



U.S. DEPARTMENT OF
ENERGY

Office of
Science

Science **for our** **Nation's** Energy Future

Energy Frontier Research Centers

Transforming the future
of energy and
the environment



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ENERGY

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Science

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Energy Frontier Research Centers

May 2011

Letter from the Director

The Energy Frontier Research Centers are a critical piece of our national investment in the fundamental science needed to achieve a 21st-century energy economy. The Department of Energy's Office of Science, the single largest supporter of basic research in the physical sciences in the United States, is the architect and sponsor of the EFRC program.

Established in 2009 after a thorough assessment by the Office of Science and the scientific community of the most fruitful opportunities in energy science, the EFRCs are now thriving. The competition for the EFRCs was extraordinarily intense, and the 46 centers selected for awards represent truly bold attempts to advance scientific understanding in many areas crucial to energy technologies. Their efforts will lay the scientific groundwork for fundamental advances in solar energy, biofuels, transportation, energy efficiency, electricity storage and transmission, carbon capture and sequestration, and nuclear energy.

The EFRCs are defined by their multidisciplinary composition and their collaborative character, which sparks new approaches to problems and breakthrough discoveries. Today EFRC researchers are also taking advantage of new capabilities in nanotechnology, high-intensity light sources, neutron scattering sources, supercomputing, and other advanced instrumentation, much of it developed over the past decade and available at our unparalleled suite of open-access user facilities. We are inspired by the vigor and focus of the literally thousands of senior investigators, postdocs, and students who have chosen to devote their professional lives and education to advancing energy science.

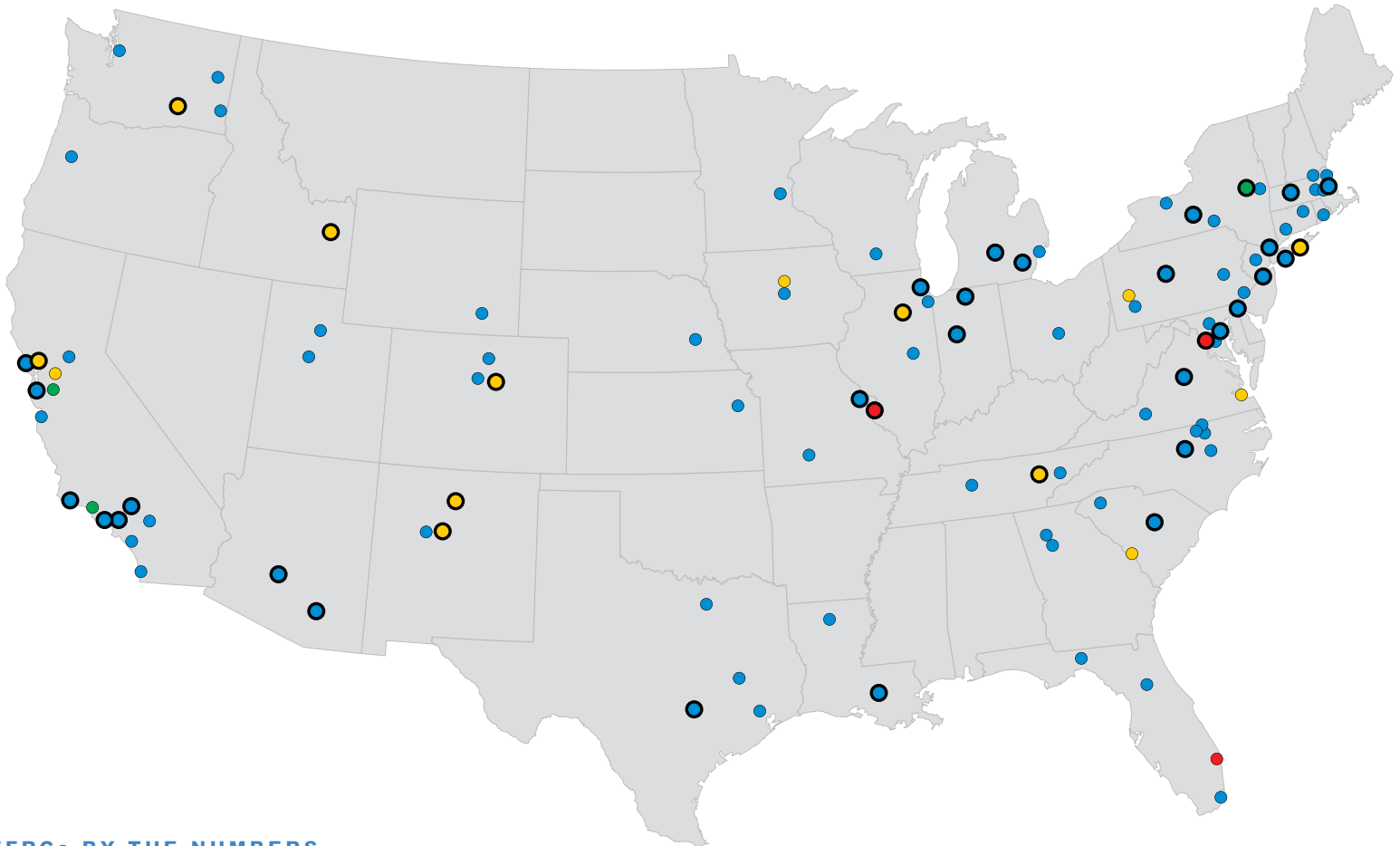
The Office of Science is proud of the early achievements of the EFRCs detailed in this brochure, and looks forward with great anticipation to the results they produce in the coming years in service to the nation.



William F. Brinkman
Director, Office of Science

KEY

- **Lead Institution**
- **Partner Institution**
- University
- National Laboratory
- Industry
- Not-for-profit



EFRCs BY THE NUMBERS

46 Lead Institutions

(31 universities, 12 DOE national laboratories, 2 not-for-profit organizations, 1 corporate research laboratory.)

Approximately **115** institutions, from **35** states plus the District of Columbia, are participating.

On the order of **860** senior investigators and involving, on a full- or part-time basis, an additional estimated **2,000** researchers, including postdoctoral associates, graduate students, undergraduate students, and technical staff.

ARIZONA

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

Center for Interface Science: Solar Electric Materials (CISSEM)
University of Arizona

CALIFORNIA

Center for Energy Efficient Materials (CEEM)
University of California, Santa Barbara

Center for Energy Nanoscience (CEN)
University of Southern California

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

Center for Nanoscale Control of Geologic CO₂ (NCGC)
Lawrence Berkeley National Laboratory

Center on Nanostructuring for Efficient Energy Conversion (CNEEC)
Stanford University

Light-Material Interactions in Energy Conversion (LMI)
California Institute of Technology

Molecularly Engineered Energy Materials (MEEM)
University of California, Los Angeles

COLORADO

Center for Inverse Design (CID)
National Renewable Energy Laboratory

DELAWARE

Catalysis Center for Energy Innovation (CCEI)
University of Delaware

DISTRICT OF COLUMBIA

Center for Energy Frontier Research in Extreme Environments (EFree)
Carnegie Institution of Washington

IDAHO

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

ILLINOIS

Argonne-Northwestern Solar Energy Research Center (ANSER)
Northwestern University

Center for Electrical Energy Storage (CEES)
Argonne National Laboratory

Institute for Atom-Efficient Chemical Transformations (IACT)
Argonne National Laboratory

Non-equilibrium Energy Research Center (NERC)
Northwestern University

INDIANA

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

Materials Science of Actinides (MSA)
University of Notre Dame

LOUISIANA

Center for Atomic-Level Catalyst Design (CALCD)
Louisiana State University

MARYLAND

Nanostructures for Electrical Energy Storage (NEES)
University of Maryland

MASSACHUSETTS

Center for Excitonics (CE)
Massachusetts Institute of Technology

Polymer-Based Materials for Harvesting Solar Energy (PHaSE)
University of Massachusetts, Amherst

Solid-State Solar-Thermal Energy Conversion Center (S³TEC)
Massachusetts Institute of Technology

MICHIGAN

Center for Solar and Thermal Energy Conversion (CSTEC)
University of Michigan

Revolutionary Materials for Solid State Energy Conversion (RMSSEC)
Michigan State University

MISSOURI

Center for Advanced Biofuel Systems (CABS)
Donald Danforth Plant Science Center

Photosynthetic Antenna Research Center (PARC)
Washington University in St. Louis

NEW JERSEY

Combustion Energy Frontier Research Center (CEFRC)
Princeton University

NEW MEXICO

Center for Advanced Solar Photophysics (CASP)
Los Alamos National Laboratory

Center for Materials at Irradiation and Mechanical Extremes (CMIME)
Los Alamos National Laboratory

EFRC for Solid State Lighting Science (SSLS)
Sandia National Laboratories

NEW YORK

Center for Electrocatalysis, Transport Phenomena and Materials for Innovative Energy Storage (CETM)
General Electric Global Research

Center for Emergent Superconductivity (CES)
Brookhaven National Laboratory

Energy Materials Center at Cornell (emc²)
Cornell University

Northeastern Center for Chemical Energy Storage (NECCES)
Stony Brook University

Re-Defining Photovoltaic Efficiency Through Molecule Scale Control (RPEMSC)
Columbia University

NORTH CAROLINA

Solar Fuels and Next Generation Photovoltaics (UNC)
University of North Carolina

PENNSYLVANIA

Center for Lignocellulose Structure and Formation (CLSF)
Pennsylvania State University

SOUTH CAROLINA

Heterogeneous Functional Materials Center (HeteroFoam)
University of South Carolina

TENNESSEE

Center for Defect Physics (CDP)
Oak Ridge National Laboratory

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

TEXAS

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

Understanding Charge Separation and Transfer at Interfaces in Energy Materials (CST)
University of Texas at Austin

VIRGINIA

Center for Catalytic Hydrocarbon Functionalization (CCHF)
University of Virginia

WASHINGTON

Center for Molecular Electrocatalysis (CME)
Pacific Northwest National Laboratory

Centers ordered alphabetically by state of the lead institution and then by center name

EFRC Program Overview

In August 2009, the Office of Science established 46 Energy Frontier Research Centers. The EFRCs are collaborative research efforts intended to accelerate high-risk, high-reward fundamental research, the scientific basis for transformative energy technologies of the future.

These Centers involve universities, national laboratories, nonprofit organizations, and for-profit firms, singly or in partnerships, selected by scientific peer review. They are funded at \$2 to \$5 million per year for a total planned DOE commitment of \$777 million over the initial five-year award period, pending Congressional appropriations. These integrated, multi-investigator Centers are conducting fundamental research focusing on one or more of several “grand challenges” and use-inspired “basic research needs” recently identified in major strategic planning efforts by the scientific community. The purpose of the EFRCs is to integrate the talents and expertise of leading scientists in a setting designed to accelerate research that transforms the future of energy and the environment.

Research Areas

Basic Research Needs To Assure A Secure Energy Future is a monumental report based on a week-long Basic Energy Sciences Advisory Committee workshop held in 2002. The report inspired a series of follow-on “Basic Research Needs” workshops that together attracted more than 1,500 participants from universities, industry and DOE laboratories. The 46 EFRC awards span the full range of energy research challenges described in the resulting Basic Energy Sciences workshop reports (see science.energy-gov/bes/news-and-resources/reports/basic-research-needs/). In addition, this process helped to identify a number of fundamental grand challenges in energy science, summarized in the report, *Directing Matter and Energy: Five Challenges for Science and the Imagination*.

Basic Research Needs Reports

- Advanced Nuclear Energy Systems
- Carbon Capture: Beyond 2020
- Catalysis for Energy
- Clean and Efficient Combustion of 21st-Century Transportation Fuels
- Electrical Energy Storage
- Geosciences: Facilitating 21st-Century Energy Systems
- The Hydrogen Economy
- Materials under Extreme Environments
- Solar Energy Utilization
- Solid State Lighting
- Superconductivity

Grand Challenges for Energy Science

- How do we control materials processes at the level of electrons?
- How do we design and perfect atom- and energy-efficient syntheses of revolutionary new forms of matter with tailored properties?
- How do remarkable properties of matter emerge from the complex correlations of atomic or electronic constituents and how can we control these properties?
- How can we master energy and information on the nanoscale to create new technologies with capabilities rivaling those of living things?
- How do we characterize and control matter away—especially very far away—from equilibrium?

Contents

Energy Frontier Research Centers

- 1 Center for Bio-Inspired Solar Fuel Production (BISfuel)
- 2 Center for Interface Science: Solar Electric Materials (CISSEM)
- 3 Center for Energy Efficient Materials (CEEM)
- 4 Center for Energy Nanoscience (CEN)
- 5 Center for Gas Separations Relevant to Clean Energy Technologies (CGS)
- 6 Center for Nanoscale Control of Geologic CO₂ (NCGC)
- 7 Center on Nanostructuring for Efficient Energy Conversion (CNEEC)
- 8 Light-Material Interactions in Energy Conversion (LMI)
- 9 Molecularly Engineered Energy Materials (MEEM)
- 10 Center for Inverse Design (CID)
- 11 Catalysis Center for Energy Innovation (CCEI)
- 12 Center for Energy Frontier Research in Extreme Environments (EFree)
- 13 Center for Materials Science of Nuclear Fuel (CMSNF)
- 14 Argonne-Northwestern Solar Energy Research Center (ANSER)
- 15 Center for Electrical Energy Storage (CEES)
- 16 Institute for Atom-Efficient Chemical Transformations (IACT)
- 17 Non-equilibrium Energy Research Center (NERC)
- 18 Center for Direct Catalytic Conversion of Biomass to Biofuels (C³Bio)
- 19 Materials Science of Actinides (MSA)
- 20 Center for Atomic-Level Catalyst Design (CALCD)
- 21 Nanostructures for Electrical Energy Storage (NEES)
- 22 Center for Excitonics (CE)
- 23 Polymer-Based Materials for Harvesting Solar Energy (PHASe)
- 24 Solid-State Solar-Thermal Energy Conversion Center (S³TEC)
- 25 Center for Solar and Thermal Energy Conversion (CSTEC)
- 26 Revolutionary Materials for Solid State Energy Conversion (RMSSEC)
- 27 Center for Advanced Biofuel Systems (CABS)
- 28 Photosynthetic Antenna Research Center (PARC)
- 29 Combustion Energy Frontier Research Center (CEFRFC)
- 30 Center for Advanced Solar Photophysics (CAPS)
- 31 Center for Materials at Irradiation and Mechanical Extremes (CMIME)
- 32 EFRC for Solid State Lighting Science (SSLS)
- 33 Center for Electrocatalysis, Transport Phenomena and Materials
for Innovative Energy Storage (CETM)
- 34 Center for Emergent Superconductivity (CES)
- 35 Energy Materials Center at Cornell (emc²)
- 36 Northeastern Center for Chemical Energy Storage (NECCES)
- 37 Re-Defining Photovoltaic Efficiency Through Molecule Scale Control (RPEMSC)
- 38 Solar Fuels and Next Generation Photovoltaics (UNC)
- 39 Center for Lignocellulose Structure and Formation (CLSF)
- 40 Heterogeneous Functional Materials Center (HeteroFoAM)
- 41 Center for Defect Physics in Structural Materials (CDP)
- 42 Fluid Interface Reactions, Structures and Transport Center (FIRST)
- 43 Center for Frontiers of Subsurface Energy Security (CFSES)
- 44 Understanding Charge Separation and Transfer at Interfaces
in Energy Materials (CST)
- 45 Center for Catalytic Hydrocarbon Functionalization (CCHF)
- 46 Center for Molecular Electrocatalysis (CME)

*Centers ordered alphabetically by
state of the lead institution and then
by center name*

EFRC Research Topic Index

| | |
|----------------------------|--|
| Actinides | 12, 13, 19 |
| Biofuels | 11, 16, 18, 20, 27, 28, 29, 39 |
| Carbon capture | 5, 9, 27 |
| Carbon sequestration | 6, 43 |
| Catalysis | 1, 7, 8, 11, 14, 16, 18, 20, 27, 33, 35, 38, 42, 45, 46 |
| Charge transport | 1, 2, 4, 7, 9, 14, 15, 17, 21, 22, 23, 24, 25, 27, 28, 30, 32, 33, 35, 36, 37, 38, 40, 42, 44, 46 |
| Combustion | 29 |
| Defects | 7, 10, 12, 13, 21, 24, 25, 31, 32, 34, 35, 36, 41, 44 |
| Electrical energy storage | 3, 7, 9, 12, 15, 17, 21, 33, 34, 35, 36, 38, 40, 42, 44, 45, 46 |
| Extreme environment | 6, 12, 13, 19, 29, 31, 41, 42, 43 |
| High performance computing | 4, 5, 6, 10, 13, 15, 17, 29, 31, 39, 41, 42, 43 |
| Hydrogen | 1, 7, 12, 14, 20, 29, 33, 35, 38, 46 |
| Inorganic materials | 1, 2, 5, 6, 7, 8, 10, 11, 13, 14, 15, 16, 17, 19, 20, 21, 22, 23, 24, 25, 26, 28, 30, 31, 32, 34, 35, 36, 37, 38, 40, 41, 42, 43, 44, 45, 46 |
| Interfaces | 2, 4, 5, 6, 7, 14, 15, 16, 17, 20, 21, 23, 24, 25, 31, 33, 35, 36, 37, 38, 39, 40, 41, 42, 43, 44 |
| Matter by design | 4, 5, 7, 8, 9, 10, 11, 13, 14, 15, 16, 17, 18, 19, 20, 23, 24, 25, 26, 31, 35, 36, 37, 39, 40, 41, 42, 44, 46 |
| Membranes | 5, 9, 28, 33, 35, 39, 40 |
| Nuclear | 13, 19, 31, 41, 43 |
| Organic materials | 1, 2, 3, 4, 5, 9, 11, 14, 15, 16, 17, 18, 21, 22, 23, 25, 27, 28, 29, 33, 35, 37, 38, 39, 44, 45, 46 |
| Oxides | 1, 2, 4, 6, 7, 8, 9, 10, 11, 12, 14, 15, 16, 20, 21, 25, 31, 35, 36, 38, 40, 42, 44, 45 |
| Photosynthesis | 1, 7, 8, 14, 22, 27, 28, 38 |
| Polymers | 2, 3, 4, 5, 6, 9, 14, 17, 18, 21, 22, 23, 25, 33, 35, 37, 38, 44 |
| Rare earth elements | 12, 24, 32 |
| Semiconductors | 1, 2, 3, 4, 7, 8, 10, 12, 14, 21, 22, 23, 24, 25, 26, 30, 32, 35, 37, 38, 40, 42, 44, 45 |
| Separations | 5, 17, 19 |
| Smart grid | 34 |
| Solar fuels | 1, 4, 7, 8, 14, 27, 28, 38, 42 |
| Solar photovoltaic | 2, 3, 4, 7, 8, 9, 10, 14, 17, 22, 23, 24, 25, 30, 32, 37, 38, 44 |
| Solar thermal | 24, 25, 26 |
| Solid state lighting | 3, 4, 8, 22, 32 |
| Superconductivity | 12, 34 |
| Thermoelectric | 3, 17, 24, 25, 26 |
| Ultrafast science | 4, 14, 24, 25, 28, 30, 41, 44 |

