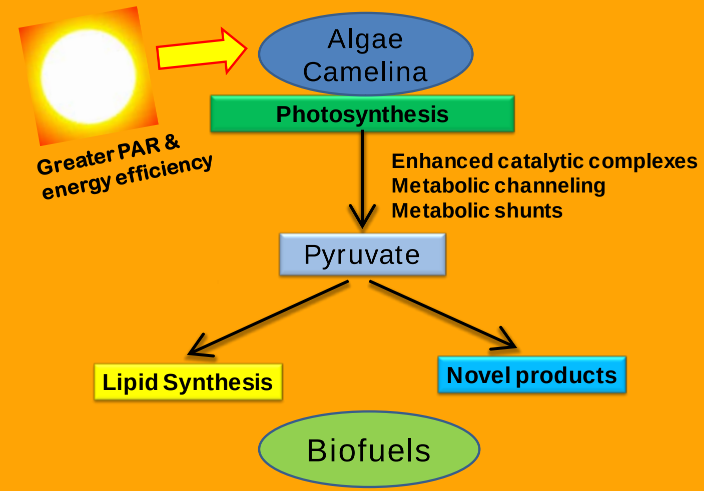
Biomass feedstocks vary considerably by source, and their transformation entails complex, multiscale reactions and processes. Based on a fundamental understanding of the *underlying* chemistry, CCEI develops novel catalytic materials and processes to set the foundations for the operation of modern biorefineries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

Center for 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

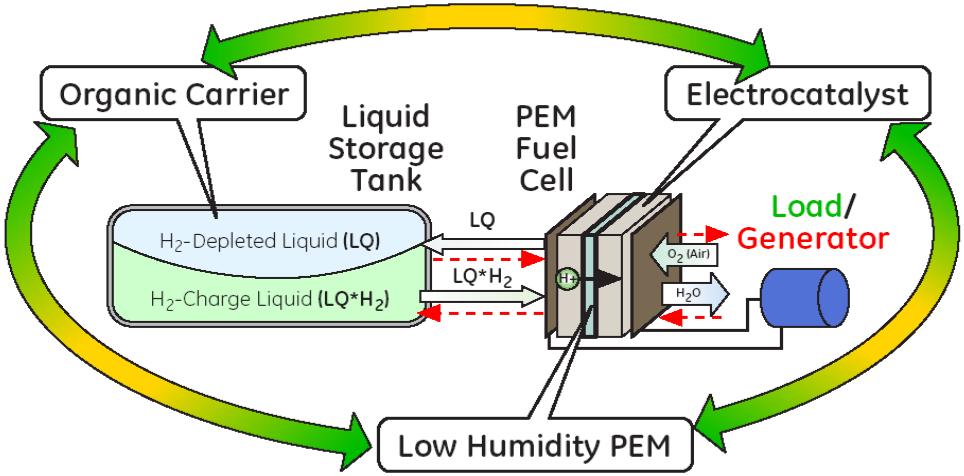
To achieve our objectives we will: 1) employ novel protein catalysts that increase the thermodynamic and kinetic efficiencies of photosynthesis and oil biosynthesis in algae and the oil seed crop, camelina, 2) engineer metabolic networks to enhance flux and channeling towards lipid synthesis, and 3)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

Revised on 10/01/2013

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

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 liquid organic hydrogen carriers
- Low humidity proton exchange membranes, selective transport of protons in the presence of fuels
- Compatibility of cell components

Approaches: Combination of modeling, synthetic chemistry and electrochemistry

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

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

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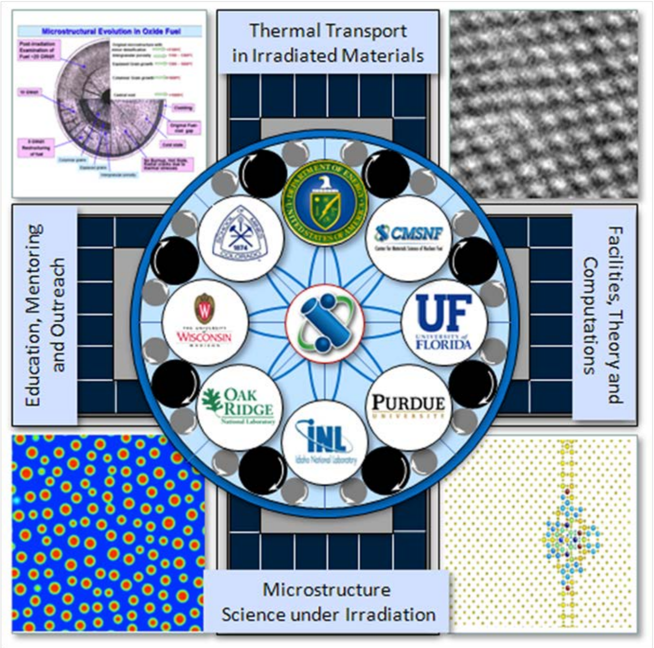
Center for Materials Science of Nuclear Fuel

Todd Allen (Idaho National Laboratory)

Vision

CMSNF will develop a first-principles-based understanding of *impact of complex defect structures on thermal transport in irradiated nuclear fuels*, with UO_2 as a model fuel system.



Research Plan and Directions

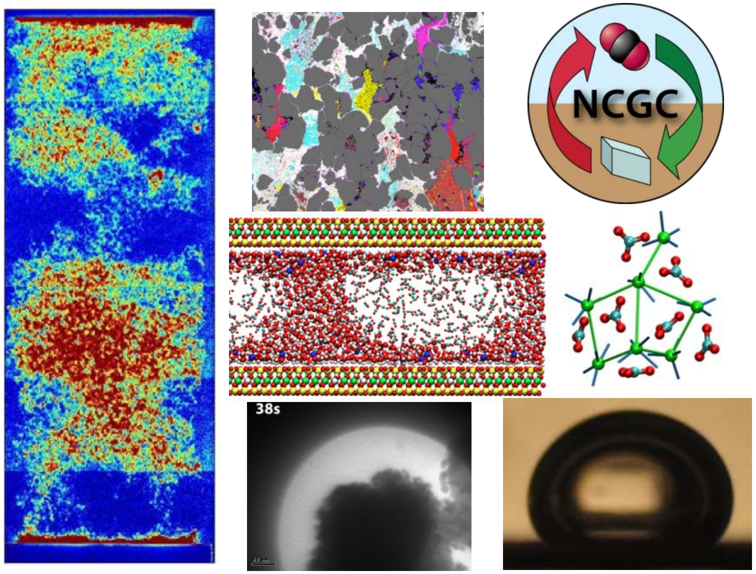
The research objectives of the center are:

- To achieve an understanding of the impact of complex defect structures on thermal transport in irradiated oxide fuel from first principles.
- To achieve the above for the case of irradiation induced defects in oxide fuel. As such, the center will also achieve a first-principles based understanding of the effects of irradiation on stoichiometry and microstructure in oxide fuel.
- By achieving these above goals, the center will also establish a new research direction that integrates the physics of thermal transport and the physics of defect and microstructure in irradiated oxide fuel.