Center for Bio-Inspired Solar Fuel Production (BISfuel)

Director

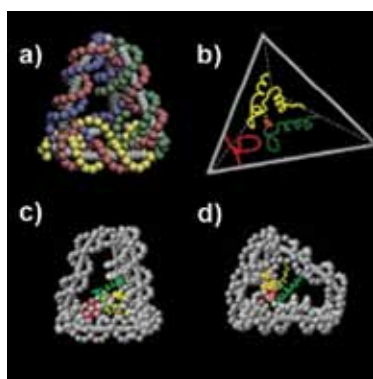
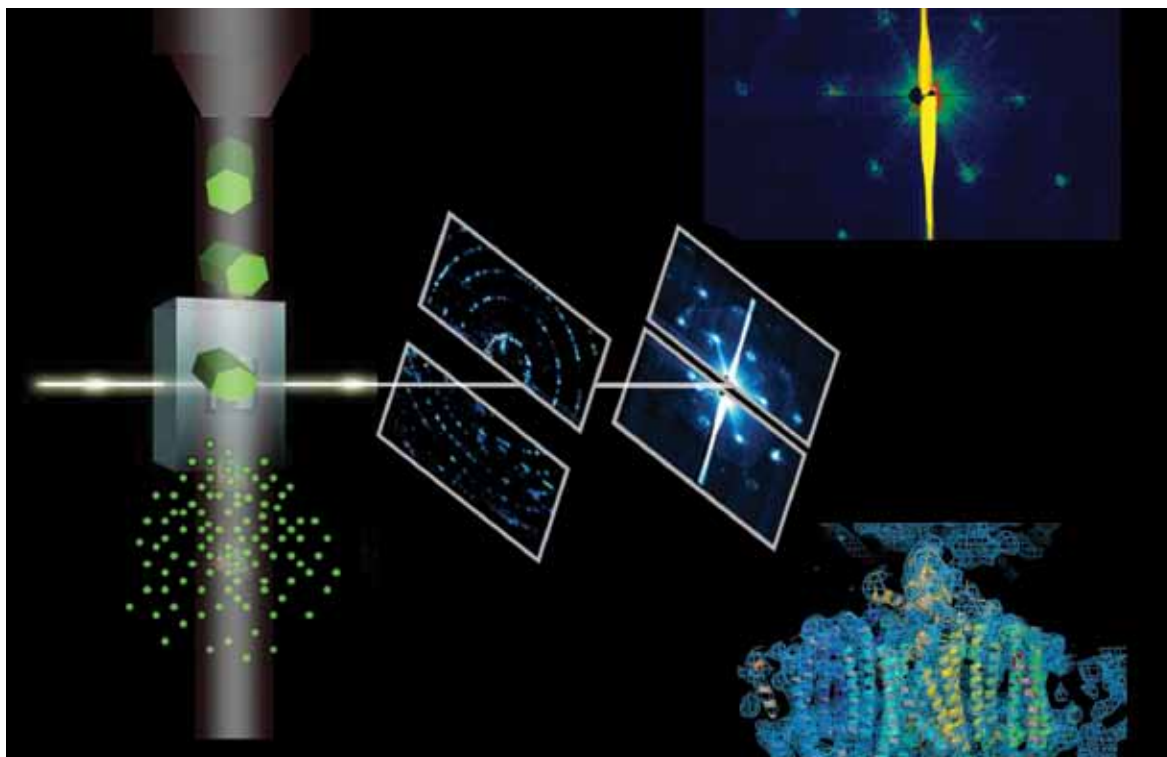
Devens Gust

Lead Institution

Arizona State University

Research Topics

catalysis, solar fuels, photosynthesis, hydrogen, charge transport, organic materials, inorganic materials, semiconductors, oxides



ABOVE: DNA self-assembles into a structural framework that binds peptide molecules at well-defined locations. The peptides organize a metal-ion based water oxidation catalyst inspired by those found in photosynthetic organisms. **TOP:** Femtosecond X-ray methods are being developed to determine the structures of small, fragile crystals of proteins and DNA using DOE's Linac Coherent Light Source.

Mission

To construct a complete system for solar-powered production of hydrogen fuel via water splitting. Design principles are drawn from the fundamental concepts that underlie photosynthetic energy conversion.

Achievements

Photosynthesis is the best-tested, largest-scale process on earth for solar fuel production. Researchers at BISfuel are using the physical and chemical principles underlying photosynthesis as a blueprint for the design of artificial analogs of natural light-gathering antennas and reaction centers that convert light energy into electrochemical energy. They are also seeking bio-inspired catalysts that use light energy to split water into hydrogen and oxygen. Recent achievements include: a novel nanoporous, transparent conducting metal oxide that can serve as a functional framework for assembly of a solar water-splitting system; DNA-based superstructures within which construction of bio-inspired water splitting catalysts takes place; a new X-ray method for determining the molecular structures of natural and artificial photosynthetic materials; and a detailed comparison of the efficiencies of photosynthesis and conventional photovoltaics for fuel production that will guide the development of artificial photosynthesis.

Center for Interface Science: Solar Electric Materials (CISSEM)

Director

Neal R. Armstrong

Lead Institution

University of Arizona

Partner Institutions

Georgia Institute of Technology

National Renewable Energy

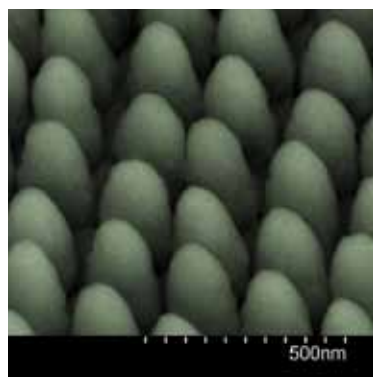
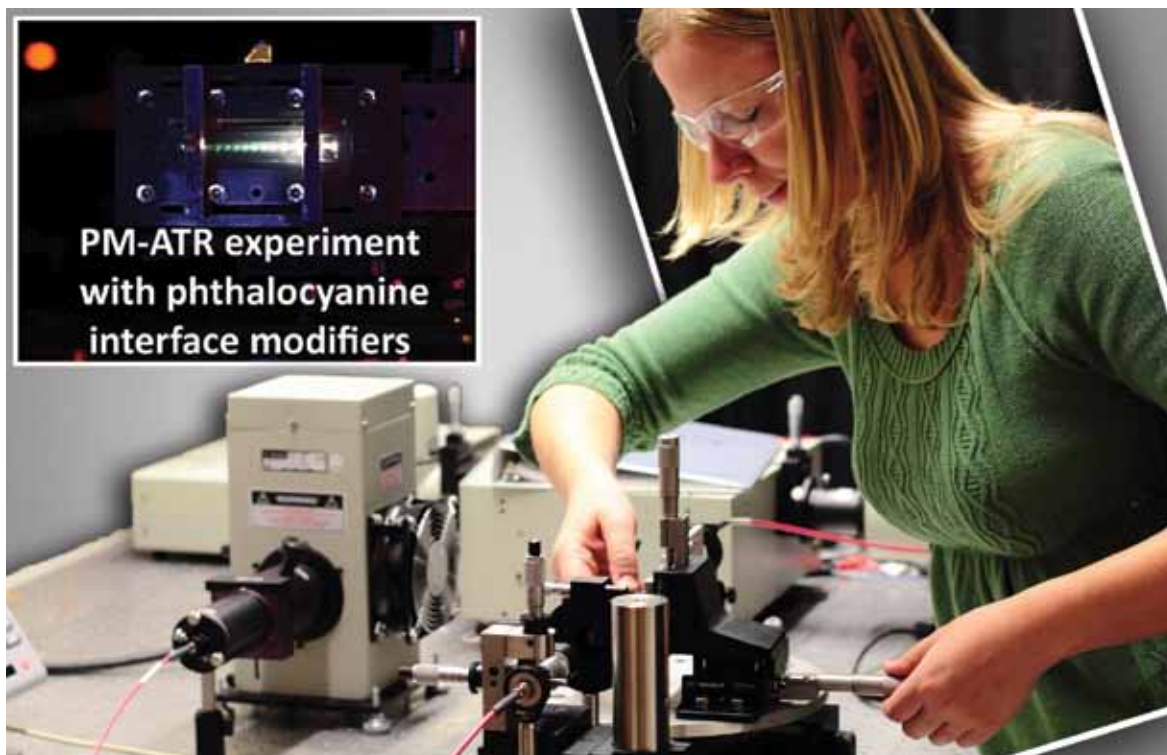
Laboratory

Princeton University

University of Washington

Research Topics

solar photovoltaics, interfaces, charge transport, organic materials, inorganic materials, polymers, semiconductors, oxides



ABOVE: Electron micrograph of a silver nano-pillar electrode—a material critical to the investigation of how nano-structured interfaces affect PV performance. **TOP:** Dr. Brooke Beam aligns a PM-ATR cell to characterize molecular orientation and electron-transfer rates at interfaces. **INSERT:** Light probing interfaces in multiple reflections in a transparent electrode.

Mission

To advance the understanding of interface science underlying solar energy conversion technologies based on organic and organic-inorganic hybrid materials; and to inspire, recruit and train future scientists and leaders in the basic science of solar electric energy conversion.

Achievements

Research at CISSEM explores the basic science underlying the development of new thin-film photovoltaic (PV) energy conversion technologies, focusing on understanding and controlling interfaces between disparate materials. The center connects 17 investigators and more than 60 students, postdocs, scientists and staff. CISSEM has developed new interface modifiers and electrical contacts, and expanded the portfolio of unique spectroscopic equipment—including new waveguide-based, potential modulated attenuated total reflectance (PM-ATR) spectroscopy—to understand both composition and energetics at critical interfaces on nanometer length scales. An innovative CISSEM program funds student and postdoc travel among CISSEM partner institutions to expand their basic science research scope through collaboration. In an annual competition, students and postdocs at different institutions jointly propose new CISSEM research projects.

Center for Energy Efficient Materials (CEEM)

Director

John Bowers

Lead Institution

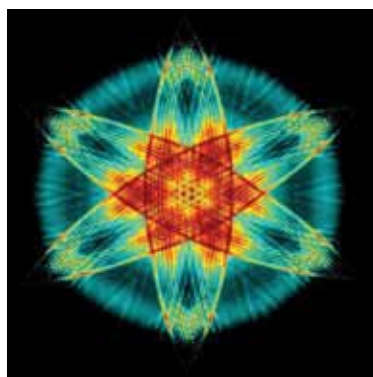
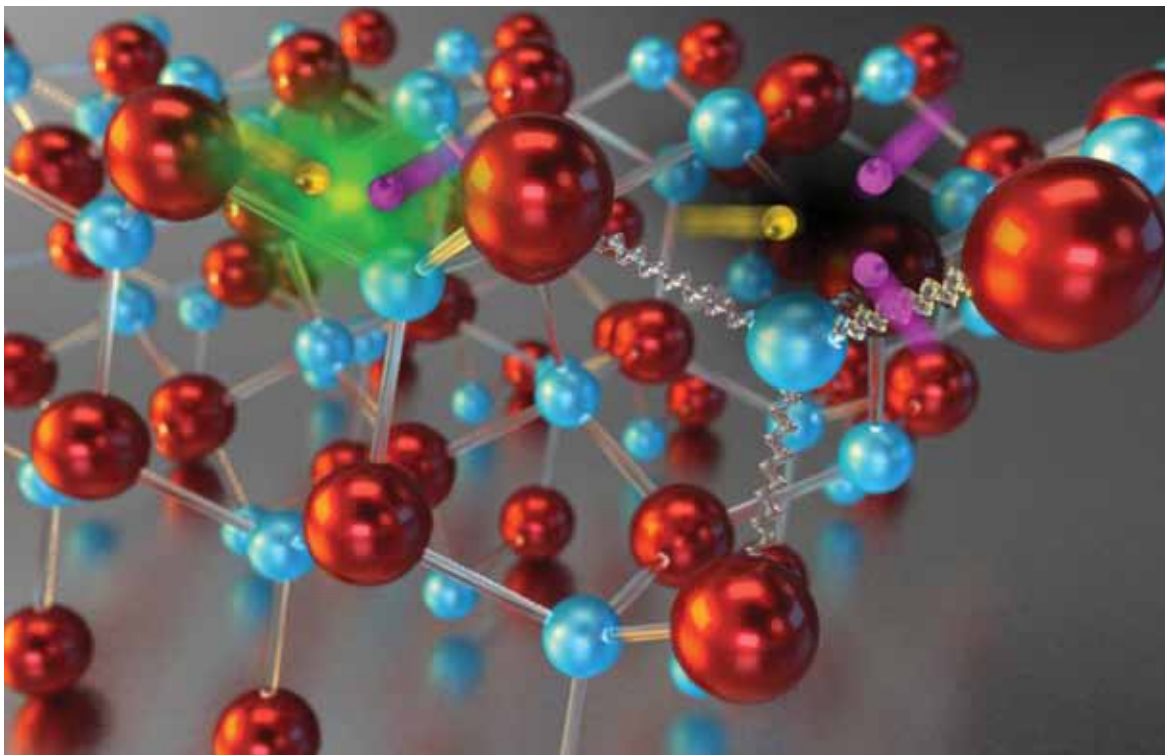
University of California,
Santa Barbara

Partner Institutions

University of California, Santa Cruz
Harvard University
Los Alamos National Laboratory
National Renewable Energy
Laboratory

Research Topics

solar photovoltaics, solid state lighting,
thermoelectric, organic materials,
polymers, semiconductors



ABOVE: Sharp diffraction patterns, such as this one, convey information about the periodic structure and dimensions of photonic crystals. **TOP:** An artists' rendition of the electronic interactions responsible for some light emitting diodes (LEDs) being less efficient than others.

Mission

To discover and develop materials that control the interactions between light, electricity, and heat at the nanoscale for improved solar energy conversion, solid-state lighting, and conversion of heat into electricity.

Achievements

CEEM's achievements include the development of a new class of organic materials that can be used for making low-cost, thin-film, plastic solar cells. CEEM researchers have also developed novel methods of stacking multiple solar cells, each absorbing a different color of light so that a larger fraction of the sun's energy can be converted to electricity. In another effort, CEEM has investigated methods for embedding grating structures in materials that improve the coupling of light out of light emitting diodes (LEDs) or into solar cells. Additionally, researchers have developed a process for growing semiconductors containing nanometer sized particles of rare earth materials to control and enhance the generation of electricity from waste heat.

Center for Energy Nanoscience (CEN)

Director

P. Daniel Dapkus

Lead Institution

University of Southern California

Partner Institutions

University of Illinois, Urbana–

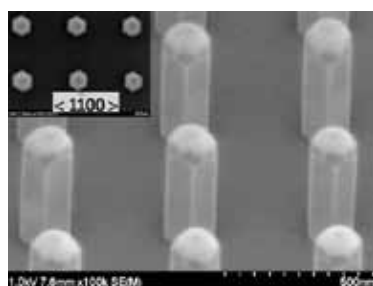
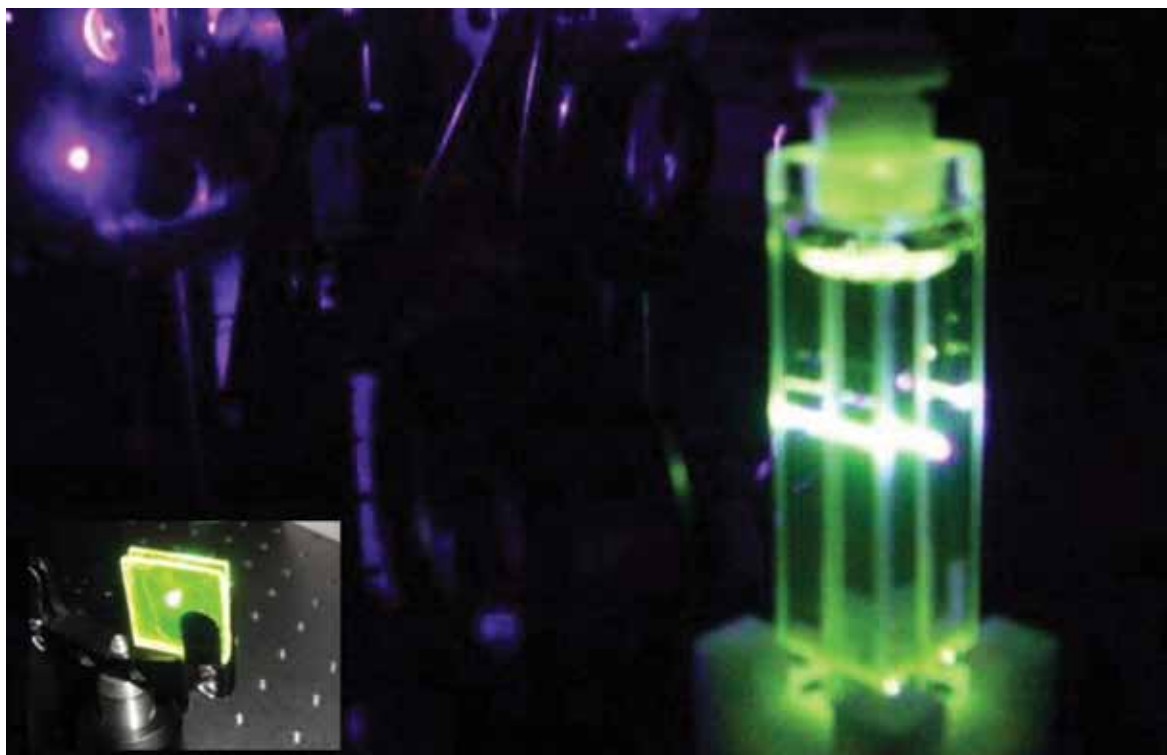
Champaign

University of Michigan

University of Virginia

Research Topics

solar photovoltaics, solar fuels, solid state lighting, interfaces, matter by design, charge transport, ultrafast science, high performance computing, organic materials, polymers, semiconductors, oxides



ABOVE: An array of hexagonal, rod-shaped gallium nitride nanowires. Ultra-thin light-emitting regions of indium gallium nitride deposited on the six walls of the nanowire efficiently generates visible light whose color is tuned by adjusting the nanowire dimensions.

TOP: Luminescence from diphenyltetracene (DPT) in solution and in thin films (inset) stimulated with ultrafast laser light helps researchers understand triplet exciton formation and improve organic photovoltaic efficiency.