Center for Nanoscale Control of Geologic CO_2 (NCGC)

Donald J. DePaolo
(Lawrence Berkeley National Laboratory)

VISION: **The NCGC objectives are to understand molecular, nano-scale, and pore network scale processes that affect flow, dissolution, and precipitation in subsurface rock formations during emplacement of supercritical CO_2; and ultimately to manipulate and control those processes to enhance storage security and efficiency**



***RESEARCH DIRECTION*:** **Properties and interactions of minerals with CO_2-brine mixed fluids are measured at elevated temperature and pressure, and effects at interfaces and in confined nanoscale pore spaces determined. Novel experimental and computational approaches, and unique DOE experimental facilities (ALS, SNS, NERSC, Molecular Foundry) are used to image and simulate pore structure, mineral surfaces, molecular - to - pore scale processes, carbonate mineral growth, and wetting properties.**

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

The purpose of this center is to explore, optimize and exploit the unique physics of solution-processed nanomaterials 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

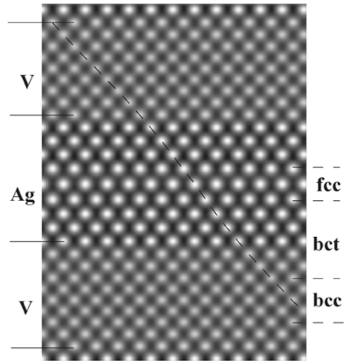
Our approach is to focus on controlled exploitation of novel physical phenomena that arise in nanomaterials, such as carrier multiplication, engineered carrier dynamics and carrier-carrier coupling, and defect-tolerant excitonic transport. The desired outcome of this work is low-cost photovoltaics with conversion efficiencies that *reach or exceed thermodynamic limits* based on <u>nanostructures fabricated via scalable chemical methods</u>.

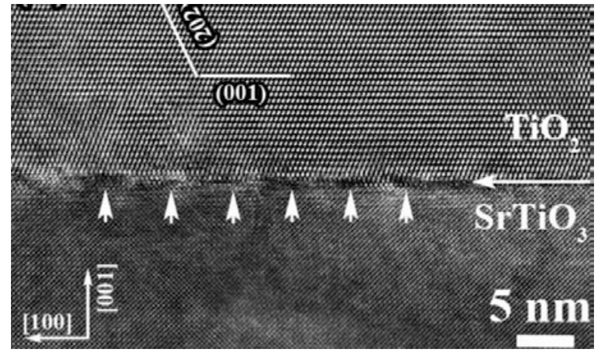
Los Alamos NATIONAL LABORATORY EST.1943 | NREL NATIONAL RENEWABLE ENERGY LABORATORY | GEORGE MASON UNIVERSITY

Center for Materials at Irradiation and Mechanical Extremes (CMIME)

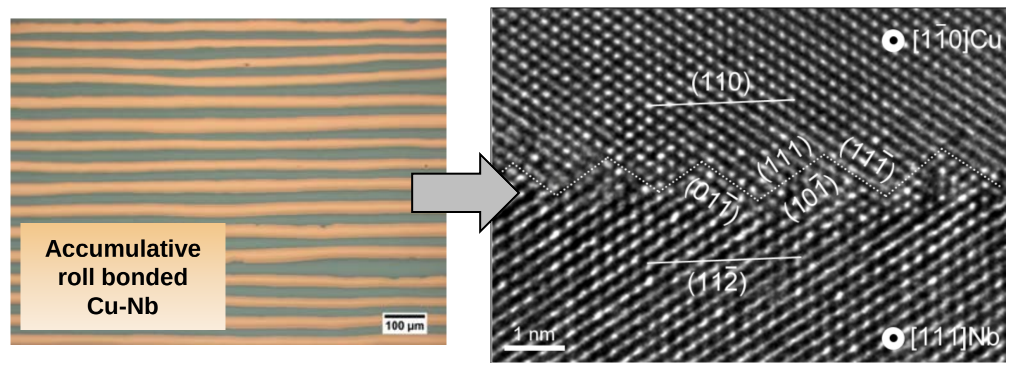
Amit Misra (Los Alamos National Lab)

The purpose of this EFRC is to understand, at the atomic scale, the interactions of defects at interfaces in materials subjected to extreme radiation doses and mechanical stress in order to synthesize new interface-dominated materials with tailored response under such extreme conditions.





Atomic structures of interfaces from some of the model systems explored in this EFRC

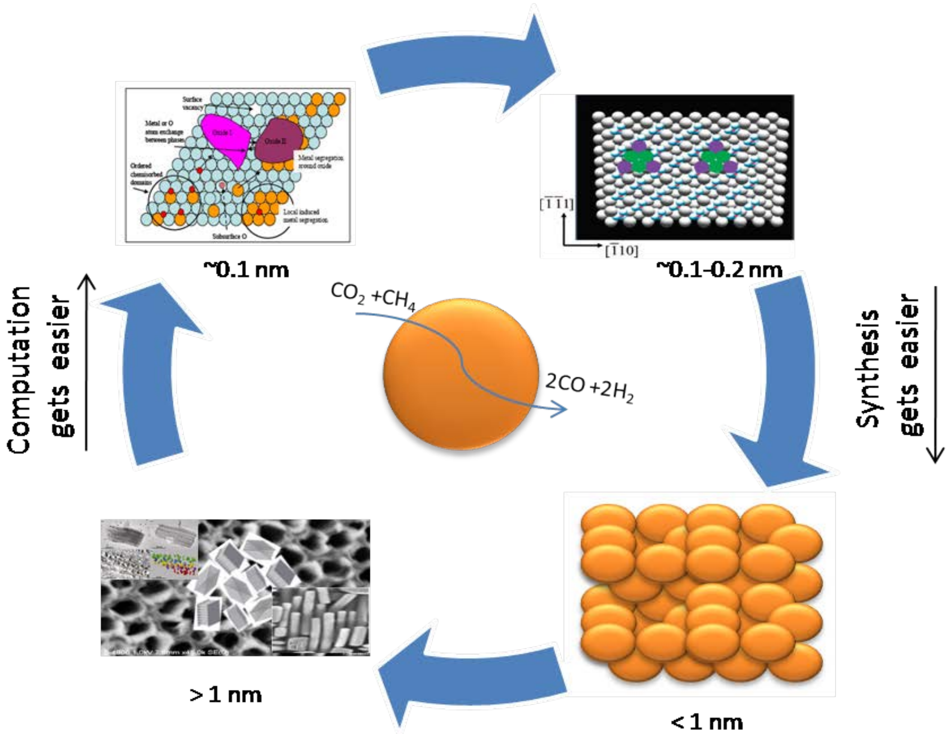


RESEARCH PLAN AND DIRECTIONS:

CMIME is developing quantitative relationships between the atomic structure and energetics of interfaces and radiation or mechanical damage evolution in materials. These quantitative relations are *figures-of-merit* that can be used to rank different solid-solid interfaces in terms of the ability of an interface to control defect evolution, and thereby enable structural materials design for the next generation of nuclear power reactors, transportation, energy and defense applications.