Mission

To explore the light absorption and emission in organic and nanostructure materials and their hybrids for solar energy conversion and solid state lighting.

Achievements

In solar cells, some of the energy from sunlight (particularly the blue light) is used inefficiently. Research at CEN is exploring exciton fission—in which the original excitation caused by the light is then split into two excitations that together preserve the total energy carried by the light. In some organic molecules this energy splitting occurs efficiently while also creating excitations (referred to as “triplet excitons”) that travel further in the material and are easier to harvest as electrical current. Researchers at CEN have studied the rates of these processes using ultrafast optical techniques and will use the information to produce more efficient solar cells.

CEN researchers are also developing nanowire light emitting diode (LED) structures to understand and eliminate the reduction in efficiency that occurs at high currents in conventional LEDs. By changing the dimensions of the nanowires, they have also been able to adjust the color of the generated light.

Center for Gas Separations Relevant to Clean Energy Technologies (CGS)

Director

Berend Smit

Lead Institution

University of California, Berkeley

Partner Institutions

University of California, Davis

University of California, Los Angeles

University of Minnesota

Lawrence Berkeley National

Laboratory

National Energy Technology

Laboratory

Texas A&M University

Research Topics

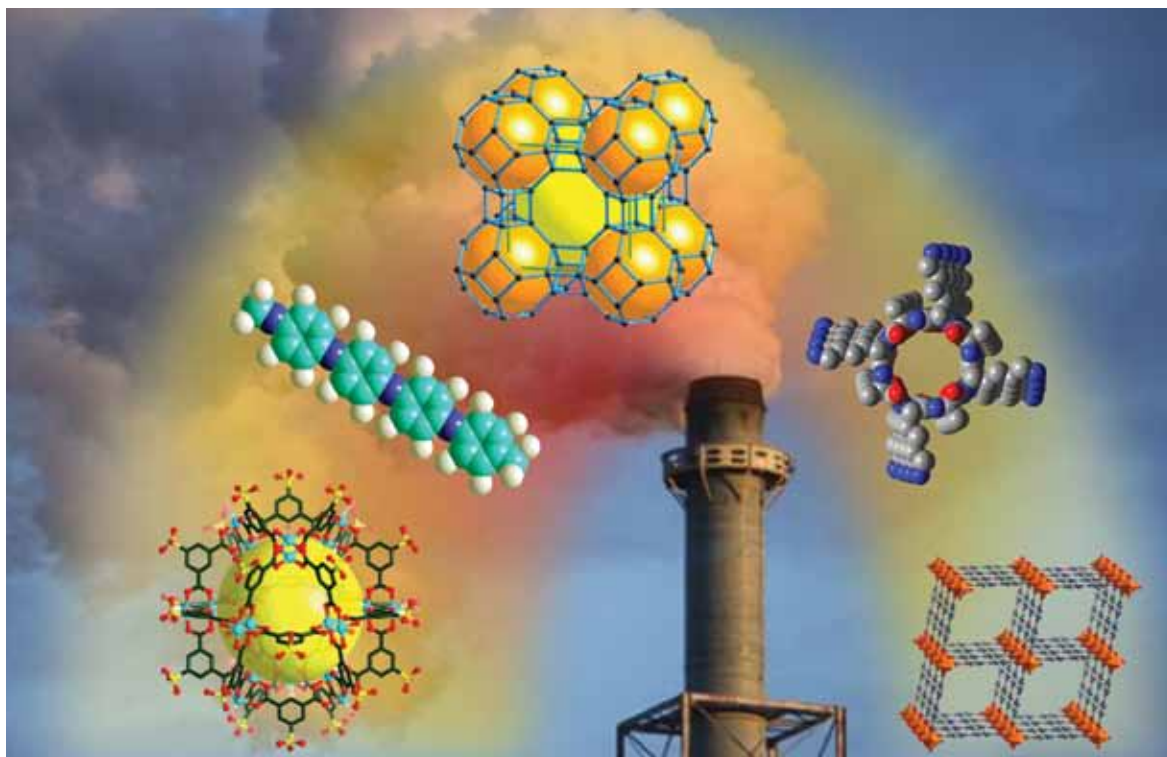
separations, membranes, carbon

capture, matter by design, high

performance computing, organic

materials, inorganic materials,

polymers



ABOVE: The pores of a metal-organic framework, as experienced by gas molecules and calculated by computer simulations. **TOP:** The structure of some representative materials developed at CGS (clockwise): metal-organic polyhedron, polyaniline, zeolitic imidazolate framework, cyclic-peptide nanotube, metal-organic framework.

Mission

To develop new strategies and materials that allow for energy efficient gas separations based on molecule-specific chemical interactions, with a focus on carbon capture.

Achievements

CGS has developed new materials with outstanding performance for separating carbon dioxide from other gases. One type of material involves microporous crystals formed by metal atoms linked by organic units—so-called metal-organic frameworks, or MOFs. Combining different metals and linkers leads to an enormous number of new materials. Other materials are based on polymer membranes, which act as highly efficient molecular sieves. The challenge is to find exactly the “right” material—one that selectively removes CO₂ from flue gas with minimal impact on the efficiency of a coal-fired power plant. To support the design of these new materials, researchers at CGS are developing experimental and computational techniques to understand and predict the relationship between material structure and performance.

Center for Nanoscale Control of Geologic CO₂ (NCGC)

Director

Donald J. DePaolo

Lead Institution

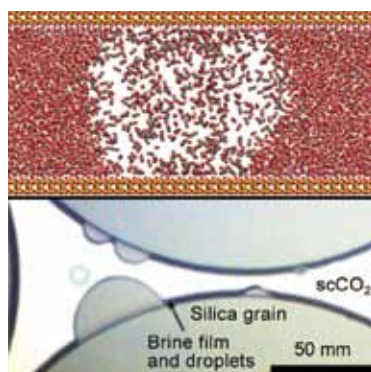
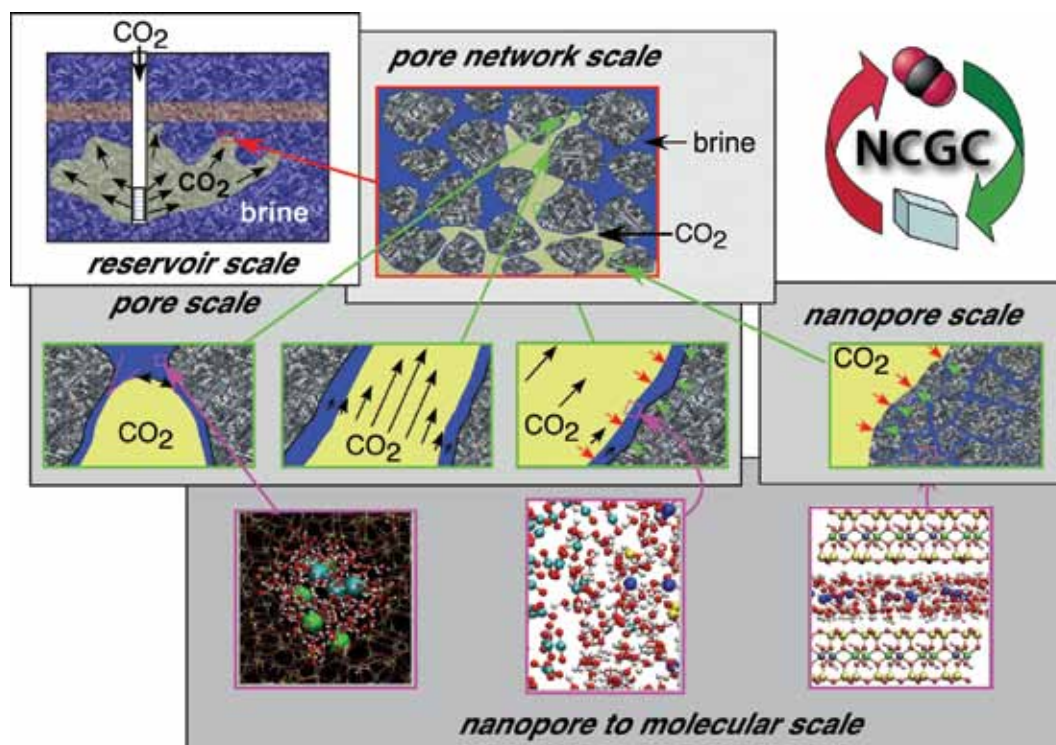
Lawrence Berkeley National
Laboratory

Partner Institutions

University of California, Davis
Lawrence Livermore National
Laboratory
Massachusetts Institute of Technology
Oak Ridge National Laboratory
Ohio State University
Washington University in St. Louis

Research Topics

extreme environment, carbon
sequestration, interfaces, high
performance computing, inorganic
materials, polymers, oxides



ABOVE: (top) Simulation of water and CO₂ between quartz surfaces (15 nm wide cell, cyan: C, red: O, white: H, yellow: Si). (bottom) Micrograph of silica pore with trapped CO₂ (white), brine-films and bridges (85 bar, 45°C).

TOP: The CO₂ distribution in a reservoir is controlled by the underlying pore network. Important processes include capillary breakthrough, multiphase flow, diffusive exchange and reactions across CO₂-water interfaces.

Mission

To use new investigative tools, combined with experiments and computer simulations, to build a fundamental understanding of molecular-to-pore-scale processes in fluid-rock systems, and to demonstrate the ability to control critical aspects of flow, transport, and mineralization in porous rock media as applied to geologic sequestration of CO₂.

Achievements

The efficacy of geologic CO₂ storage can only be assessed with a detailed understanding of molecular, nanoscale and pore scale processes in geologic formations, and the effects of confinement, pressure and temperature on the relevant material properties. The unique character of this Center derives from its focus on CO₂-rich fluids, use of specialized analytical facilities at the participating institutions, and multidisciplinary approach. A major goal is to establish strategies for controlling flow, dissolution, and precipitation in deep subsurface rock formations to achieve efficient filling of pore space with injected supercritical CO₂, with maximum solubility and mineral trapping and near- zero leakage through caprocks, the outer rock crust. The investigations will also provide the scientific basis for improved long-term predictions of reactive transport of CO₂-rich fluid that will help ensure storage for 1000 years or more into the future.

Center on Nanostructuring for Efficient Energy Conversion (CNEEC)

Directors

Fritz Prinz and Stacey Bent

Lead Institution

Stanford University

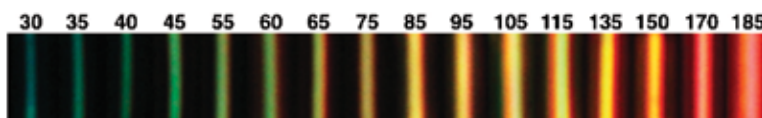
Partner Institutions

Carnegie Institution for Science
Technical University of Denmark
HRL Laboratories

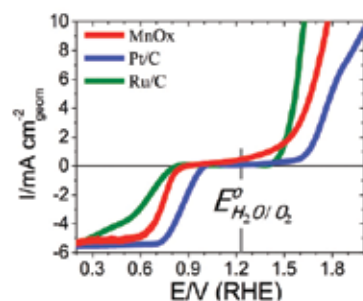
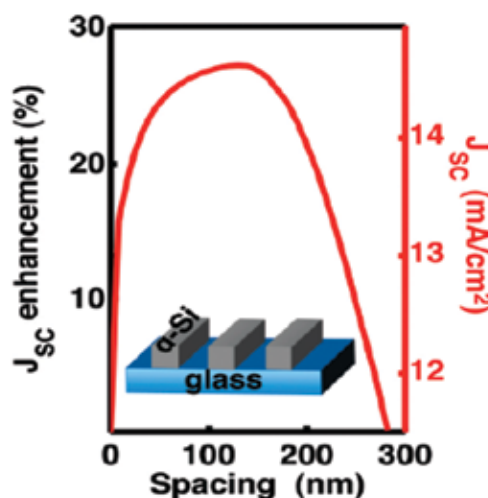
Research Topics

catalysis, solar photovoltaic, solar fuels, photosynthesis, electrical energy storage, defects, hydrogen, interfaces, matter by design, charge transport, inorganic materials, semiconductors, oxides

Optical Resonances in Si nanowires



Enhancing performance of PV cells



ABOVE: Nanostructured manganese oxide (MnO_x) catalysts exhibit bifunctional activity for both oxygen reduction and oxygen evolution reactions comparable to the precious-metal platinum and ruthenium containing catalysts. **TOP:** Under white light, 30 – 185 nm diameter silicon nanowires exhibit tunable optical resonances. A simulation of a solar cell made of amorphous-silicon nanobeams shows a 25 percent increase in the electric current.

Mission

To understand how nanostructuring can enhance efficiency for energy conversion and to solve fundamental cross-cutting problems in advanced energy conversion and storage systems.

Achievements

Research at CNEEC provides the scientific foundation for physical and chemical phenomena that underlie key energy conversion and storage processes. By developing scientific concepts and tools to fabricate and characterize nanostructured materials, CNEEC researchers optimize charge transport, light absorption, reaction kinetics, and thermodynamics to achieve breakthroughs in energy conversion efficiency.

Research achievements include the design of one-dimensional silicon (Si) nanostructures to manage photons, or light packets, in order to enhance the conversion of light collection to electric current, while using less than half of the semiconductor materials used in current solar cells. In another area, bifunctional catalysts containing earth-abundant, non-precious metals show high activity for the oxygen reduction and evolution reactions that play critical roles in the efficiencies of fuel cells and solar fuel reactors.

Light-Material Interactions in Energy Conversion (LMI)

Director

Harry Atwater

Lead Institution

California Institute of Technology

Partner Institutions

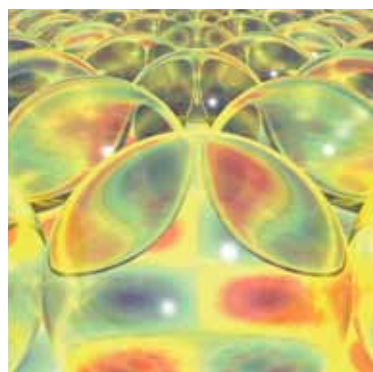
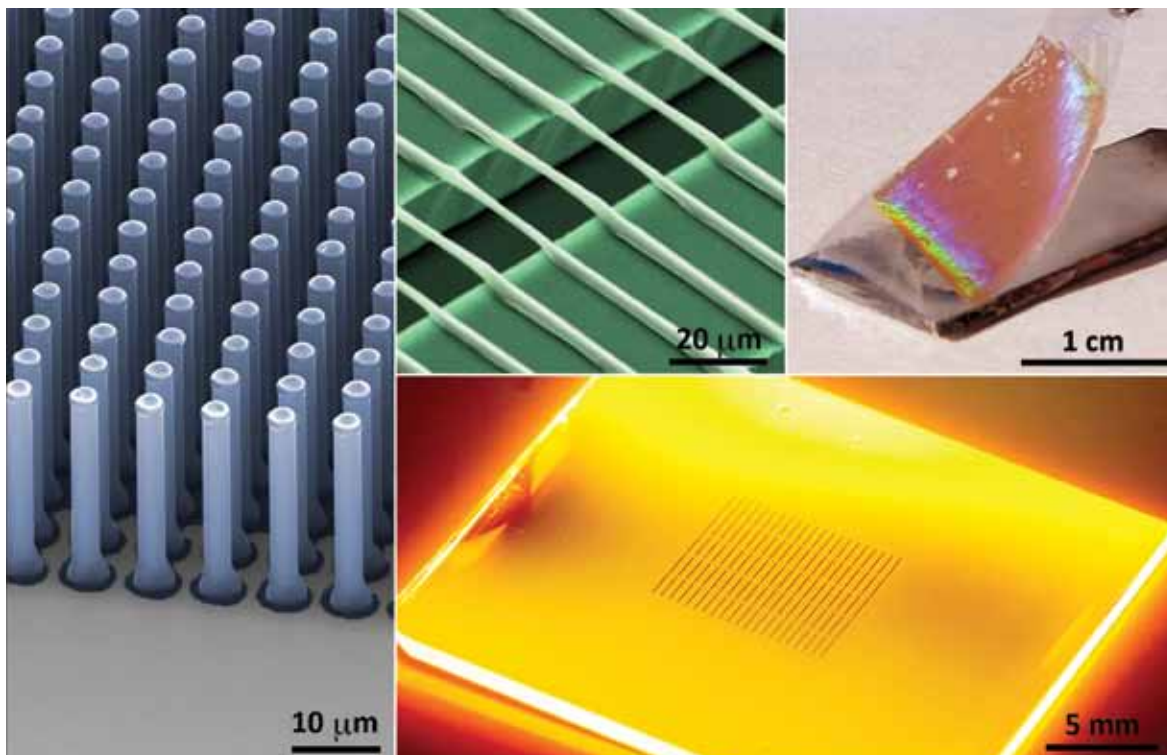
University of California, Berkeley

University of Illinois, Urbana-

Champaign

Research Topics

catalysis, solar photovoltaic, solar fuels, solid state lighting, photosynthesis, matter by design, inorganic materials, semiconductors, oxides



ABOVE: Simulations are used to compute light absorption in silicon solar cells coated with nanospheres. The small glass spheres could enable efficient coupling of sunlight to ultrathin semiconductor layers, significantly increasing solar cell efficiency. **TOP:** LMI synthesized (clockwise from left): silicon micro-wire arrays; transparent, conductive microelectrodes; 3-D, flexible, silicon photonic crystals in plastic; and luminescent waveguide solar concentrators.

Mission

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.

Achievements

The LMI has a strong focus on the design and characterization of complex photonic materials to enable revolutionary advances in photovoltaic energy conversion and fuel synthesis from sunlight. Research within the LMI spans a broad range of activities from fundamental theoretical advances and creative optical design to innovative material synthesis, device fabrication, and novel characterization techniques. Recent achievements include the demonstration of enhanced light absorption in silicon micro-wire array solar cells; realization of flexible photovoltaic concentrators based on microscale silicon solar cells embedded in luminescent waveguides; refinement of theoretical single-junction solar cell efficiency taking into account light-trapping effects; and development of advanced fabrication techniques to build complex, three-dimensional materials with unprecedented photonic, electronic and phononic properties.