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

"Theoretical investigations guiding experiments on reactive surfaces"



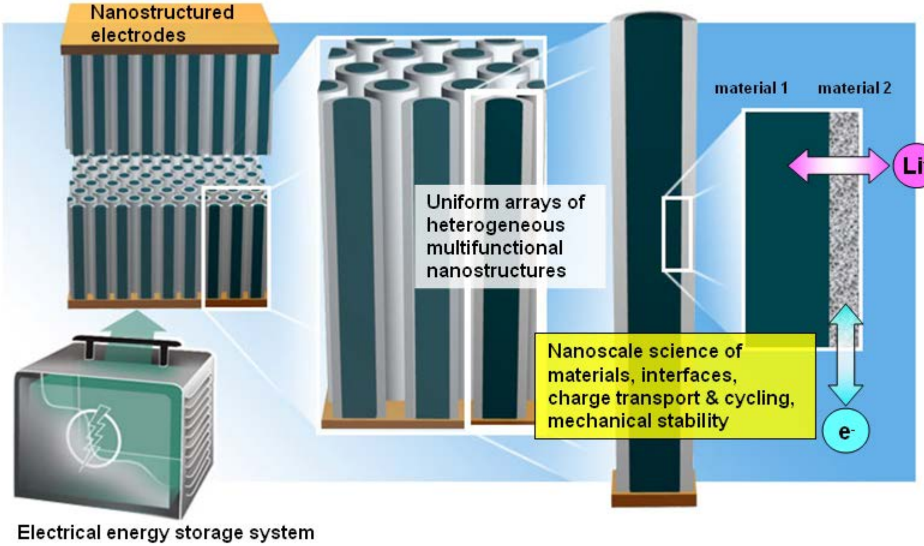
RESEARCH PLAN AND DIRECTIONS

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

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



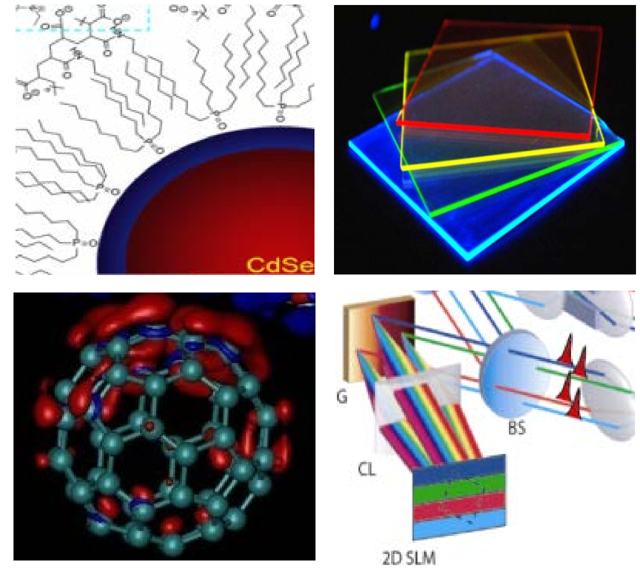
The Center…

- ***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.**

Center for Excitonics
Marc Baldo (MIT)

<u>Electronics vs Excitonics</u>

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:

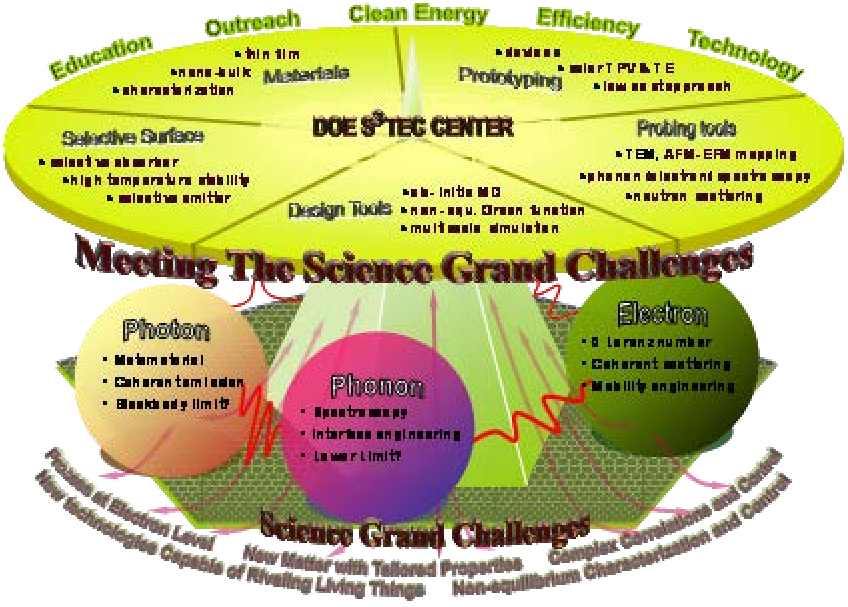
(1) Understand, control and exploit exciton transport

(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 thermal energy conversion technologies.

Revised on 02/12/2013

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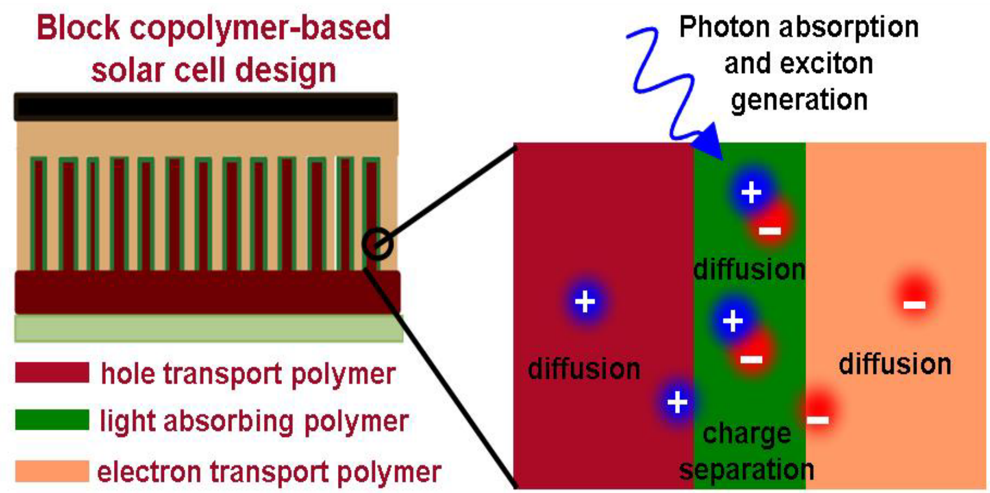
Polymer-Based Materials for Harvesting Solar Energy (PHaSE)

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

PHaSE's 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.



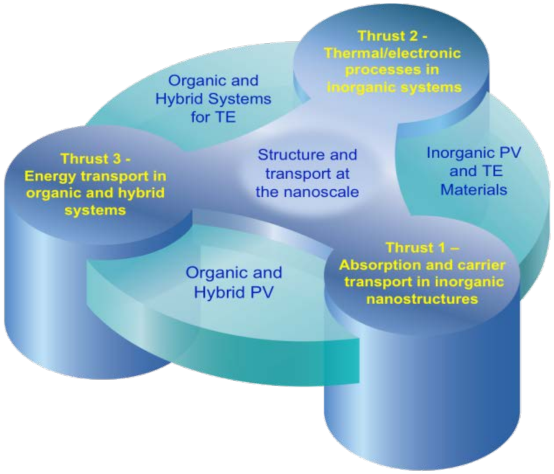
RESEARCH PLAN AND DIRECTIONS

Organic-based photovoltaics are relatively inexpensive and easy to fabricate, with energy conversion efficiencies and performance lifetimes that continue to improve. PHaSE's interdisciplinary research teams seek to maximize conversion of light to electrical charges by making new and better materials, and finding effective ways to assemble them in devices. Such basic research developments are crucial to yield economically viable polymer photovoltaics.

CENTER FOR SOLAR AND THERMAL ENERGY CONVERSION

Peter F. Green (University of Michigan)

Design and synthesize new materials for high efficiency photovoltaic (PV) and thermoelectric (TE) devices, predicated on new fundamental insights into equilibrium and non-equilibrium processes, including quantum phenomena, that occur in materials over various spatial and temporal scales.