Molecularly Engineered Energy Materials (MEEM)

Director

Vidvuds Ozolins

Lead Institution

University of California, Los Angeles

Partner Institutions

University of California, Berkeley

Eastern Washington University

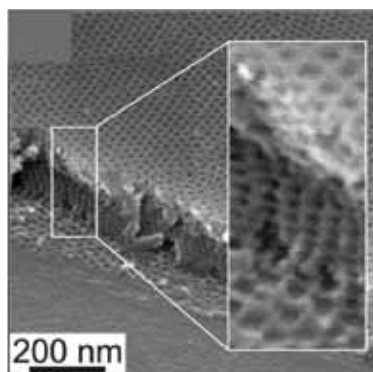
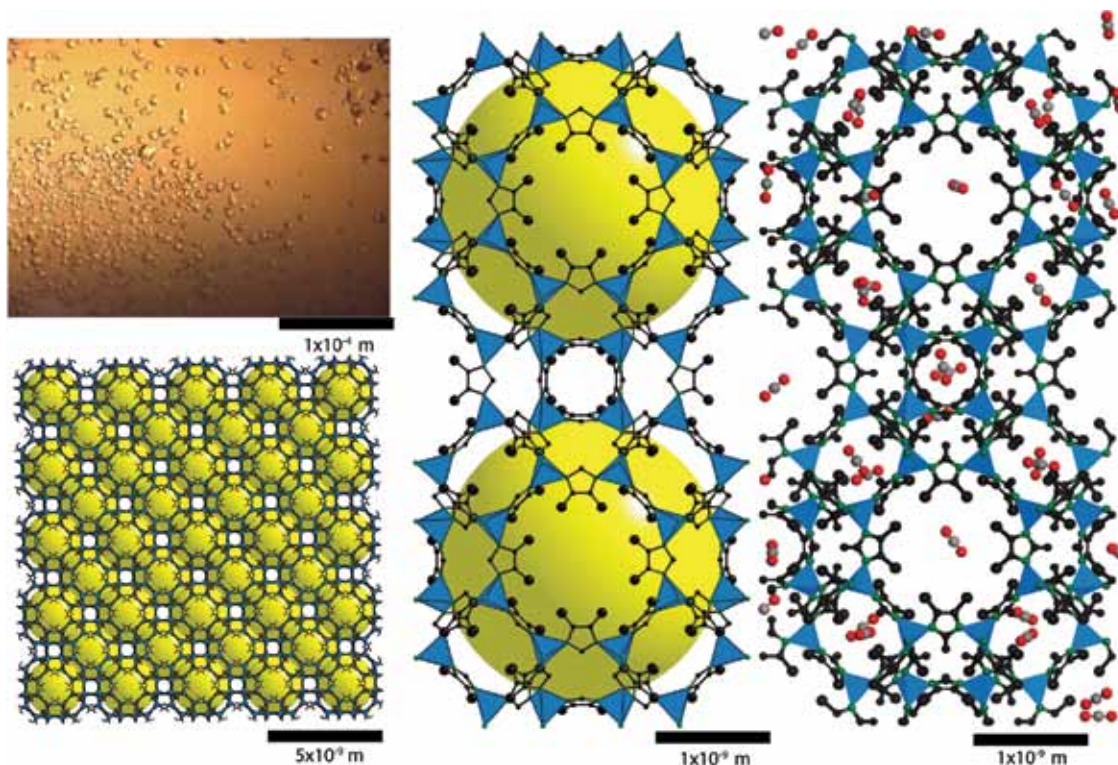
University of Kansas

National Renewable Energy

Laboratory

Research Topics

solar photovoltaics, electrical energy storage, membranes, carbon capture, matter by design, charge transport, organic materials, polymers, oxides



ABOVE: Porous architecture of niobium oxide, a unique high-performance material for next-generation supercapacitors. The pores are about 15 nm in diameter and extend uniformly throughout the material. **TOP:** ZIF-25, a new material for capturing carbon dioxide in an interconnected three-dimensional framework of very small pores. Each pore is less than 3 nm, or three billionths of a meter in diameter.

Mission

To acquire a fundamental understanding and control of nanoscale material architectures for conversion of solar energy to electricity, electrical energy storage, and separation/capture of greenhouse gases.

Achievements

Researchers at MEEM are creating new zeolitic imidazolate frameworks, or ZIFs, materials with ultra-high internal surface areas that can capture greenhouse gases such as carbon dioxide, CO₂. In a collaboration between computational and experimental research groups, MEEM scientists have designed and synthesized new types of ZIFs with ultra-high densities of small pores tailored for unprecedented performance in CO₂ uptake. In another development, MEEM researchers have achieved enhanced energy storage by creating new materials with highly ordered pore-solid architectures. Their interconnected porosity enables an electrolyte to reach the redox-active walls, ensuring that all of the material is effectively storing energy. In the case of niobium oxide, the resulting energy density increases by a factor of three compared to nonporous materials. Moreover, the crystallographic orientation of the solid walls further enhances energy storage.

Center for Inverse Design (CID)

Director

Bill Tumas (Interim)

Lead Institution

National Renewable Energy
Laboratory

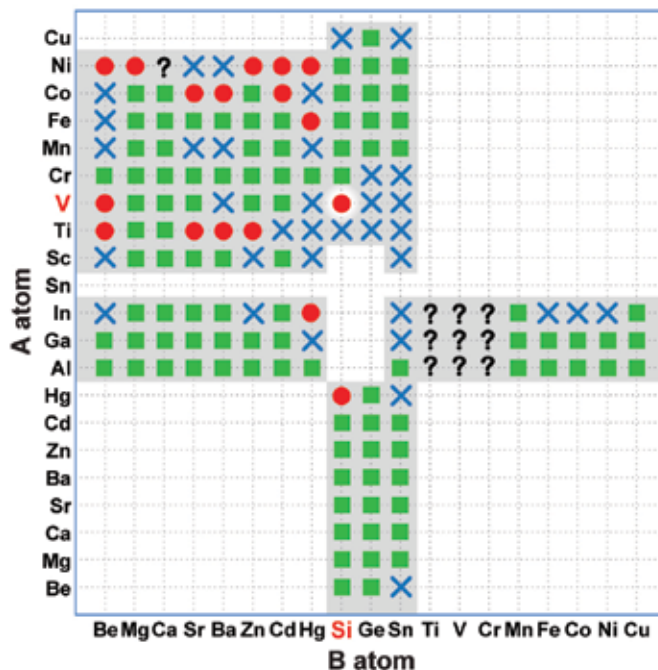
Partner Institutions

Northwestern University
Oregon State University
Stanford University

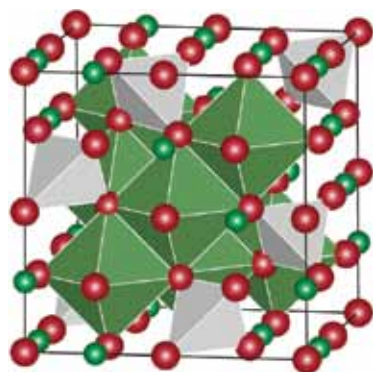
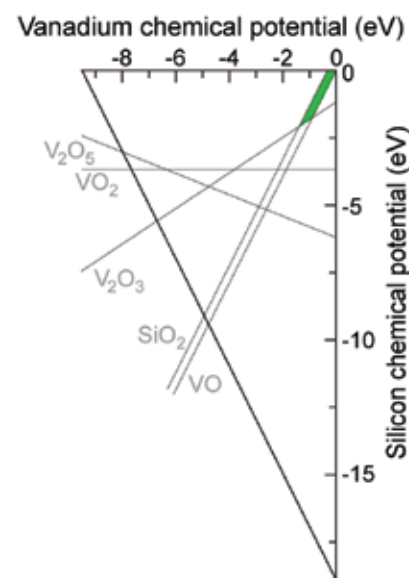
Research Topics

solar photovoltaics, defects, matter by
design, high performance computing,
inorganic materials, semiconductors,
oxides

Reported (■); Missing-but-unstable (X);
Missing-and-predicted-stable (●) A_2BO_4 Compounds



Stability Range (green sliver) of
Newly Predicted V_2SiO_4



ABOVE: A_2BO_4 spinel structure
(A-green; O-red). **TOP:** Quantum
mechanical calculations of postulated
 A_2BO_4 compounds and their many
possible “competing” phases (right)
leads to identification of previously
missed materials. In the matrix (left),
materials marked with red dots are
predicted stable; those with blue x's
are not stable.

Mission

To replace trial-and-error methods used in the development of materials for solar energy conversion with an inverse design approach powered by theory and computation.

Achievements

The Center for Inverse Design is realizing its “materials by design” challenge with discovery-class approaches to produce new materials with new functionalities. Materials with a formula of A_2BX_4 , where A, B, and X are different elements, are a large, important family of electro-optical ternary compounds for transparent conducting oxides and solar-cell absorbers used in solar cells, and contain Earth-abundant elements with $X = O, S, Se, \text{ or } Te$. For example, of the 164 oxide possibilities in this A_2BX_4 class ($X = O$; see matrix above), only 101 are reported. What happened to the other 63? Were they missing for a “good” reason (i.e., unstable; X in matrix) or for no good reason (i.e., stable; dot in matrix)? This discovery of missing materials is a major accomplishment of the Center. This case includes the discovery of 17 new, stable oxides and the determination that the other 36 are not stable and thus, do not exist. Analogous discoveries have also been made for the other “X” compounds.

Catalysis Center for Energy Innovation (CCEI)

Director

Dion Vlachos

Lead Institution

University of Delaware

Partner Institutions

University of Massachusetts, Amherst

University of Minnesota

California Institute of Technology

University of Pennsylvania

Princeton University

Lehigh University

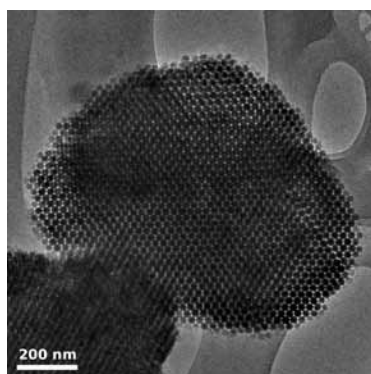
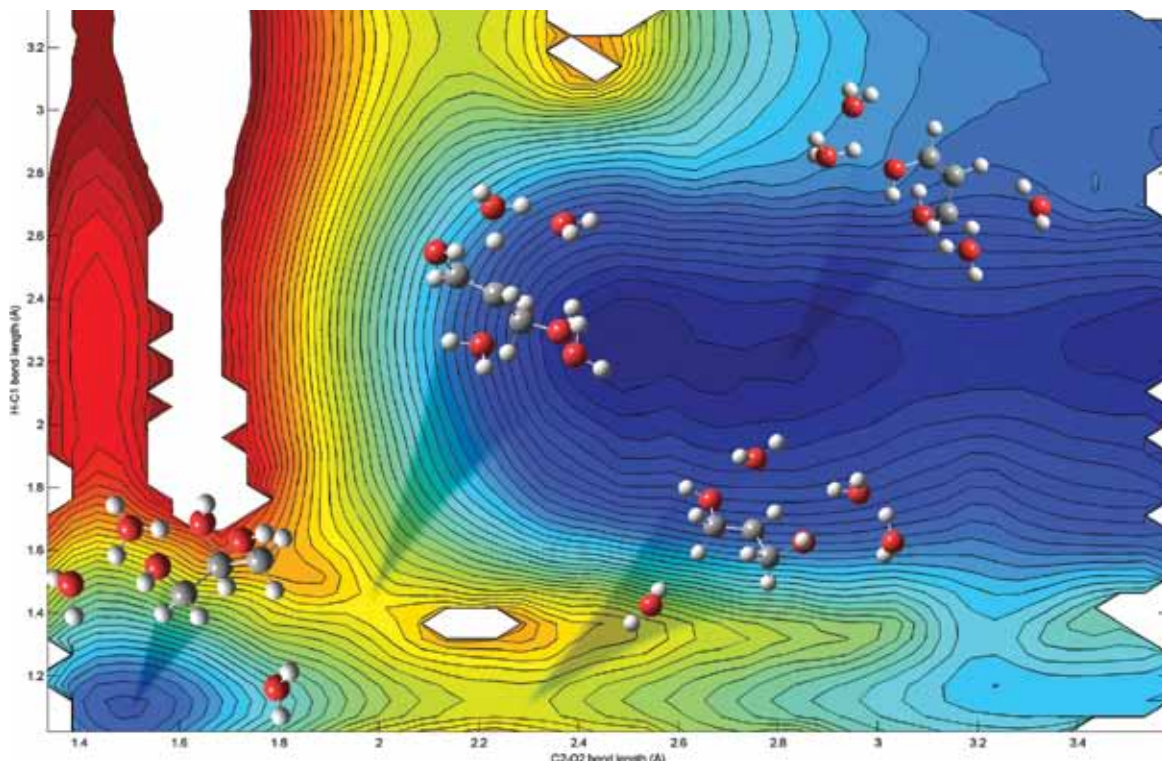
University of Southern California

North Carolina State University

Brookhaven National Laboratory

Research Topics

catalysis, biofuels, matter by design,
organic materials, inorganic materials,
oxides



ABOVE: Tin-beta zeolite isomerizes glucose to fructose followed by dehydration to hydroxymethylfurfural, a value-added intermediate. Depicted is a mesoporous zeolite. **TOP:** Computations reveal the mechanism of acid-catalyzed dehydration of biomass derivatives along the free energy landscape. Depicted is the conversion of glycerol toward acrolein.

Mission

To design and characterize novel catalysts for the efficient conversion of the complex molecules comprising biomass into chemicals and fuels.

Achievements

Researchers at CCEI have developed a novel catalyst to efficiently convert biomass-derived sugars into chemicals and fuels. The recent push for renewable chemicals and fuels has revitalized interest in carbohydrate chemistry. A particularly important and difficult reaction is the isomerization of glucose to fructose, an intermediate step in the conversion of biomass to value-added products. CCEI researchers have shown that the use of tin-beta zeolite as a catalyst for this reaction offers significant advantages over traditional enzyme catalysts. It is unaffected by impurities that harm enzyme activity and is compatible with harsh environments, such as acidic solutions. This development could have a very significant impact on the production of renewable chemicals and fuels.

Energy Frontier Research in Extreme Environments (EFree)

Director

Ho-kwang Mao

Lead Institution

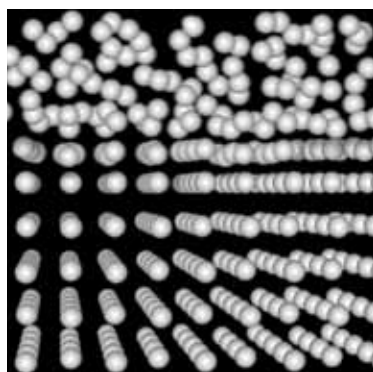
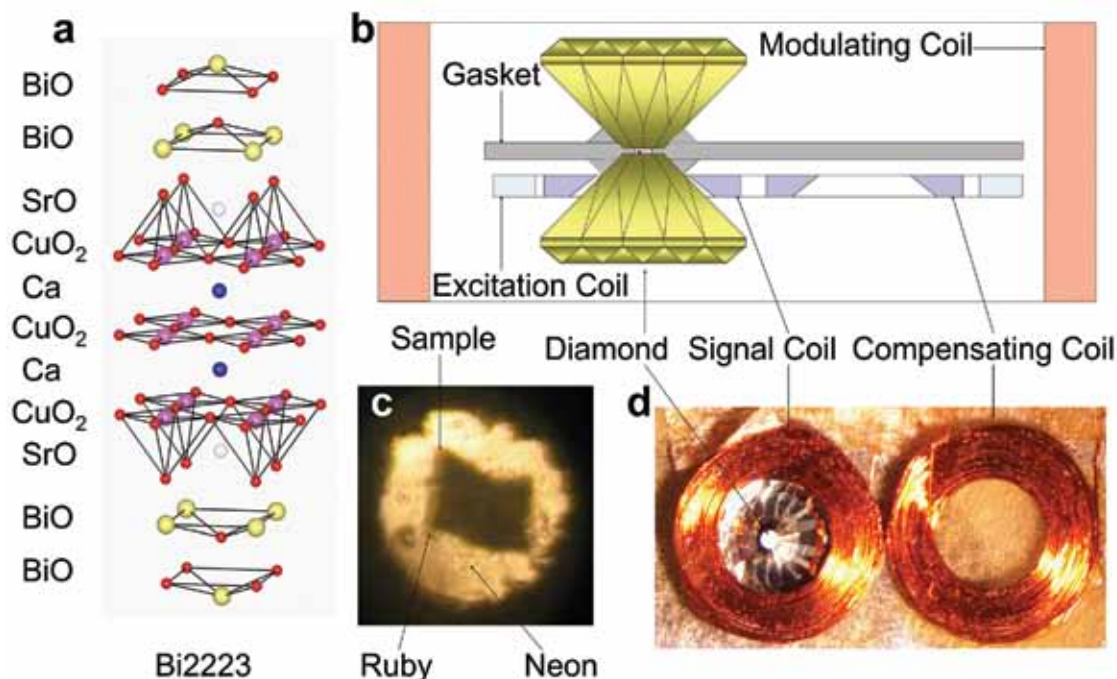
Carnegie Institution of Washington

Partner Institutions

Argonne National Laboratory
Arizona State University
California Institute of Technology
Cornell University
Florida International University
Jefferson National Laboratory
Lawrence Livermore National Laboratory
Missouri State University
Pennsylvania State University
Stanford University
University of Texas at Austin

Research Topics

electrical energy storage, superconductivity, extreme environment, defects, hydrogen, ultrafast science, inorganic materials, rare earth elements, semiconductors, oxides, actinides



ABOVE: Lithium, a highly mobile atom, is a vital component of batteries. The mobility is greatly enhanced by pressure, reducing the melting point by more than 50%. **TOP:** The creation of superconductors with the highest transition temperatures (T_c) is one of the great science quests that could reduce energy losses in transmission lines. Subjecting a bismuth-based superconductor to high pressures results in an unusual T_c increase of 36% to 136 K.

Mission

To accelerate the discovery and creation of energy-relevant materials using extreme pressures and temperatures.

Achievements

The extreme pressure-temperature studies at EFree provide a route to discovering new materials with enhanced performance for energy applications. Collaborations among EFree scientists of complementary expertise have led to significant achievements. EFree theoreticians have calculated and predicted elements and compounds with favorable properties for energy storage and transport. Experimentalists have developed novel techniques to probe properties of materials in real time under extreme environments. Together, they have reported exceptionally high superconductivity temperatures, record-low melting temperatures, and record-high electronic energy levels. The fundamental understanding that researchers have gained of the transitions from insulator to metal from direct observations at high pressures may help them design better materials for energy production, storage and transfer. Novel nanomaterials and superhard mesoporous diamonds, initially discovered at high pressures, have now been synthesized by EFree so that they are stable at ambient conditions.

Center for Materials Science of Nuclear Fuels (CMSNF)

Director

Todd Allen

Lead Institution

Idaho National Laboratory

Partner Institutions

Argonne National Laboratory

Colorado School of Mines

University of Florida

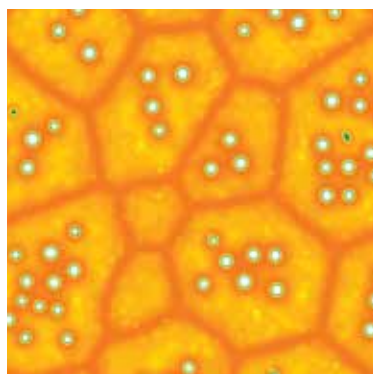
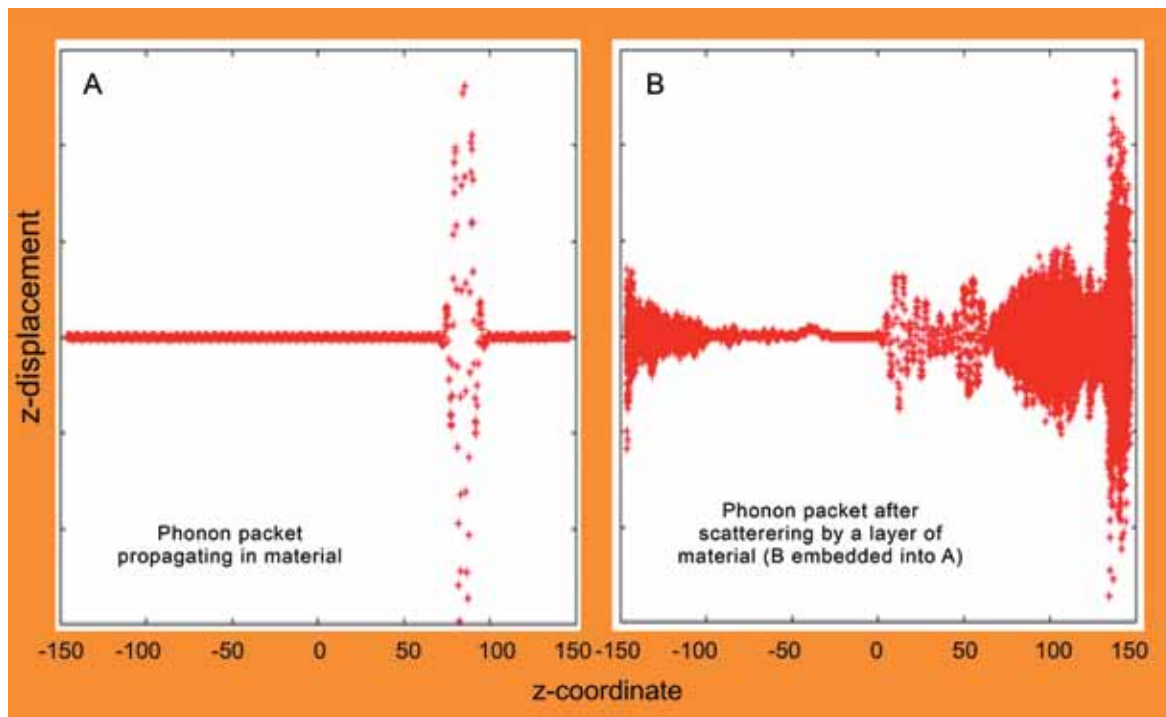
Florida State University

Oak Ridge National Laboratory

University of Wisconsin

Research Topics

nuclear, extreme environment, defects, matter by design, high performance computing, inorganic materials, actinides



ABOVE: Model prediction of void nucleation under irradiation. **TOP:** A packet of phonons in silicon (material A) propagate and interact with a thin slab of silica (material B) embedded along its trajectory, resulting in a complex scattering of the heat transferring phonons (right). The outcome of similar scattering events at voids and dislocations will provide input to the simulations of thermal transport in uranium oxide.

Mission

To achieve a first-principles based understanding of the effect of irradiation-induced defects and microstructures on thermal transport in oxide nuclear fuels.

Achievements

Scientists at CMSNF are developing capabilities to link models that describe nanometer-sized phenomena to models that describe important physical properties in nuclear fuel. The specific nanometer-sized phenomena these models predict are the formation of defects in irradiated nuclear fuel. Key physical properties include the physical dimensions of a sample and the ability to transfer heat. Researchers at CMNSF have successfully developed a model that describes how nanometer-sized pockets empty of atoms, known as voids, are formed under irradiation and how those voids block heat flow, also known as phonon transport. Contrary to the previously held beliefs, CMSNF scientists discovered that the time evolution of the formation of voids during irradiation differs from the time evolution of the increase in material volume, known as swelling. From a heat transfer point of view, voids act to block the carriers of heat (phonons) in the material. CMSNF scientists are now investigating in greater detail how the voided spaces limit heat flow. These results may ultimately help improve the performance of fuel in nuclear reactors under normal and accident scenarios.

Argonne-Northwestern Solar Energy Research (ANSER) Center

Director

Michael R. Wasielewski

Lead Institution

Northwestern University

Partner Institutions

Argonne National Laboratory

University of Chicago

University of Illinois, Urbana-
Champaign

Yale University

Research Topics

catalysis, solar photovoltaics, solar fuels, photosynthesis, hydrogen, interfaces, matter by design, charge transport, ultrafast science, organic materials, inorganic materials, polymers, semiconductors, oxides



ABOVE: Organic photovoltaic cell connected to a solar cell analyzer and tested under illumination that mimics sunlight. **TOP:** ANSER graduate student Charusheela Ramanan characterizes light-driven charge separation in new molecules and materials for solar energy conversion using ultrafast laser technology.

Mission

To revolutionize our understanding of molecules, materials and methods necessary to create dramatically more efficient technologies for solar fuels and electricity production.

Achievements

ANSER researchers have developed new molecules, materials and fundamental insights into systems for solar fuels and electricity production. They have made advances in understanding how to couple light-driven charge separation to catalysts that use earth-abundant elements to generate hydrogen by splitting water molecules. Using the Advanced Photon Source at DOE's Argonne National Laboratory, ANSER researchers have found that placing light-absorbing molecules in ordered layers is essential to significantly increase the efficiency of the solar energy to electricity conversion in plastic solar cells. ANSER researchers have also overcome the electronic limitations for using ordinary "rust" (hematite, $\alpha\text{-Fe}_2\text{O}_3$), which is a solar absorber and water oxidation catalyst. They have put hematite to work in photoelectrochemical cells for solar energy conversion by designing a new route to intricately folded Fe_2O_3 electrodes based on atomic layer deposition.

Center for Electrical Energy Storage (CEES)

Director

Michael Thackeray

Lead Institution

Argonne National Laboratory

Partner Institutions

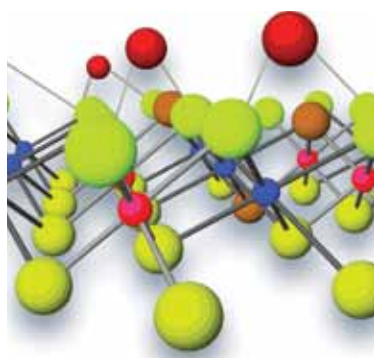
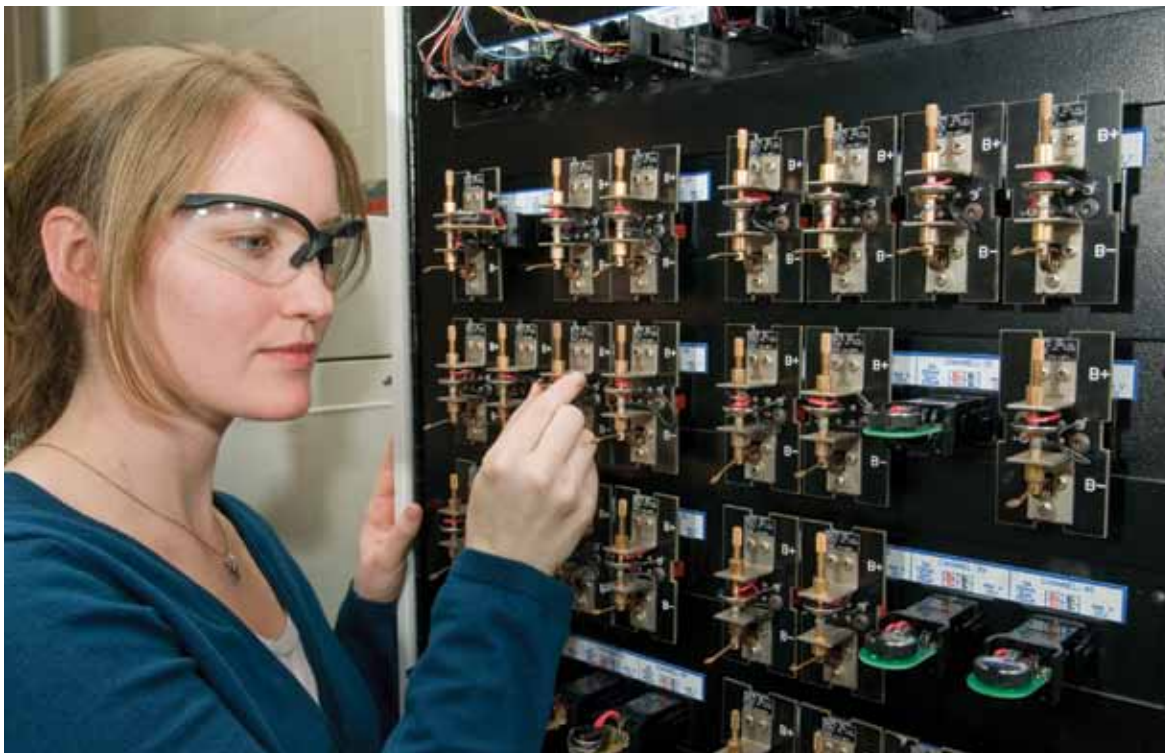
University of Illinois, Urbana–

Champaign

Northwestern University

Research Topics

electrical energy storage, interfaces, matter by design, charge transport, high performance computing, organic materials, inorganic materials, oxides



ABOVE: CEES uses advanced molecular-scale approaches, including both experiments and high-level theory, to obtain a new understanding of the electrode-electrolyte interface, critical to achieving a much higher level of performance of lithium-ion batteries and other energy storage materials.

TOP: CEES Scientist Lynn Trahey loads a coin-sized cell on a testing unit used to evaluate electrochemical cycling performance in batteries.

Mission

To acquire a fundamental understanding of interfacial phenomena controlling electrochemical processes that will enable dramatic improvements in the properties and performance of energy storage devices, notably Li ion batteries.

Achievements

The ideal battery for energy storage combines high energy and power output, extended lifetimes and safe operation. These properties are ultimately controlled by the transport of ions, for example lithium, and electrons into the battery electrodes and by the stability of the interfaces separating the electrodes from the electrolyte solution. The high reactivity of lithium battery electrodes can lead to unwanted chemical reactions, loss of storage capacity and even spontaneous combustion. CEES seeks to identify radical improvements in battery capabilities through the creation of novel, stabilized electrode-electrolyte architectures and a better understanding of the processes that occur at the electrified interface. Recent achievements include the improved understanding of how lithium is inserted into electrodes; use of microscale electrode structures to extend reversibility and lifetime; development of autonomous repair and shutdown capabilities for safer operation; and surface modification and nanostructuring of electrode materials for higher power.

Institute for Atom-efficient Chemical Transformations (IACT)

Director

Christopher L. Marshall

Lead Institution

Argonne National Laboratory

Partner Institutions

Brookhaven National Laboratory

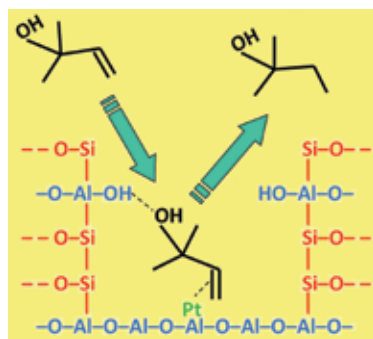
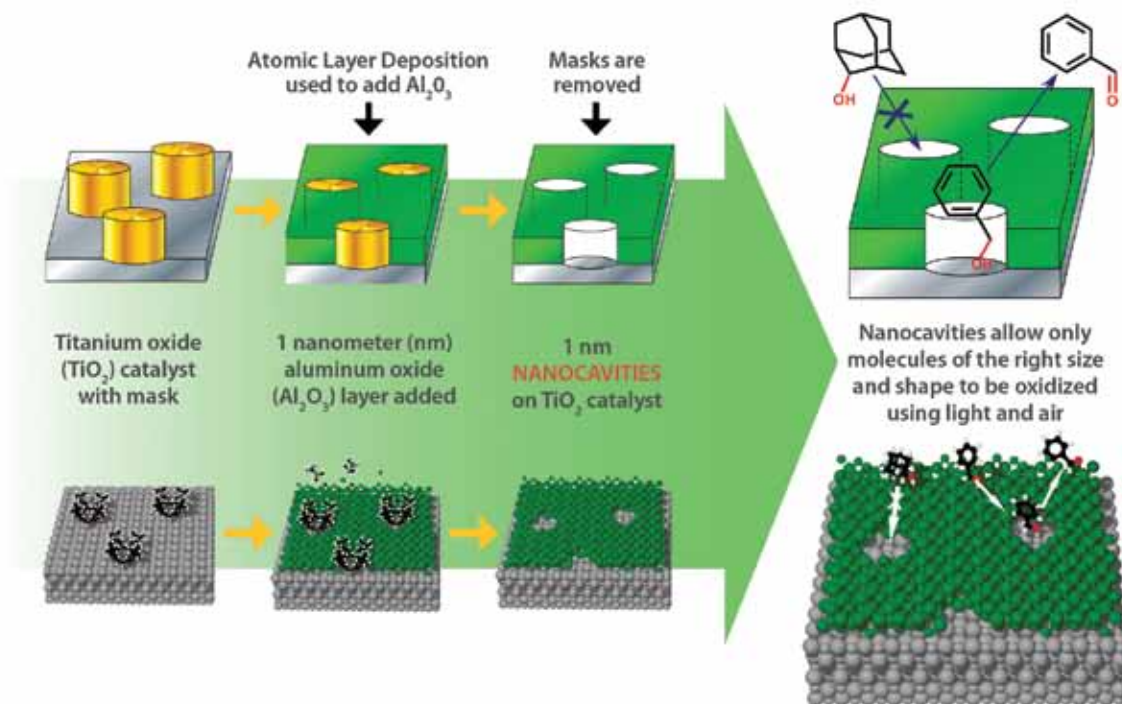
Northwestern University

Purdue University

University of Wisconsin at Madison

Research Topics

catalysis, biofuels, interfaces, matter by design, organic materials, inorganic materials, oxides



ABOVE: By using different components on the walls of the nanocavities, IACT researchers create inorganic catalysts that can hold biomass materials in place while the metal at the bottom performs the required reaction. **TOP:** Individual molecular masks on a titanium dioxide (TiO_2) catalyst allows cavities of less than one nanometer in diameter to be grown in a layer less than one nanometer thick. The "nanocavity" catalyst only reacts with specific molecules.

Mission

To address key catalytic conversions that could improve the efficiency of producing fuels from biomass. IACT 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.

Achievements

Catalysts enable production of most of today's fuels and chemical products. However, many catalysts react unselectively, limiting their usefulness. Scientists and engineers from IACT have developed a new technique that modifies catalysts to react selectively only with molecules of a certain size and shape. In the reaction shown above, titanium oxide materials oxidize alcohols into valuable products using only light and air. Normally, this reaction is unselective, but "nanocavity" layers permit only alcohol molecules of the right shape to reach the catalyst surface and react. By decreasing the energy requirement and the waste associated with making a chemical product, these new "nanocavity" catalysts are now finding uses in other chemical reactions that are important to meeting the nation's energy needs.

Non-equilibrium Energy Research Center (NERC)

Director

Bartosz A. Grzybowski

Lead Institution

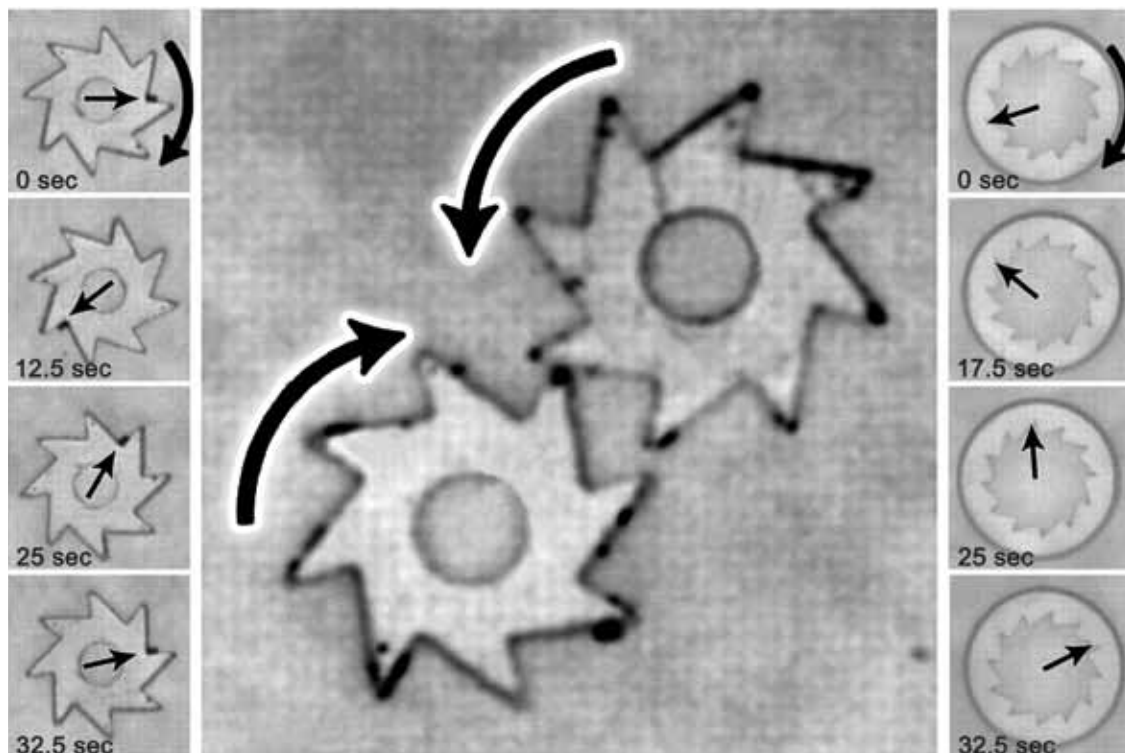
Northwestern University

Partner Institutions

Harvard University
University of Michigan
Ohio State University
Pennsylvania State University

Research Topics

solar photovoltaics, thermoelectrics, separations, electrical energy storage, interfaces, matter by design, charge transport, high performance computing, polymers, inorganic materials, organic materials



ABOVE: An example of an adaptive material in which magenta and violet colors reflect different modes of organization of nanoparticles irradiated with light of different wavelength. **TOP:** The first-ever micromachine powered by random motions of the surrounding bacteria. Bacterial motions are "rectified" by the geometry of the rotating gears.