RESEARCH OBJECTIVES AND DIRECTIONS

Research in CSTEC falls in three synergistic and collaborative thrusts, under a unifying concept: *structure and transport at the nanoscale.* Thrust 1: exploit unique quantum effects at the nanoscale to achieve high efficiency solar energy conversion. Thrust 2: to understand and to exploit fundamental mechanisms and processes to achieve high figures of merit in thermoelectric (inorganic, hybrid or molecular) materials. Thrust 3: investigate the molecular and structural origins of energy conversion phenomena in organic and hybrid material systems.

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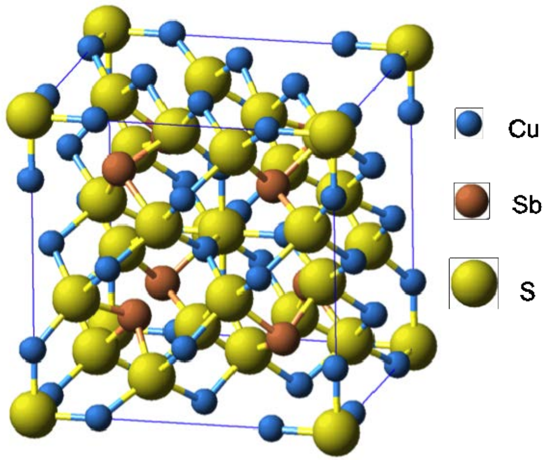
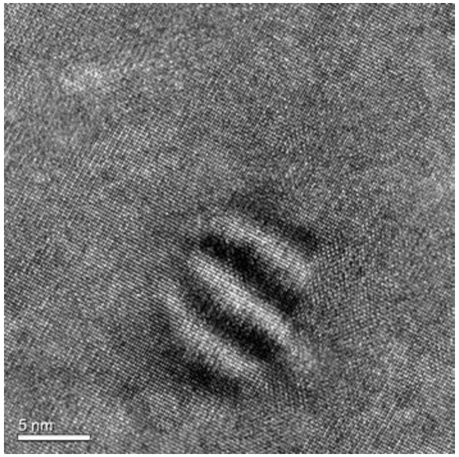
Revolutionary Materials for Solid State Energy Conversion (RMSSEC)

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**

MICHIGAN STATE UNIVERSITY | NORTHWESTERN UNIVERSITY | THE OHIO STATE UNIVERSITY | M | UCLA | WAYNE STATE UNIVERSITY | OAK RIDGE NATIONAL LABORATORY Managed by UT-Battelle for the Department of Energy | [efrc] RMSSEC Revolutionary Materials for Solid State Energy Conversion

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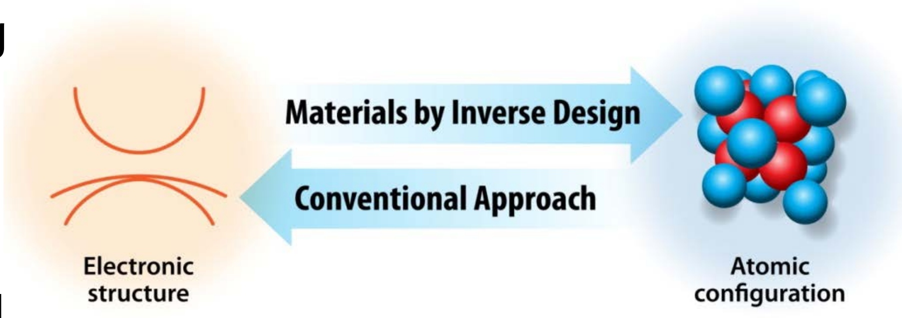
Center for Inverse Design

Bill Tumas (National Renewable Energy Laboratory)

VISION: Revolutionary materials discovery—leading to developing better and even entirely new materials more rapidly—by (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) employing combinatorial and targeted materials synthesis to realize such new materials experimentally.



The "materials by inverse design" approach (left to right), as compared to the conventional approach (right to left)

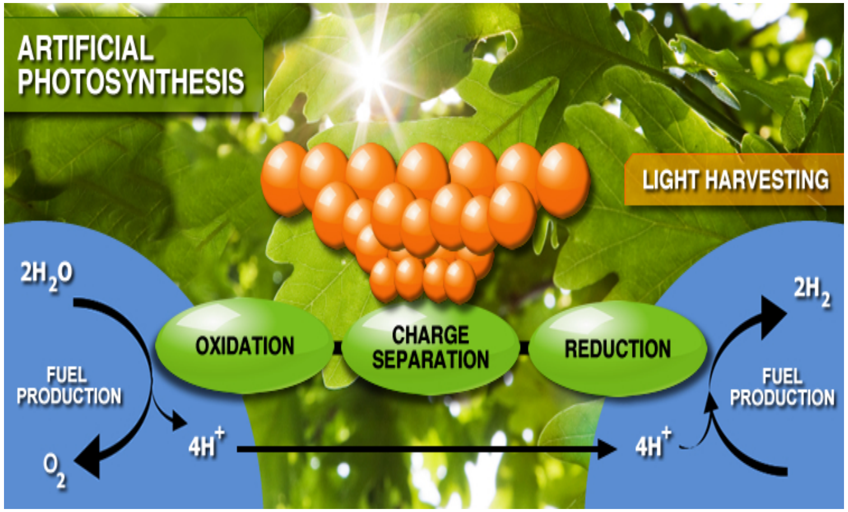
RESEARCH PLAN AND DIRECTIONS

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 are optimized in the design of new semiconductor absorbers, transparent conductors, and nanostructures for energy sustainability. We study predictions iteratively using 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.

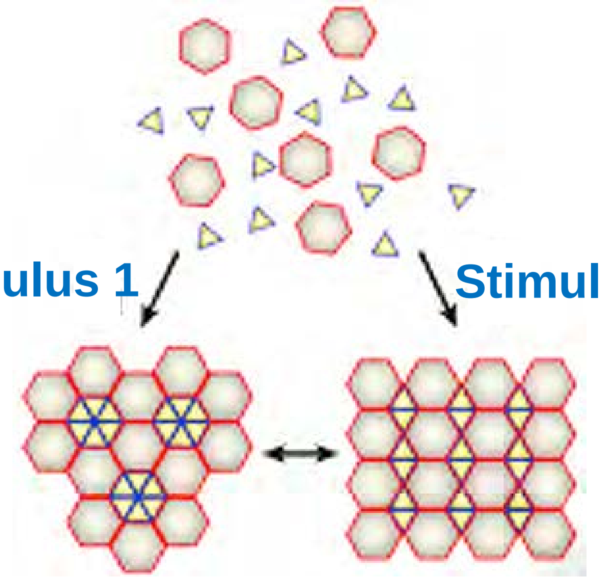


RESEARCH PLAN AND DIRECTIONS

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

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 far-from-equilibrium that are relevant to solar energy conversion, catalysis, and storage of electricity and hydrogen. These "adaptive" materials, while structurally robust, are able to change and optimize their own performance in response to external stimuli.



RESEARCH PLAN AND DIRECTIONS

By translating the theoretical description into the design and synthesis of specific non-equilibrium systems, identify the rules/requirements under which artificial materials and systems become least dissipative and, therefore, most energetically efficient.

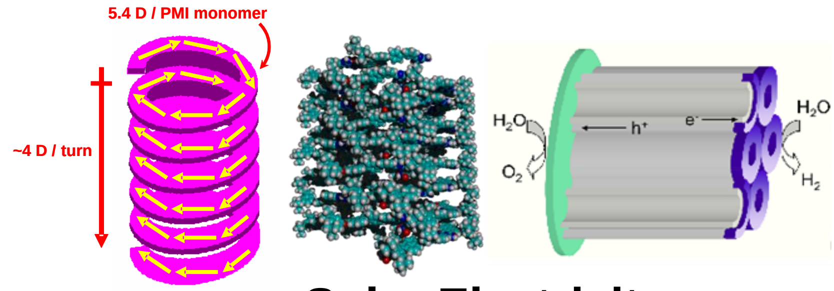
Argonne-Northwestern Solar Energy Research (ANSER) Center

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.

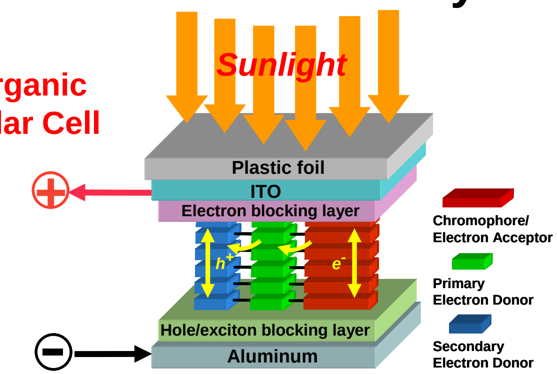
Solar Fuels

Artificial Photosynthetic Systems

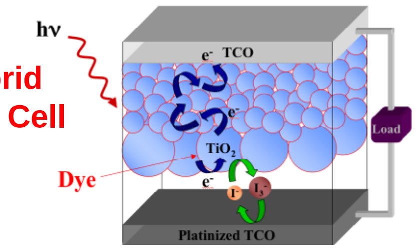


Solar Electricity

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.

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

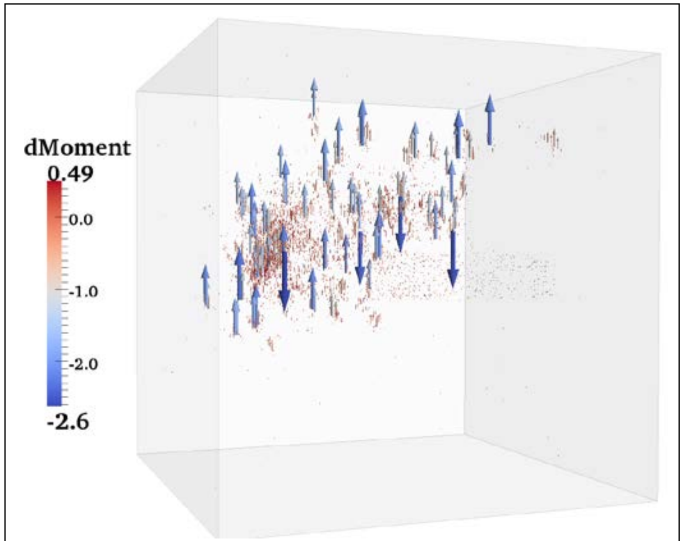
The Materials Science of Actinides EFRC seeks to understand and control, at the nanoscale, materials that contain actinides (radioactive heavy elements such as uranium and plutonium) to lay the scientific foundation for advanced nuclear energy systems.

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 (CDP)
G. Malcolm Stocks (Oak Ridge National Laboratory)

The Center for Defect Physics aims to develop a quantitative understanding of the mechanisms of defect formation, evolution and interactions that determine material behavior under irradiation. This research will provide the knowledge base and validated models of the critical parameters and processes that will accelerate the development of radiation tolerant materials for use in the extreme environments encountered in next generation nuclear energy systems.



Multi-Million Atom Quantum Simulations of Defect Production in Irradiated Fe

The CDP is using novel nano-scale experimental and quantum-informed theoretical techniques to probe the processes that control *Defect Formation and Short-Term Evolution Under Irradiation* and *Dislocation Interactions with Radiation Produced Defects* in iron-based alloys. By achieving unprecedentedly small experimental and large theoretical length scales, the CDP provides fundamental understanding of the controlling unit events.

Oak Ridge National Laboratory · The Ames Laboratory · Carnegie Mellon · Illinois · The Ohio State University · Berkeley University of California · The University of Georgia · The University of Tennessee

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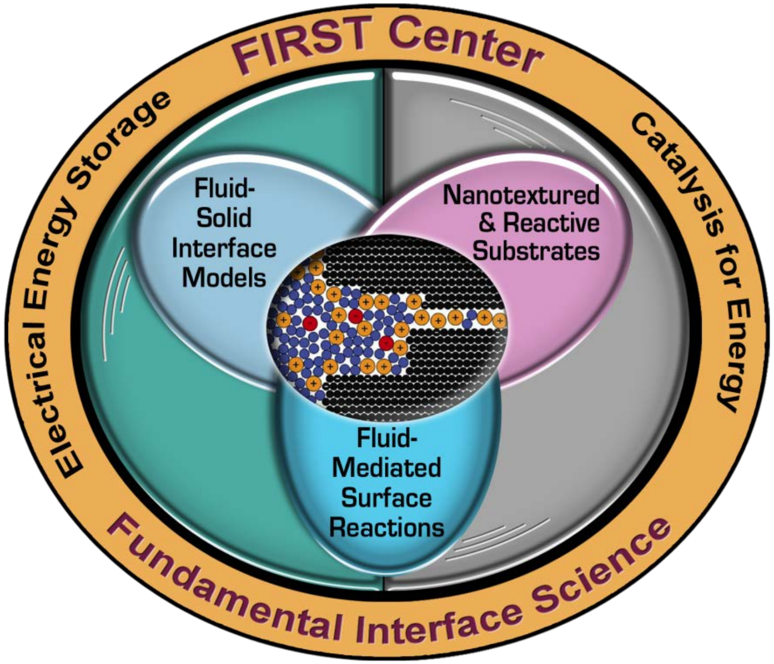
Fluid Interface Reactions, Structures and Transport (FIRST) Center
David J. Wesolowski (Oak Ridge National Lab)

FIRST Center Mission Statement:

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



RESEARCH PLAN AND DIRECTIONS

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

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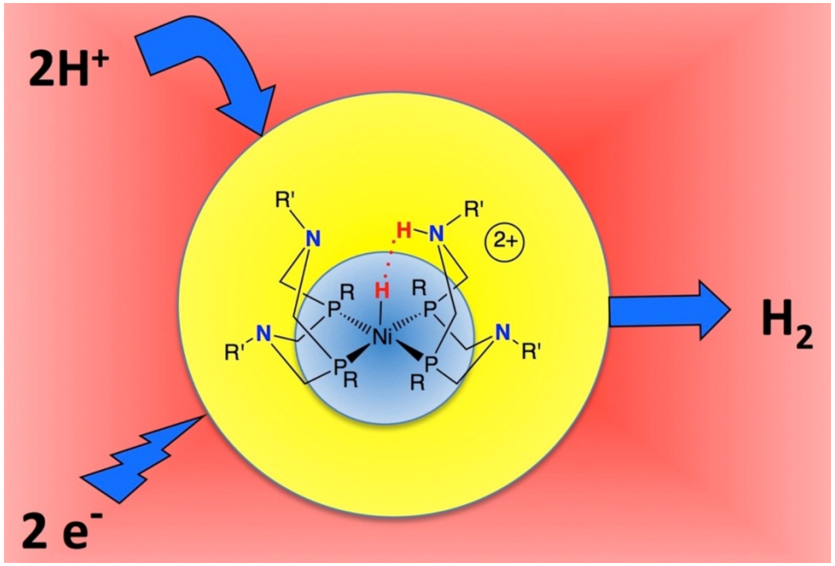
Center for Molecular Electrocatalysis (CME)

R. Morris Bullock
(Pacific Northwest National Laboratory)

Our vision is to develop a fundamental understanding of proton transfer reactions that will lead to transformational changes in our ability to design molecular electrocatalysts that rapidly and efficiently convert electrical energy into chemical bonds in fuels, or the reverse, converting chemical energy to electrical energy.