Mission

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

Achievements

NERC's interdisciplinary team has synthesized and characterized a variety of unique dissipative materials and systems that harness energy from their surroundings and transform it into mechanical, chemical, or electrical work. Examples include molecular-scale machines based on mechanically interlocked molecules, polymeric materials which under mechanical stress can drive chemical reactions, light-switchable and controllable catalysts, nanostructured materials that internally reconfigure in response to light and act as batteries, supercapacitors or photoconductors, as well as microscopic machines in which random motions of the surrounding molecules or microorganisms are rectified into mechanical work. This experimental effort goes hand-in-hand with the theoretical studies aimed at understanding how external free-energy fluxes can be best coupled to self-organization into metastable states, and how dissipation of the delivered energy can be minimized.

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

Director

Maureen McCann

Lead Institution

Purdue University

Partner Institutions

Argonne National Laboratory

National Renewable Energy

Laboratory

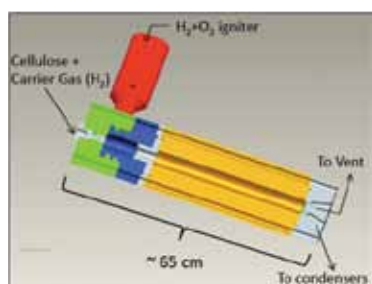
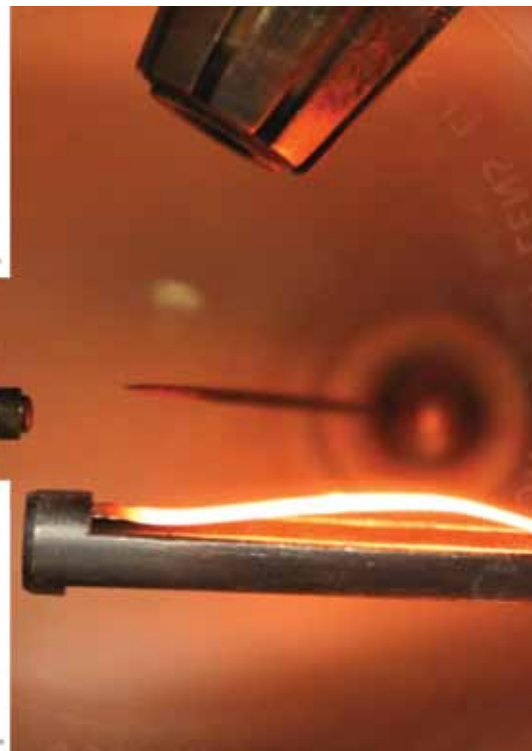
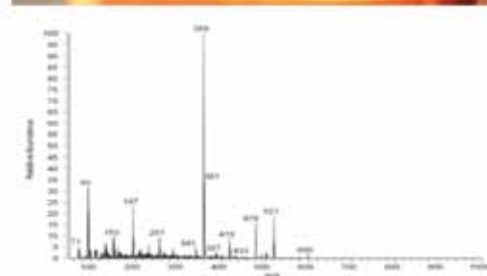
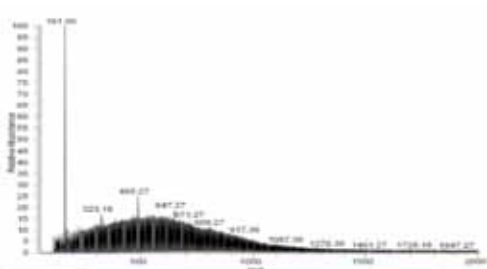
Northeastern University

University of Tennessee

Research Topics

catalysis, biofuels, matter by design,

organic materials, polymers



ABOVE: In collaboration with aerospace scientists at Purdue, C³Bio's chemical engineers have built and tested a high-pressure, low-residence-time hydro-pyrolysis unit—a "Rocket Reactor" to convert biomass compounds into fuel molecules. **TOP:** Mass spectrometer analysis of reaction products from cellulose pyrolysis. The charts represent high residence-time (upper) and low residence-time (lower) spectra.

Mission

To develop transformational knowledge and technologies to optimize the efficiency and effectiveness of biomass conversion to advanced biofuels through rational and synergistic design of both physical and chemical conversion processes and the biomass itself.

Achievements

Pyrolysis heats biomass to very high temperatures where a gas forms and then condenses into bio-oil. However, the bio-oil is highly corrosive and contains too much oxygen as well as a wide range of other undesirable products. C³Bio researchers have developed new mass spectrometry methods to measure the reaction products in the gas phase. Using a precisely controlled pyroprobe instrument, C³Bio evaluates the the products that come from cellulose. Instead of the thousands of products observed during conventional pyrolysis, they observe a few discrete masses using fast hydro-pyrolysis—a heating rate of 1000K per second in the presence of hydrogen. By varying gas temperature and flow rate, researchers can control the types of products that form. Removing unwanted oxygen from biomass, a key step in developing energy-rich fuels, may now be feasible.

Materials Science of Actinides (MSA)

Director

Peter Burns

Lead Institution

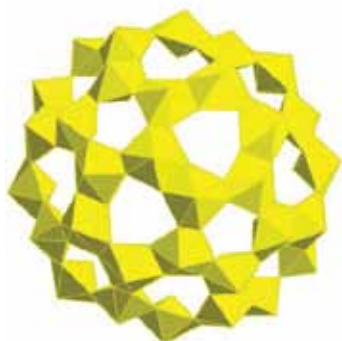
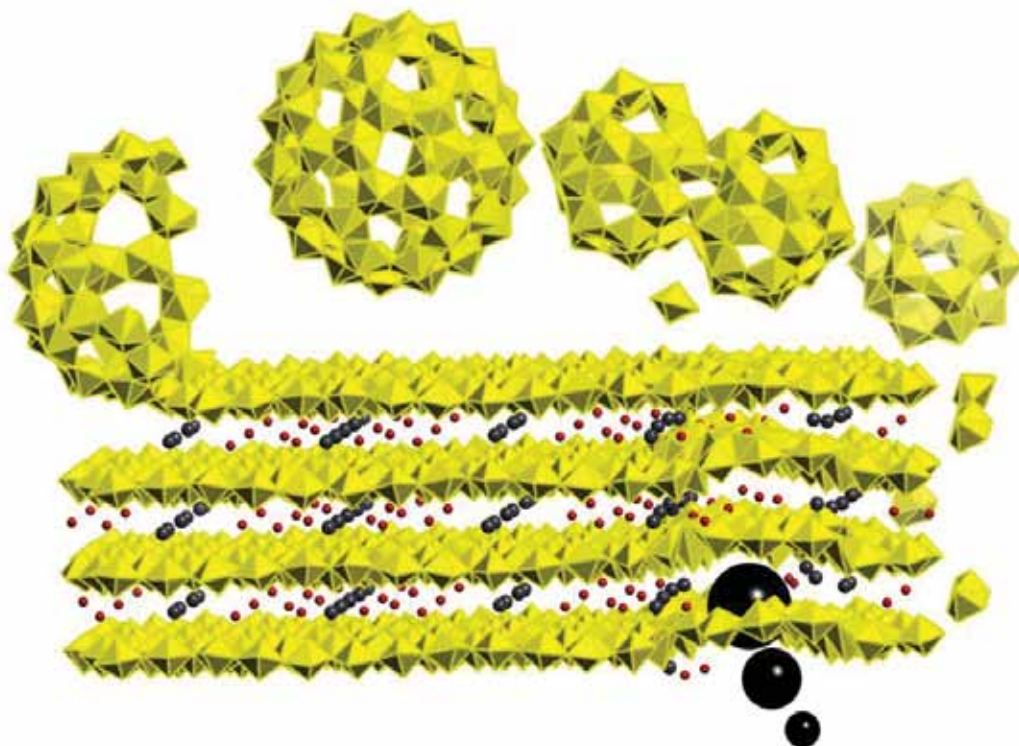
University of Notre Dame

Partner Institutions

University of California, Davis
George Washington University
University of Michigan
University of Minnesota
Oak Ridge National Laboratory
Pacific Northwest National Laboratory
Rensselaer Polytechnic Institute
Sandia National Laboratories
Savannah River National Laboratory

Research Topics

nuclear, extreme environment,
separations, matter by design,
inorganic materials, actinides



ABOVE: The nanocluster U_{60} contains 60 uranium atoms as well as oxygen, and has a mass about 80 times higher than that of a single uranium atom. More than 50 such clusters have been created in water over the pH range 3–13.

TOP: An artistic representation of the three research themes of the MSA EFRC: complex actinide materials, nano-scale actinide materials, and actinide materials under extreme environments.

Mission

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.

Achievements

Researchers at MSA are advancing knowledge in complex actinide materials at the nanoscale, and their behaviors at high temperatures and pressures, as well as in intense radiation fields found in reactors and nuclear waste. Actinides (including uranium, thorium and plutonium) are the fuels of nuclear energy and are major constituents in nuclear waste. Research at MSA is laying the foundation for controlling actinide materials at the nanoscale by creating more than 50 uranium materials using a new type of chemical bonding that makes molecular structures with curved shapes. These structures allow control of the chemical compositions of materials in ways that are important for the manufacturing of new types of nuclear fuels and for the recycling of nuclear materials.

Center for Atomic-Level Catalyst Design (CALCD)

Director

James J. Spivey

Lead Institution

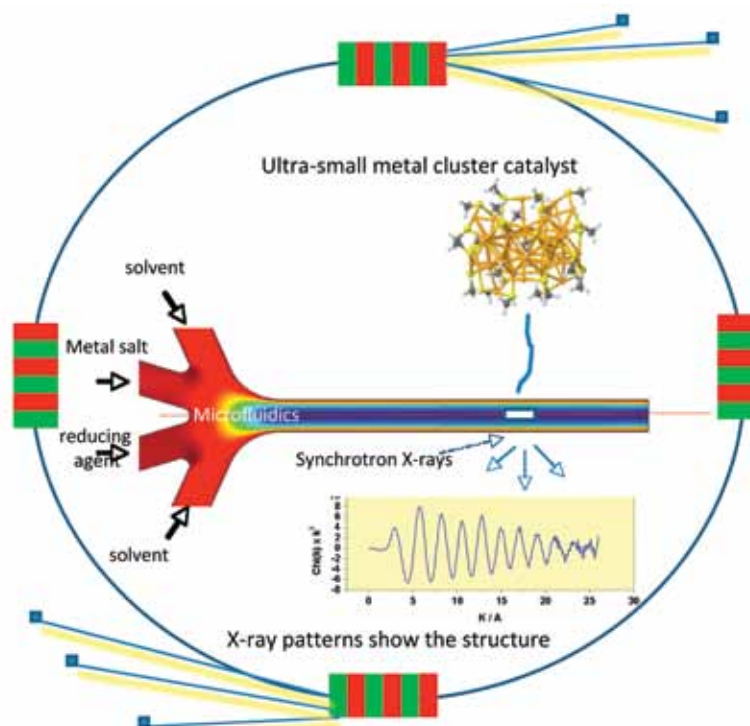
Louisiana State University

Partner Institutions

Clemson University
University of Florida
Georgia Institute of Technology
Grambling State University
Louisiana Tech University
Oak Ridge National Laboratory
Ohio State University
Pennsylvania State University
Texas A&M University
Vienna University of Technology,
Austria
University of Utrecht, Netherlands

Research Topics

catalysis, biofuels, hydrogen, interfaces,
matter by design, inorganic materials,
oxides

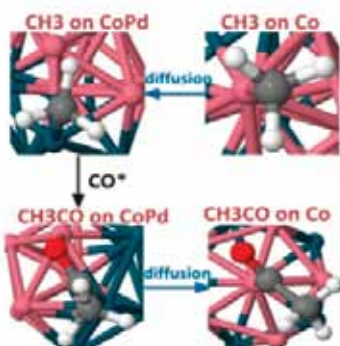


Mission

To build effective catalysts from first principles via computational catalysis and atomic-level synthesis.

Achievements

Researchers at CALCD are developing ways to make catalysts with atomic-level control of the structure. This level of control is required to match the precision of computational simulations that researchers use to follow chemical reactions. Understanding and controlling these reactions is essential to developing clean energy processes. Among other techniques, scientists carefully study the atomic-level structure using X-ray sources available at Louisiana State University and DOE's Argonne National Laboratory (ANL). As an example, CALCD investigators have teamed with colleagues at Clemson and ANL to prepare and study clusters of fewer than 50 gold atoms, which are then supported on a solid oxide. This represents a significant advance in our ability to control these clusters at an atomic level. Computational and experimental characterization of these materials is underway with the goal of demonstrating a seamless process of preparing catalysts at the atomic scale, modeling their properties and experimentally confirming both their structure and their catalytic behavior.



ABOVE: Developing computational tools for understanding surface diffusion on ultra-small multifunctional catalysts.

TOP: Developing tools that provide atomic control in synthesis and characterization of ultra-small metal cluster catalysts for a new energy future.

Nanostructures for Electrical Energy Storage (NEES)

Director

Gary Rubloff

Lead Institution

University of Maryland

Partner Institutions

University of California, Irvine

University of Florida

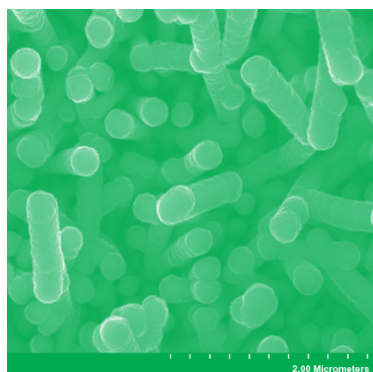
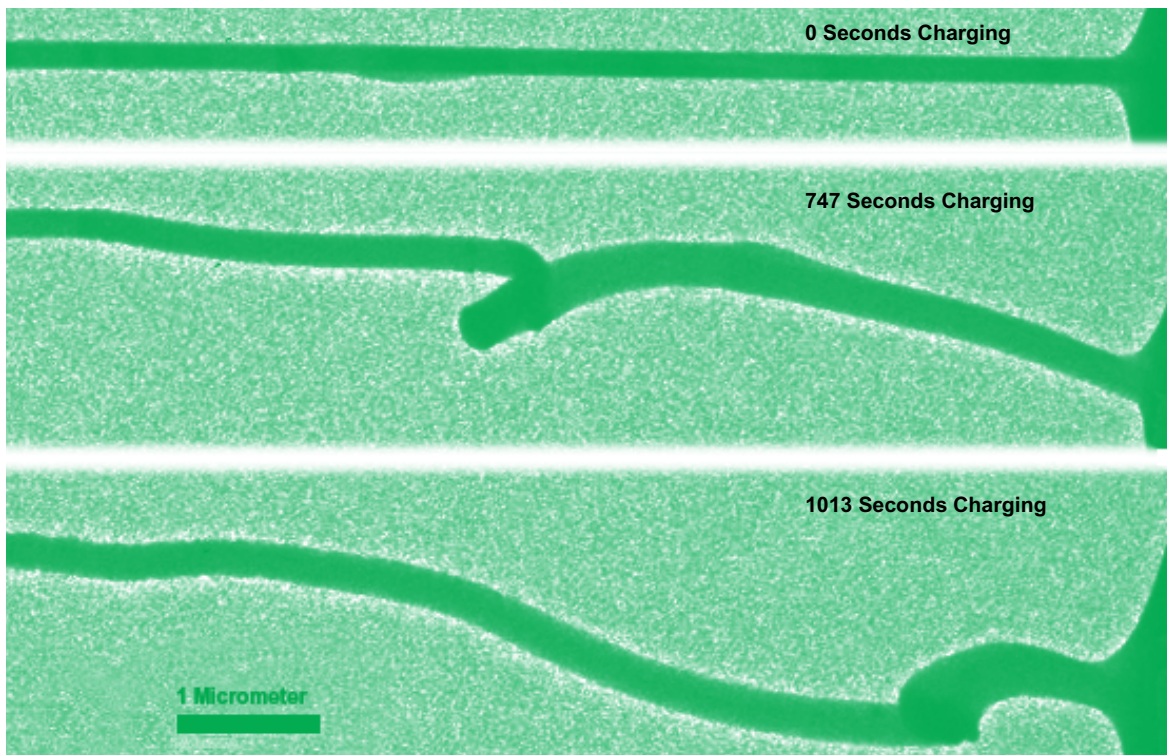
Los Alamos National Laboratory

Sandia National Laboratories

Yale University

Research Topics

electrical energy storage, defects, interfaces, charge transport, organic materials, inorganic materials, polymers, semiconductors, oxides



ABOVE: NEES researchers investigate silicon as a candidate electrode material. They coat layers of metal and silicon onto viruses, which act as templates for creating nearly identical nanowires.

TOP: Snapshots from the real-time video show the tin oxide electrode. As lithium ions moved through and reacted with the material, the wire twisted and lengthened. The movie unveiled clues about the atomic movements that cause the shape changes.

Mission

To understand and build nano-structured electrode components as the foundation for new electrical energy storage technologies.

Achievements

The first ever real-time movie of lithium ions charging a nano-sized battery may lead to safer, longer lasting, and more powerful electrical energy storage. Researchers within the multi-institutional Nanostructures for Electrical Energy Storage EFRC built and observed a nanosized electrochemical device inside an electron microscope. They watched a ceramic nanowire made of tin oxide, a promising battery electrode material, swell, lengthen, and coil as it charged. The nanowire did not break apart, unlike many ceramic materials charged in bulk form. This new atomic-scale time-resolved visualization capability will help researchers understand why electrode materials degrade after charging and discharging many times and will contribute to the design of powerful, robust and light-weight nanostructured lithium-ion batteries.