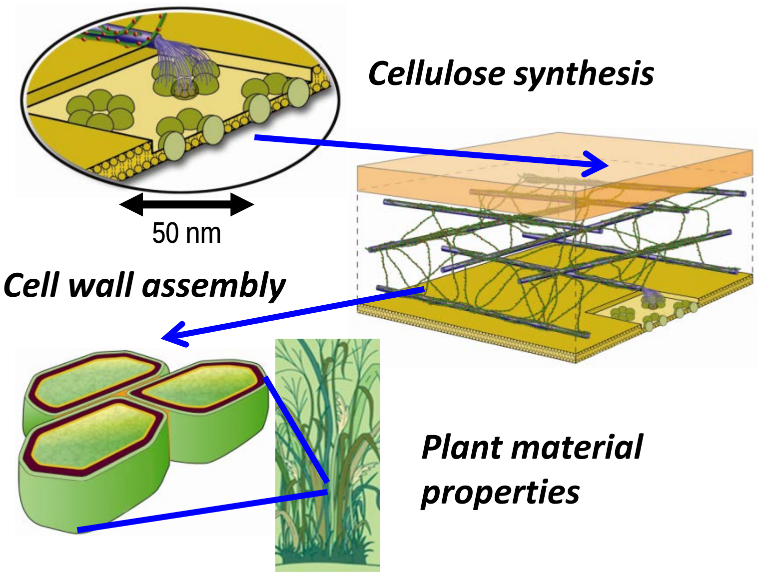


RESEARCH PLAN AND DIRECTIONS

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

Center for Lignocellulose Structure and Formation
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 nano-scale structure of this material as well as the machinery and processes underlying its formation 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)

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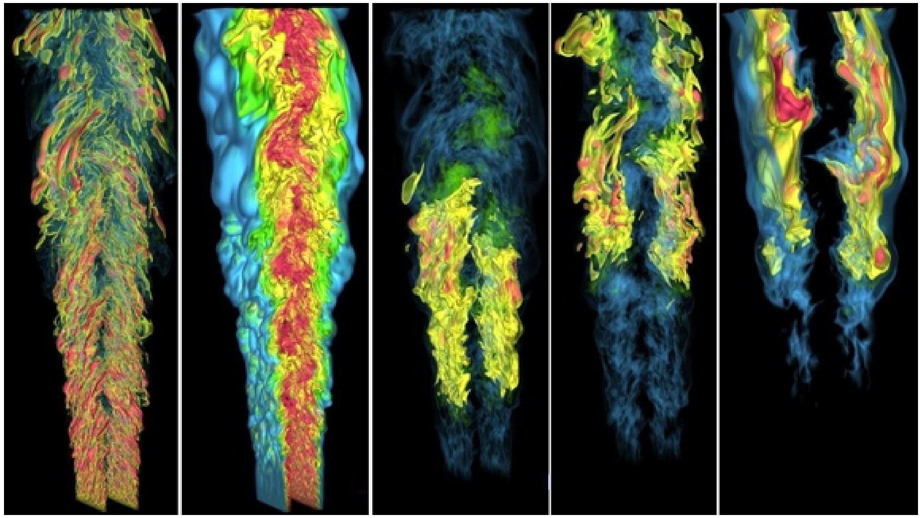
Overarching Goal

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***

PRINCETON UNIVERSITY · STANFORD ENGINEERING · THE UNIVERSITY of WISCONSIN MADISON · Argonne NATIONAL LABORATORY · Sandia National Laboratories · Massachusetts Institute of Technology · UCONN · Cornell University · USC UNIVERSITY OF SOUTHERN CALIFORNIA · UNIVERSITY OF MINNESOTA

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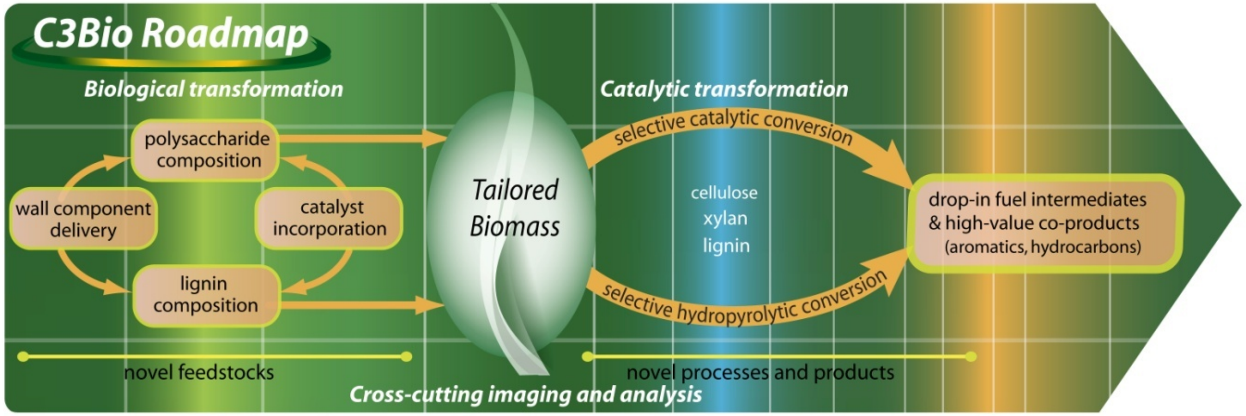
Center for Direct Catalytic Conversion of Biomass to Biofuels (C3Bio)
Maureen McCann (Purdue University)

C3Bio develops transformational knowledge and technologies for the direct conversion of plant lignocellulosic biomass to biofuels and other biobased products currently derived from oil.



RESEARCH PLAN AND DIRECTION

We will increase the energy and carbon efficiencies of converting biomass to advanced biofuels 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 how catalysts interact with biomass, and tailoring biomass for highly efficient direct catalytic conversion, we will *more than double* the carbon captured into energy-rich advanced hydrocarbon fuels and other high-value products. Our interdisciplinary teamwork bridges the complexity of biology to the selectivity of chemistry and enables solutions through engineering.

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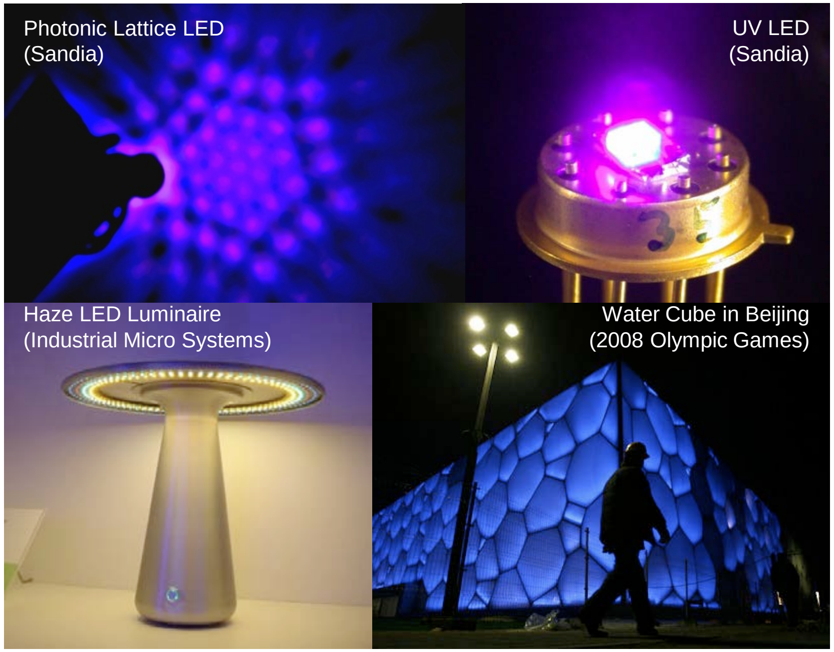
EFRC for Solid-State Lighting Science (SSLS)
Michael E. Coltrin (Sandia National Labs)

Goal: **To explore energy conversion in tailored photonic structures and materials to enable revolutionary breakthroughs in the efficiency and performance of light-emitting diode (LED) based lighting; to improve energy-efficiency in the way we light our homes and offices, which currently accounts for 20 percent of the nation's electrical energy use.**



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.**

Heterogeneous Functional Materials Center (HeteroFoaM Center)

Ken Reifsnider (University of South Carolina)

U.S. DEPARTMENT OF ENERGY | Office of Science

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 designing the functionality of nano-structural configurations 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 design and create new functional material systems.

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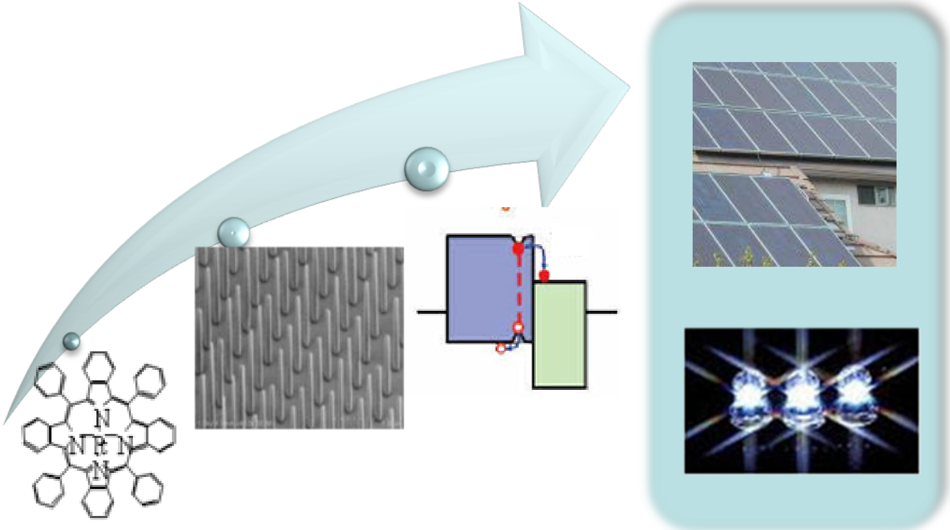
Center for Energy Nanoscience (CEN)
P. Daniel (Dan) Dapkus (USC)

The Center for Energy Nanoscience will explore organic and nano - structured 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.

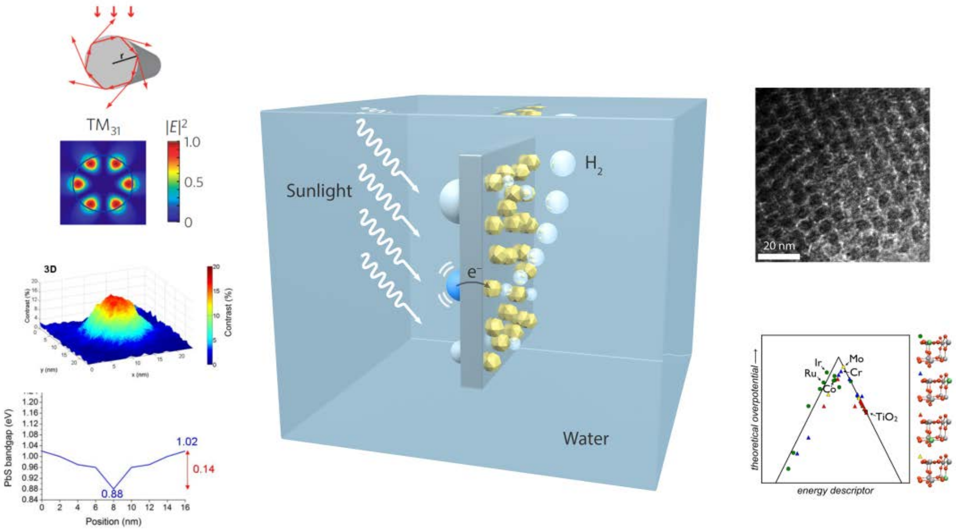


RESEARCH PLAN AND DIRECTIONS

- **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 advancing solar conversion into stored energy.



RESEARCH PLAN AND DIRECTIONS

We use nanostructuring to achieve quantum and optical confinement for light absorption and atomic-scale engineering for catalysis, each of which contributes to improved efficiency and performance in solar energy conversion into fuels.

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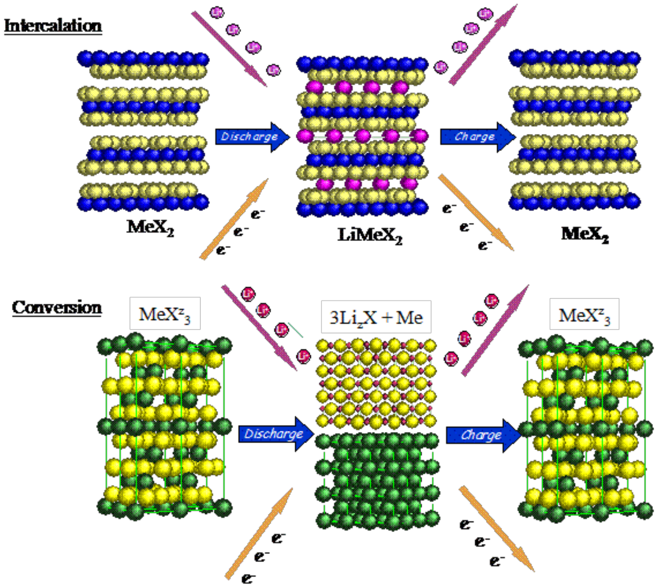
Northeastern Center for Chemical Energy Storage (NECCES)

M. Stanley Whittingham (Stony Brook University)

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

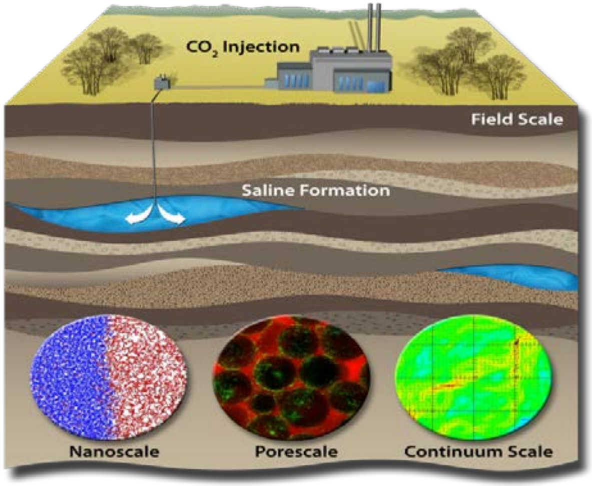


RESEARCH PLAN AND DIRECTIONS

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 methodologies to determine how electrodes function in real time, as batteries are cycled. The team will determine/control the phases formed and the role overpotential plays.

Center for Frontiers of Subsurface Energy Security
Steven Bryant (University of Texas at Austin)

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.