Center for Excitonics (CE)

Director

Marc Baldo

Lead Institution

Massachusetts Institute of Technology

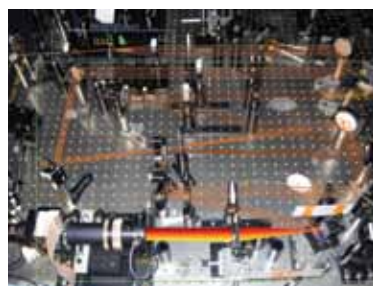
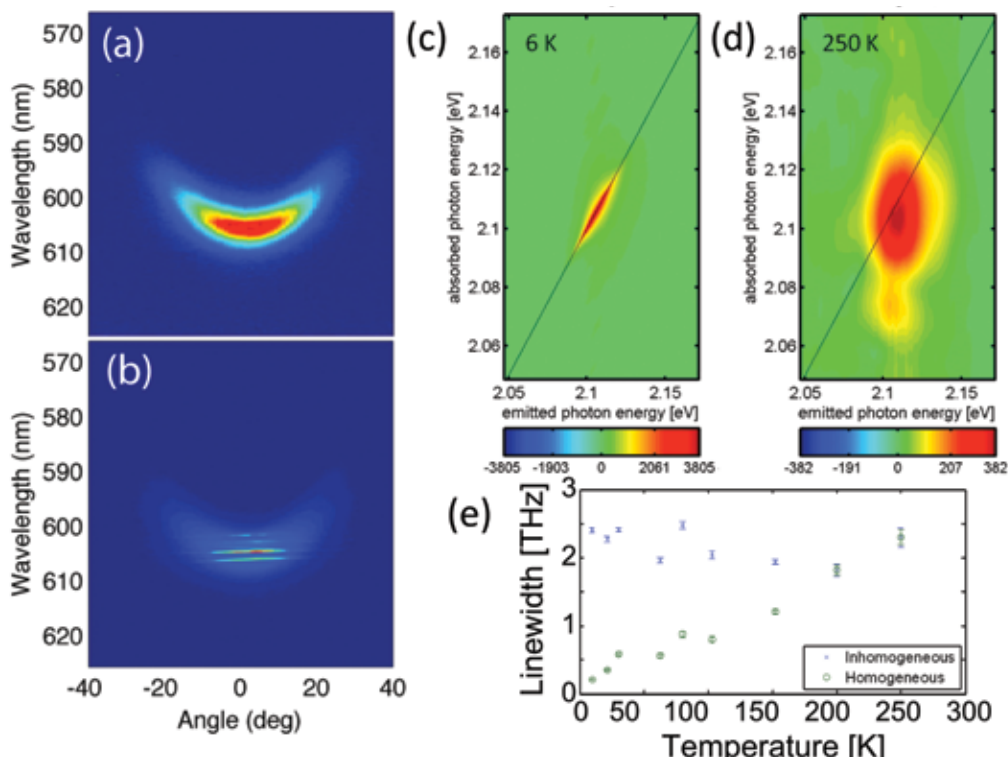
Partner Institutions

Brookhaven National Laboratory

Harvard University

Research Topics

solar photovoltaics, solid state lighting,
photosynthesis, charge transport,
organic materials, inorganic materials,
polymers, semiconductors



ABOVE: The optical system constructed to measure the processes illustrated in the diagram above. **TOP:** Emission of polaritons, or excited states of molecules, (a) below lasing threshold and (b) above threshold (logarithmic scale). Two-dimensional photon echo spectroscopy (c,d) yields an exciton coherence length exceeding 40 monomer units at low temperature, and 15 monomer units near room temperature (e).

Mission

To understand the transport of charge carriers in synthetic disordered systems, which hold promise as new materials for conversion of solar energy to electricity and electrical energy storage.

Achievements

One of the outstanding opportunities in energy research is the exploitation of new combinations of light and matter. Researchers at CE have made progress in understanding and manipulating “exciton-polariton”, hybrid states of light (photons) and excited states of molecules (excitons), for applications in lighting and solar cells. The work is based on “J-aggregates”—brightly colored dyes with a long history in photography due to their extremely high optical absorption. One recent result, shown above, is a room temperature polariton laser that employs a new architecture based on a J-aggregate. An EFRC-funded laser system and homebuilt two-dimensional optical spectroscopy system enabled the first observations of wave-like properties, or coherence, in J-aggregate excitons, a result that could help researchers understand how to better capture the energy from the sun in next-generation solar cells.

Polymer-Based Materials for Harvesting Solar Energy (PHaSE)

Directors

Thomas P. Russell and Paul M. Lahti

Lead Institution

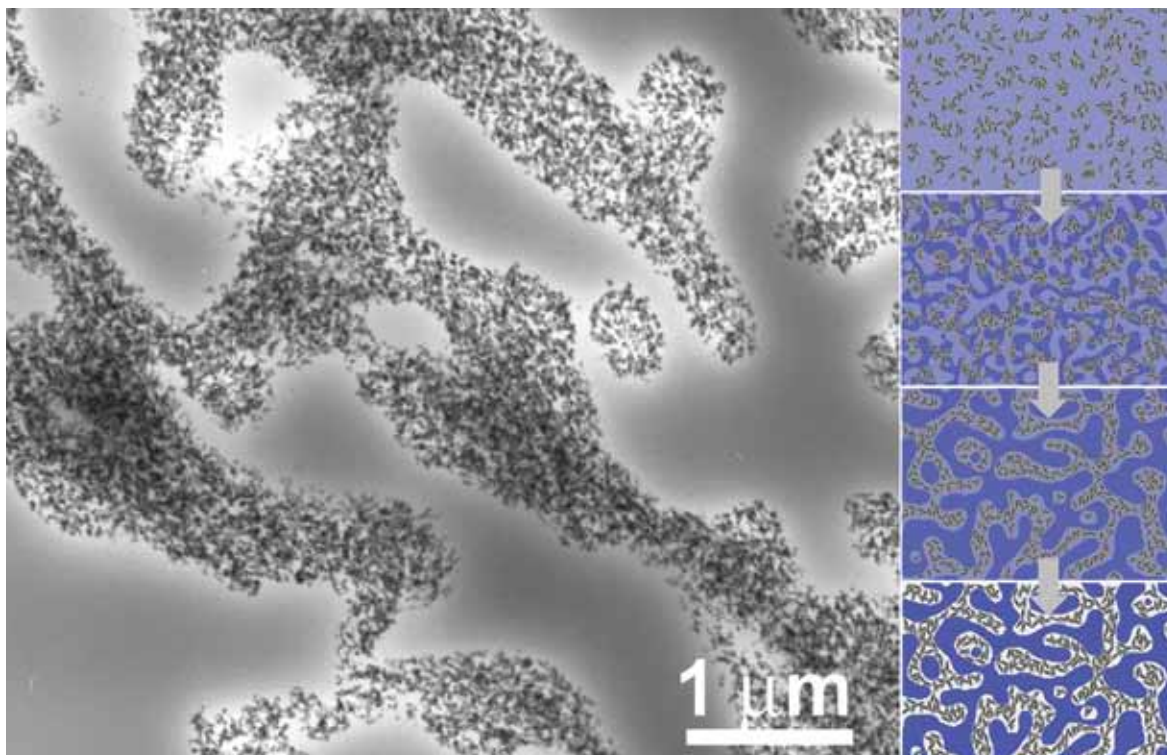
University of Massachusetts, Amherst

Partner Institutions

University of Massachusetts, Lowell
Oak Ridge National Laboratory
Pennsylvania State University
Rensselaer Polytechnic Institute
University of Pittsburgh

Research Topics

solar photovoltaics, interfaces,
photonics, matter by design, charge
transport, organic materials, inorganic
materials, polymers, semiconductors



ABOVE: Making and purifying new polymers and compounds is a first, vital step in creating new designs for solar cells. **TOP:** Conducting nanoparticles mixed with special polymers (right) gradually grow into an electrically desirable, highly branched network (close-up left).

Mission

To carry out fundamental photovoltaic-oriented research using polymeric and related materials; to maximize efficiency in the collection and harvesting of energy over a broad frequency range of the solar spectrum.

Achievements

PHaSE's interdisciplinary research teams seek to minimize loss and maximize transport of electric current in polymer ("plastic") solar cells. A synergistic loop involving the design, synthesis and assembly, physical process evaluation and device evaluation helps identify promising materials and strategies for better devices. Controlled assembly of solar cell components at the molecular level is critical for efficient energy conversion. In one example, PHaSE scientists found a way to create nano-sized channels for better electrical charge flow (top picture). Holding the conduit size-scale to tens of nanometers is essential for polymer device performance. Using model systems, researchers successfully trapped and stabilized channels as shown (arrows, right side picture), and prevented them from merging into undesirably large size-scales.

Solid-State Solar Thermal Energy Conversion Center (S³TEC)

Director

Gang Chen

Lead Institution

Massachusetts Institute of Technology

Partner Institutions

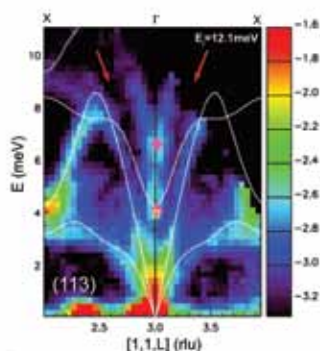
Boston College

Oak Ridge National Laboratory

Rensselaer Polytechnic Institute

Research Topics

solar photovoltaics, solar thermal, thermoelectric, defects, interfaces, matter by design, charge transport, ultrafast science, inorganic materials, rare earth elements, semiconductors



ABOVE: Neutron scattering data and calculated frequencies (white lines) on lattice vibrations at 300 K in lead telluride, a common thermoelectric material, shows a “waterfall effect” due to strong interactions between different vibrational modes in the material. **TOP:** An innovative design of solar thermoelectric generator that incorporates improved nanostructured thermoelectric materials leads to a quantum leap in solar-to-electricity conversion efficiency.

Mission

To create novel, solid-state materials for the conversion of sunlight into electricity using thermal and photovoltaic processes.

Achievements

Research at S³TEC develops the scientific and technological foundations to convert solar energy into electricity through thermal processes using solid-state energy conversion devices based on thermoelectric and photovoltaic effects. The Center recently demonstrated flat-panel solar thermoelectric generators with a 4.6 percent solar-to-electricity energy conversion efficiency at standard conditions, a level that is seven to eight times higher than previously reported values. Scientists are improving thermoelectric materials and wavelength-selective surfaces that are crucial for energy conversion efficiency. Using first-principles simulations, optical diagnosis, and neutron scattering, S³TEC researchers have mapped out the contributions of phonons with different mean free paths to the thermal conductivity. Researchers use this information to design and synthesize nanostructured thermoelectric materials.

Center for Solar and Thermal Energy Conversion (CSTEC)

Director

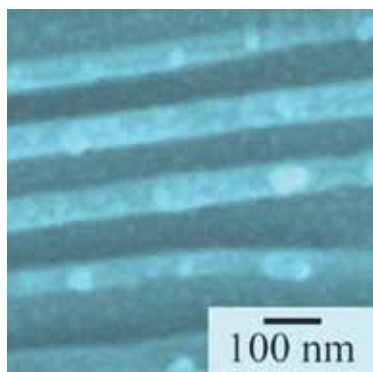
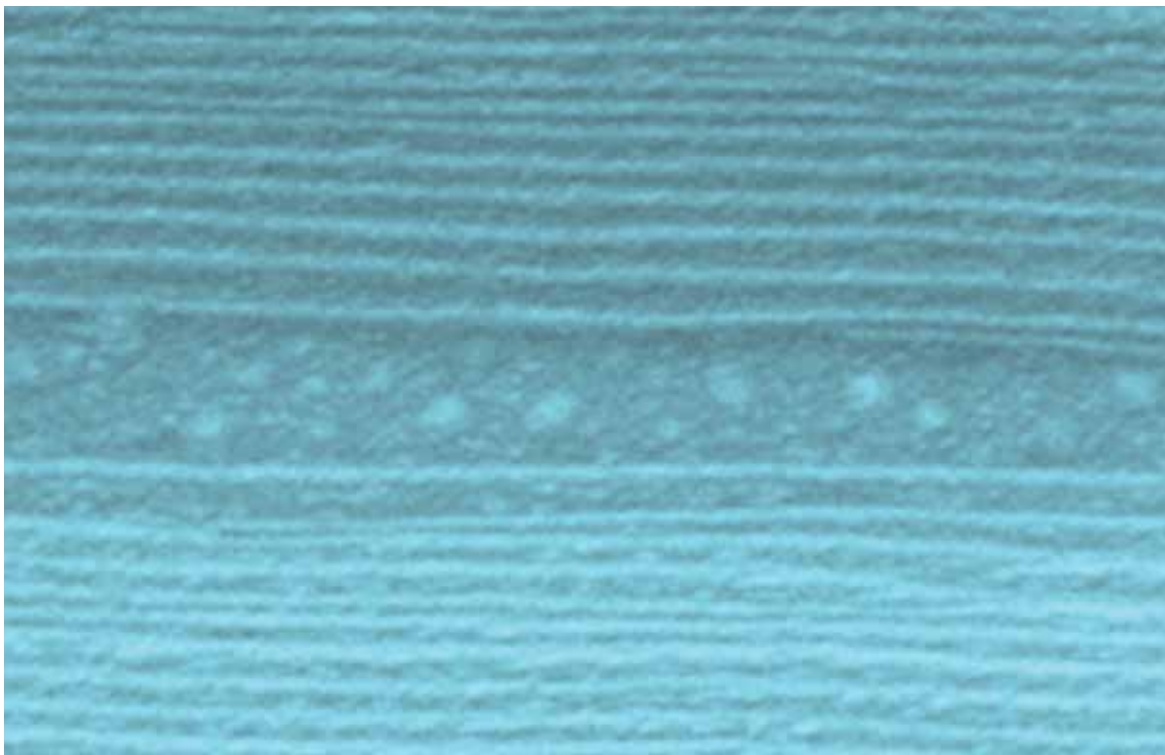
Peter F. Green

Lead Institution

University of Michigan

Research Topics

solar photovoltaics, solar thermal, thermoelectric, defects, interfaces, matter by design, charge transport, ultrafast science, organic materials, inorganic materials, polymers, semi-conductors, oxides



ABOVE: CSTEC researchers are using femtosecond-pulse lasers to modify thermoelectric materials. They can write 'nanotracks' by scanning the laser.

TOP: Scanning electron micrograph of antimony telluride after irradiating with a 100 femtosecond laser beam that induces tracks at the rate of 10 microns per second. Long tracks can be made < 50 nanometers wide. This is a fast, convenient way to create unidimensional nanostructured thermoelectric materials.

Mission

To study complex material structures on the nanoscale to identify key features for their potential use as materials to convert solar energy and heat to electricity.

Achievements

CSTEC researchers have demonstrated, for the first time, femtosecond laser-induced nanopatterning in both thin film and bulk forms of highly absorbing antimony telluride. These materials are of interest for thermoelectric energy conversion applications. After laser exposure, researchers observed long nanotracks with widths smaller than 50 nm and spacing approximately 130 nm apart, much smaller than the laser wavelength. This finding is significant because including nanostructures in thermoelectric materials is known to have favorable effects on their thermal and electronic properties, and thus may lead to enhancement of their efficiency for thermal energy conversion. The use of ultrafast laser processing for nanostructure formation is a promising avenue for further development of this family of high-performance thermoelectric materials.

Revolutionary Materials for Solid State Energy Conversion (RMSSEC)

Director

Donald T. Morelli

Lead Institution

Michigan State University

Partner Institutions

University of California, Los Angeles

University of Michigan

Northwestern University

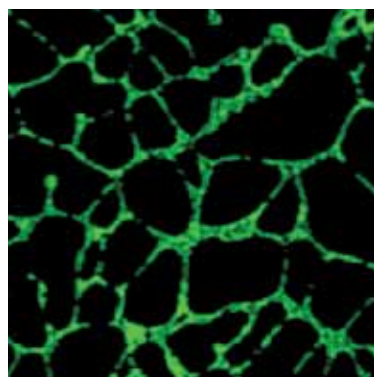
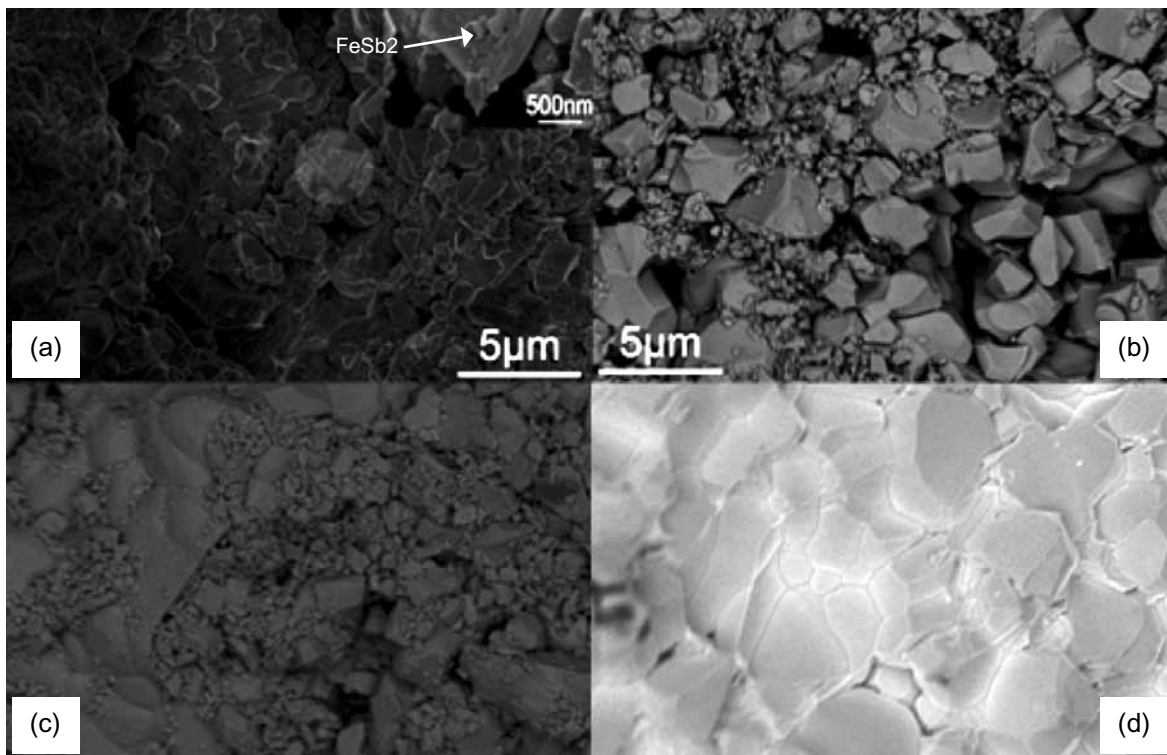
Oak Ridge National Laboratory

Ohio State University

Wayne State University

Research Topics

solar thermal, thermoelectric, matter by design, inorganic materials, semiconductors



ABOVE: Auger image of the migration of boron (green) to the grain boundaries in a cobalt-silicon thermoelectric alloy. The boron improves the thermoelectric properties by enhancing intergranular charge transport without decreasing the Seebeck coefficient. **TOP:** High resolution images of iron diantimonide/cobalt triantimonide nanocomposites exhibit fine-grained structure only when nanoscopic iron diantimonide is added (a-c).

Mission

To investigate the underlying physical and chemical principles of advanced materials for the conversion of heat into electricity.