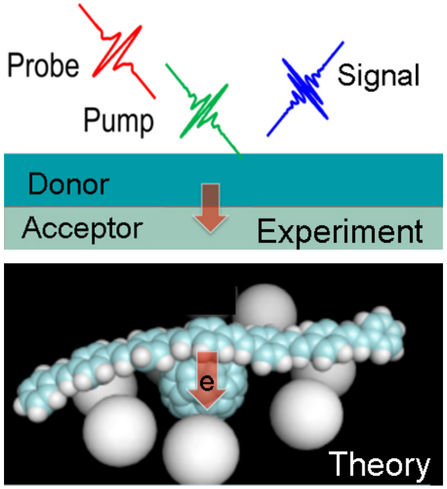
Unique aspects: The uncertainty and complexity of fluids in geologic media from the molecular scale to the basin scale.

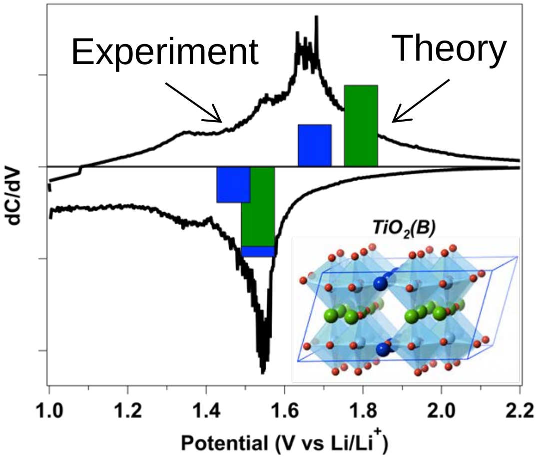
Outcome: Better understanding of long term behavior of subsurface storage.

Understanding Charge Separation and Transfer at Interfaces in Energy Materials

Peter J. Rossky (University of Texas at Austin)

We are developing a *fundamental understanding* of interfacial charge separation and transfer processes that govern the *function* of molecular energy materials, thus *enabling design* of next-generation organic "plastic" solar cells and advanced batteries.





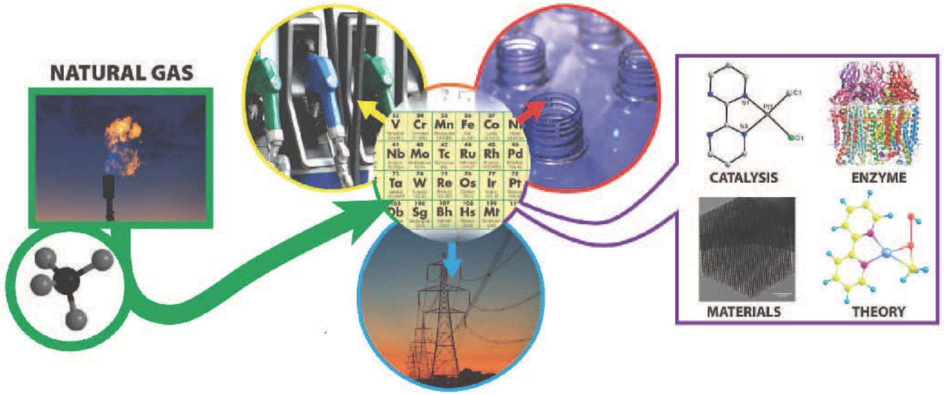
RESEARCH PLAN AND DIRECTIONS

We use *cutting-edge experimental methods* (e.g., interface-specific laser probes, *in situ* electron microscopy) *intimately coupled with frontier theoretical methods* (e.g., multiscale and quantum electronic dynamics simulation) to elucidate the mechanisms and structural basis for observed charge separation and transfer behavior in energy materials.

Center for Catalytic Hydrocarbon Functionalization (CCHF)

T. Brent Gunnoe (University of Virginia)

The goal of the CCHF is to develop next generation catalyst technologies for the conversion of fossil feedstocks to useful materials, particularly the conversion of natural gas to liquid fuel, that would reduce our dependence on oil and reduce harmful emissions.



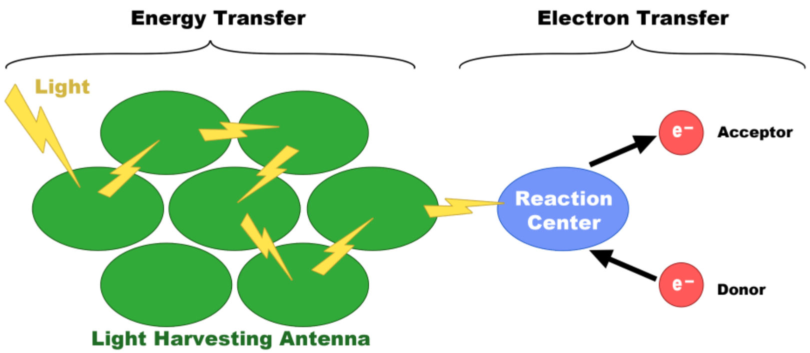
RESEARCH PLAN AND DIRECTIONS

The CCHF will combine theoretical, computational and experimental approaches to the design and study of new catalysts and catalytic processes for the selective and low-temperature conversion of hydrocarbons, particularly methane from natural gas, into liquid fuels and for the use of methane in direct low-temperature fuel cells.

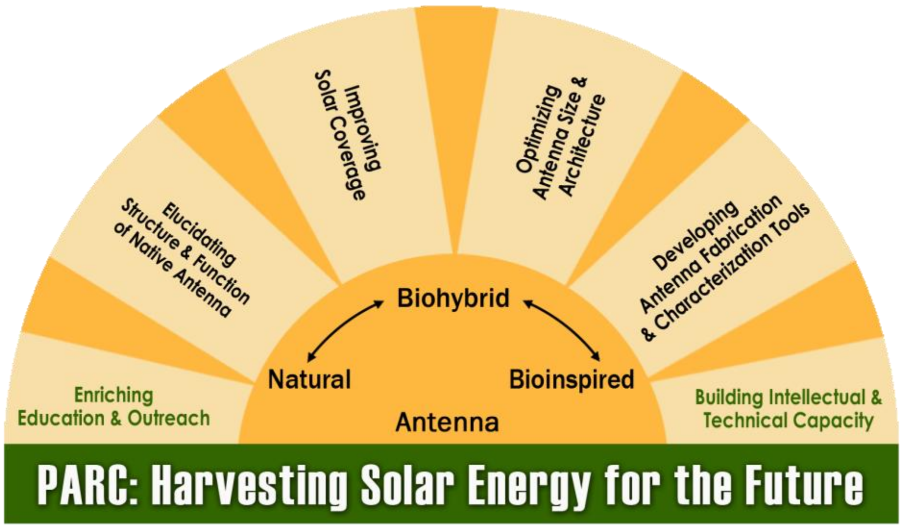
Photosynthetic Antenna Research Center (PARC)
Robert Blankenship (Washington Univ. in St. Louis)

MISSION

Maximize photosynthetic antenna efficiency in living organisms and fabricate robust micron-scale biohybrid light-harvesting systems to drive photocurrent.



VISION



GOALS

- **Tailor antenna size, composition, and spectral coverage**
- **Design and construct light-harvesting assemblies**
- **Exercise comprehensive control over light-harvesting systems**
- **Positively impact the scientific community and public**

‘GRAND CHALLENGES’ INDEX

‘BASIC RESEARCH NEEDS’ INDEX

TOPICAL INDEX

EXPERIMENTAL AND THEORETICAL METHODS INDEX