Achievements

Researchers at RMSSEC are learning how nanostructure can improve properties of semiconductors that convert waste heat to electricity, a class of materials known as thermoelectrics. In one study, they have shown that strontium telluride nanocrystals embedded coherently in a thermoelectric lead telluride host can allow for the concurrent transmission of electrical charge while blocking the flow of heat, a key combination for producing a highly efficient thermoelectric material. In a second approach, nanocomposites consisting of iron diantimonide nanoparticles dispersed in a cobalt triantimonide matrix exhibit enhanced “Seebeck coefficient,” also an important property for a good thermoelectric material. This enhancement is thought to be due to an alteration of the energy dependence of scattering of charge carriers. These and similar findings may lead to improved thermoelectric devices for energy conversion from waste heat.

Center for Advanced Biofuel Systems (CABS)

Director

Richard T. Sayre

Lead Institution

Donald Danforth Plant Science Center

Partner Institutions

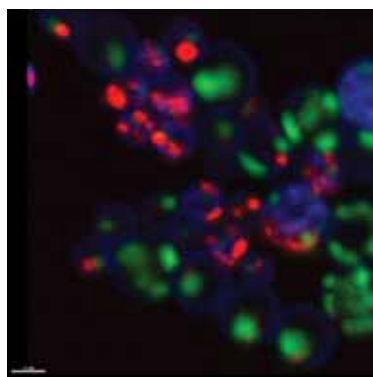
Michigan State University

University of Nebraska

Washington State University

Research Topics

catalysis, solar fuels, photosynthesis,
biofuels, carbon capture, charge
transport, organic materials



ABOVE: Fluorescence image of *Chlorella* cells shows the accumulation of oil droplets following growth in the presence of glucose. Green is auto-fluorescence from chlorophyll, red is triacylglycerol and blue is membrane phospholipids. **TOP:** Michigan State University researchers investigate the role of light in plant oil formation. The *Camelina* plant oilseeds use light that reaches them through the pod walls to fuel the production of high-energy oils.

Mission

To generate the fundamental knowledge required to increase the efficiency of photosynthesis and production of energy-rich molecules in plants.

Achievements

The high failure rate of genetic engineering efforts to improve biomass and oil yield in plants highlights deficiencies in our knowledge of plant metabolism. CABS researchers seek to identify potential bottlenecks for productivity in the oilseed plant *Camelina* and in the model alga *Chlamydomonas*. They construct metabolic models of the inputs, outputs and internal transformations of metabolites and energy during seed development and oil accumulation in algae. They use these models to quantify and understand the basis for metabolic efficiency, to identify potentially wasteful processes, and to develop novel strategies for improving biodiesel production. CABS identified specific enzymes whose levels significantly rise during glucose-induced oil production in the green alga *Chlorella*. Increasing the levels of these enzymes in *Chlamydomonas*, a different green alga, substantially enhanced net photosynthetic rates. Recent results point not only to improved yield but also promise the capability to engineer new biochemical feedstock molecules ideal for biofuels production.

Photosynthetic Antenna Research Center (PARC)

Director

Robert E. Blankenship

Lead Institution

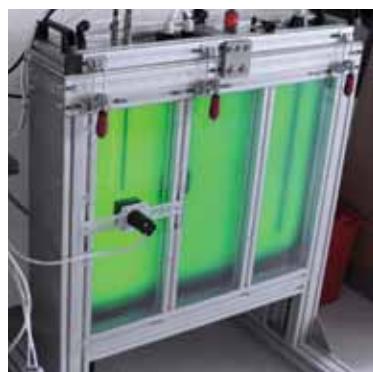
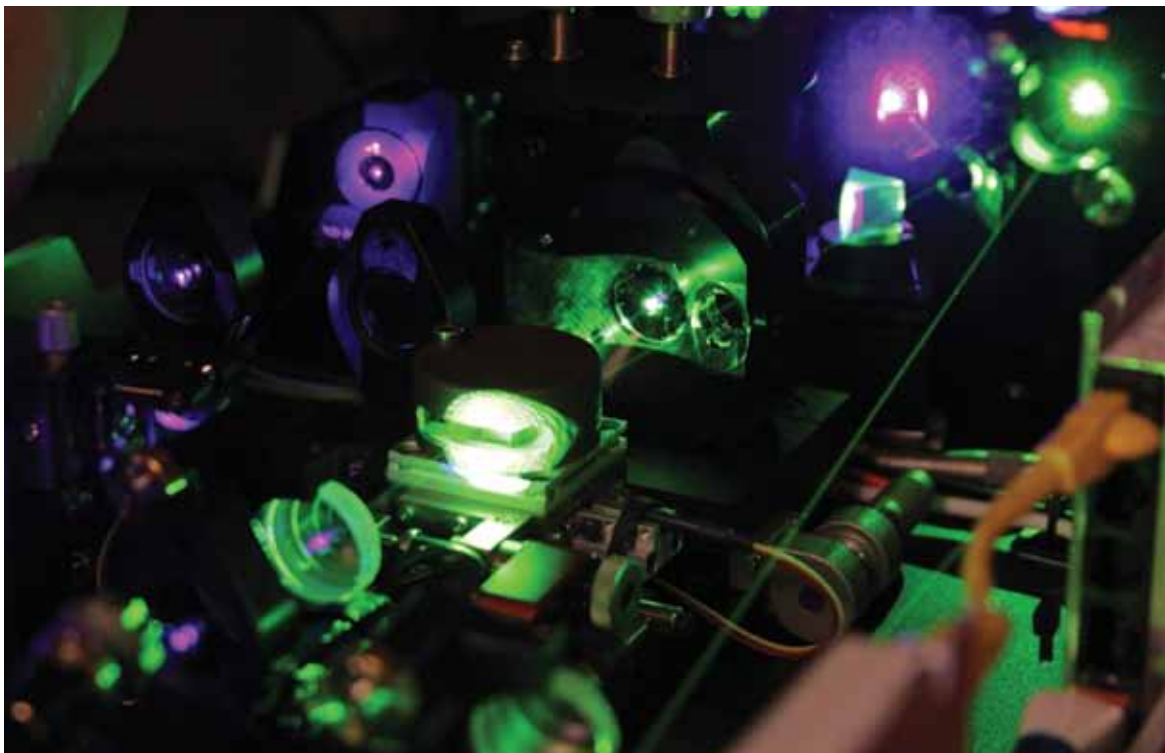
Washington University in St. Louis

Partner Institutions

University of California, Riverside
Donald Danforth Plant Science Center
University of Glasgow, UK
Los Alamos National Laboratory
North Carolina State University
Oak Ridge National Laboratory
University of Pennsylvania
Sandia National Laboratories
University of Sheffield, UK

Research Topics

solar fuels, photosynthesis, biofuels,
membranes, charge transport, ultrafast
science, organic materials, inorganic
materials



ABOVE: The PARC Photobioreactor Facility is growing a chlorophyll d-containing cyanobacterium for the purification of light-harvesting phycobilisome complexes for protein structure and light energy transfer studies. **TOP:** The optical parametric oscillator is one of four instruments in the PARC Ultrafast Laser Facility used to probe diverse natural and artificial photosynthetic antenna systems.

Mission

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

Achievements

PARC's three research themes are directed towards developing simple light-harvesting systems with efficiencies equal to or better than native photosynthetic antennas and facilitating revolutionary advances in artificial systems for solar-energy conversion. Theme 1 explores mechanisms of natural photosynthetic antennas, groups of pigment molecules that harvest light. Theme 2 investigates natural antennas on surfaces and structures forming biohybrid antennas. Theme 3 fabricates micron-scale arrays for efficient solar light harvesting, energy transfer, and trapping. Accomplishments so far include characterization of photosynthetic pigments in cyanobacteria and photosynthetic complexes in purple bacteria, development of operational biohybrid devices consisting of a bacterial antenna complex attached to an inorganic surface, and incorporation and testing of designer pigments in artificial antenna systems that could use more of the solar spectrum.

Combustion Energy Frontier Research Center (CEFRC)

Director

Chung K. Law

Lead Institution

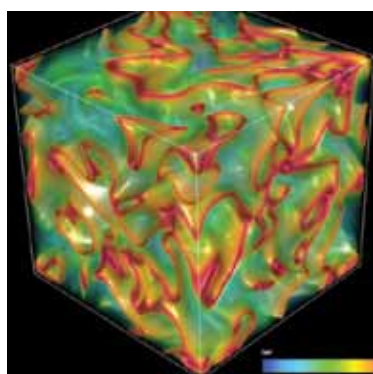
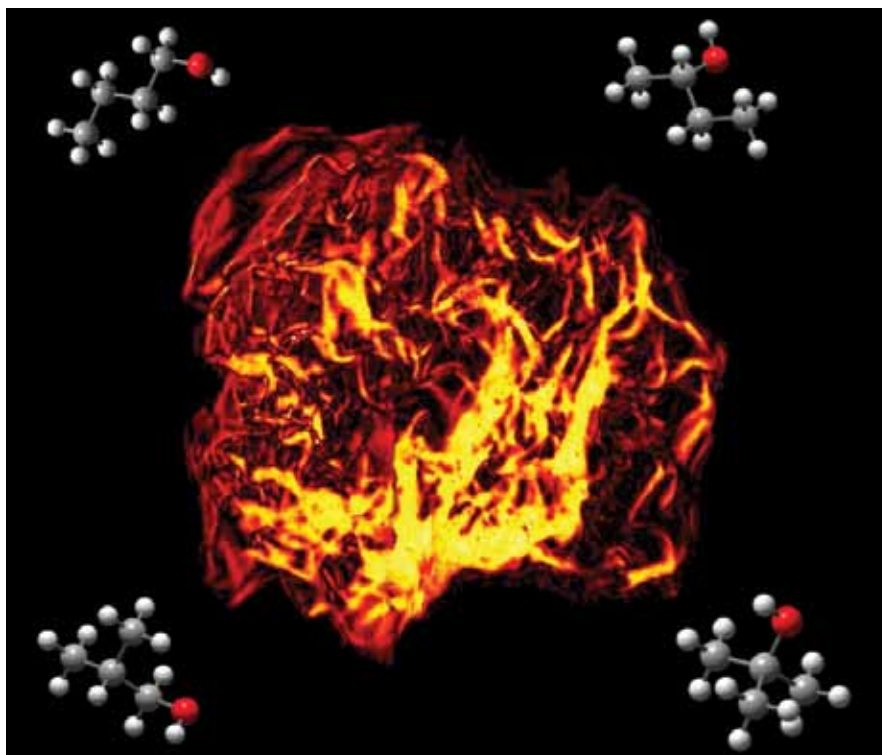
Princeton University

Partner Institutions

Argonne National Laboratory
University of Connecticut
Cornell University
Massachusetts Institute of Technology
University of Minnesota
Sandia National Laboratories
University of Southern California
Stanford University

Research Topics

biofuels, combustion, extreme environment, hydrogen, high performance computing, organic materials



ABOVE: A direct numerical simulation showing combustion fronts in a turbulent flow; different colors indicate regions of various burning intensities.

TOP: An experimental picture of a convoluted n-butanol/air flame in a turbulent flow, simulating conditions in internal combustion engines. The insets show the molecular structures of the four isomers of butanol. Carbon, hydrogen and oxygen atoms are dark grey, light grey and red respectively.

Mission

To develop a validated, predictive, multi-scale combustion modeling capability which can be used to optimize the design and operation of evolving fuels in advanced engines for transportation applications.

Achievements

Bio-butanol is under active commercial development as an engine fuel to supplement or replace ethanol. It has advantages of higher energy density, miscibility with gasoline, noncorrosiveness and reduced smog-forming emissions. Using advanced chemical reactors, laser-based diagnostics and a synchrotron light source, CEFRC researchers developed a reaction mechanism describing butanol combustion. The model is based on a multiscale investigation involving quantum chemistry calculation of elementary reaction kinetics and flame propagation in complex flows. High-fidelity computations will use this reaction mechanism to study turbulent combustion processes underlying engine environments in concert with high pressure experimentation. Further research will apply the reaction mechanism to develop predictive models of advanced engine processes burning bio-butanol or its blends with gasoline; this method could also be used for other alternative fuels.

Center for Advanced Solar Photophysics (CASP)

Director

Victor I. Klimov

Lead Institution

Los Alamos National Laboratory

Partner Institutions

National Renewable Energy

Laboratory

University of California, Irvine

Rice University

University of Minnesota

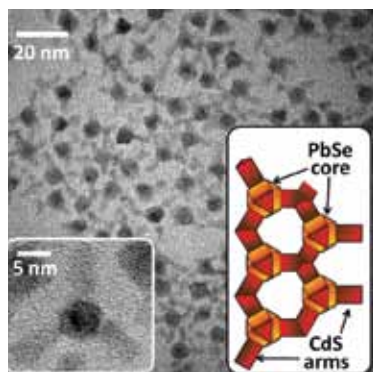
University of Colorado

Colorado School of Mines

George Mason University

Research Topics

solar photovoltaic, charge transport,
ultrafast science, inorganic materials,
semiconductors



ABOVE: CASP is developing advanced nanomaterials for next-generation solar cells. Nanoscale tetrapod heterostructures spatially separate electrons and holes between the “core” and the “arms”, resulting in improved conversion of light into electrical charges.

TOP: Fabrication of the first p-n junction photovoltaic device based on colloidal semiconductor nanocrystals (inset) is a key step towards efficient yet inexpensive solution-processed solar cells.

Mission

To capitalize on recent advances in the science of how nanoparticles interact with light to design highly efficient materials for the conversion of sunlight into electricity.

Achievements

Researchers at CASP have fabricated the first nanocrystal solar cell to feature a junction formed by electron and hole conductive layers. Highly-efficient layered structures are used for converting absorbed sunlight into electrical current and are at the heart of nearly all commercial solar cells. Researchers created the junctions by combining layers of colloidal lead sulfide and zinc oxide nanocrystals using low-cost, solution-based fabrication methods. CASP's prototype cell achieved an officially certified record-high conversion efficiency of 4.4 percent. The device operates at a voltage greater than the bulk-material energy gap that separates the conduction and valence bands. The difference in voltage is due to the influence of “quantum confinement,” unique physics that occurs in nanoscale materials. The CASP nanocrystal solar cell is also robust, maintaining over 95 percent of its efficiency after a thousand-hour solar simulator work cycle. This groundbreaking achievement puts this new class of solar cells on the map and sets the standard for future nanocrystal-based efforts.

Center for Materials at Irradiation and Mechanical Extremes (CMIME)

Director

Michael Nastasi

Lead Institution

Los Alamos National Laboratory

Partner Institutions

Carnegie Mellon University

University of Illinois, Urbana-

Champaign

Massachusetts Institute of Technology

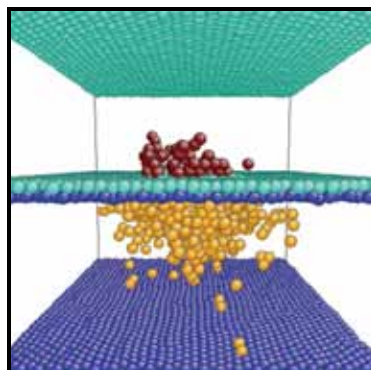
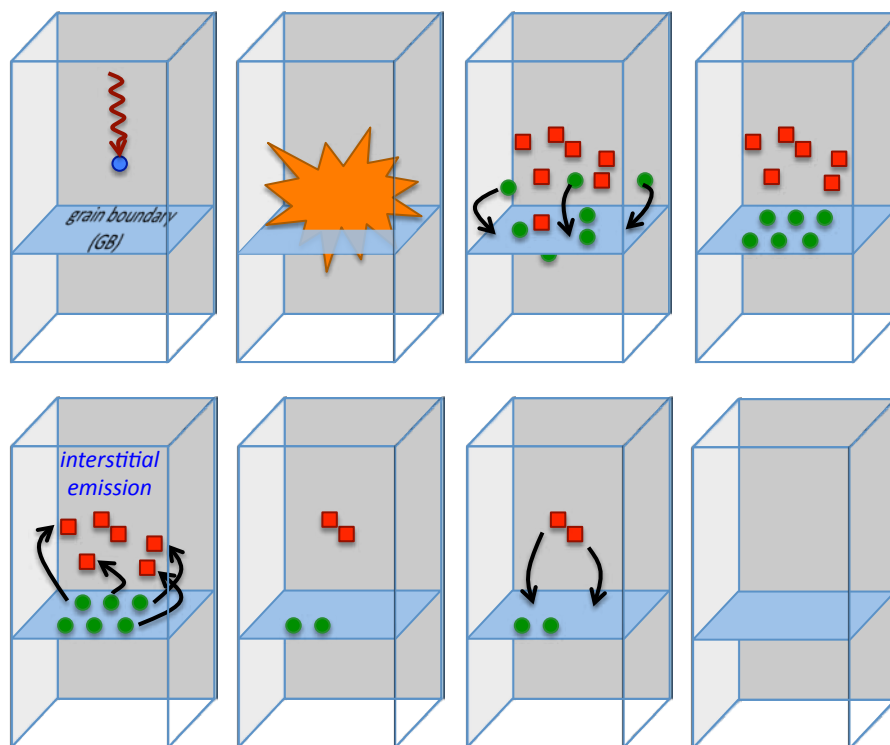
Research Topics

nuclear, extreme environment, defects,

interfaces, matter by design, high

performance computing, inorganic

materials, oxides



ABOVE: Red (Nb) and yellow (Cu) atoms are radiation-induced defects, all of which are eventually healed by the interface (green: Nb side, blue: Cu side). For clarity, perfect crystalline atoms are not shown. **TOP:** Molecular and accelerated molecular dynamics of radiation damage near a Cu grain boundary. First, the boundary is loaded with interstitials while vacancies remain behind. Eventually, interstitials unload to annihilate some vacancies.

Mission

To understand, at the atomic scale, the behavior of materials subject to extreme radiation doses and mechanical stress in order to synthesize new materials that can tolerate such conditions.

Achievements

Researchers at the CMIME, at Los Alamos National Laboratory, have discovered a promising new mechanism for reducing damage to materials in fission or fusion reactors. The mechanism enhances the “healing” of point defects created by exposure to energetic neutrons in these environments. Using a combination of modeling tools, they examined the role of grain boundaries in damage production and defect evolution. They showed that boundaries have a complex effect on damage production, reducing the number of resulting defects. Their findings may explain the radiation damage resistance found in nanostructural materials and may lead to their use in the design of improved materials for reactor applications.

Energy Frontier Research Center for Solid-State Lighting Science (SSLs)

Director

Jerry A. Simmons

Lead Institution

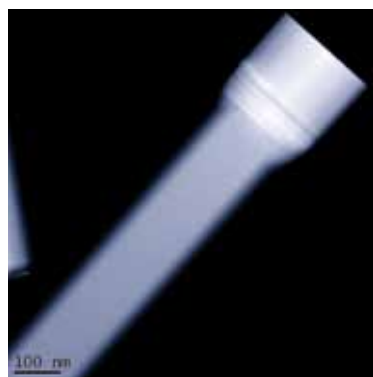
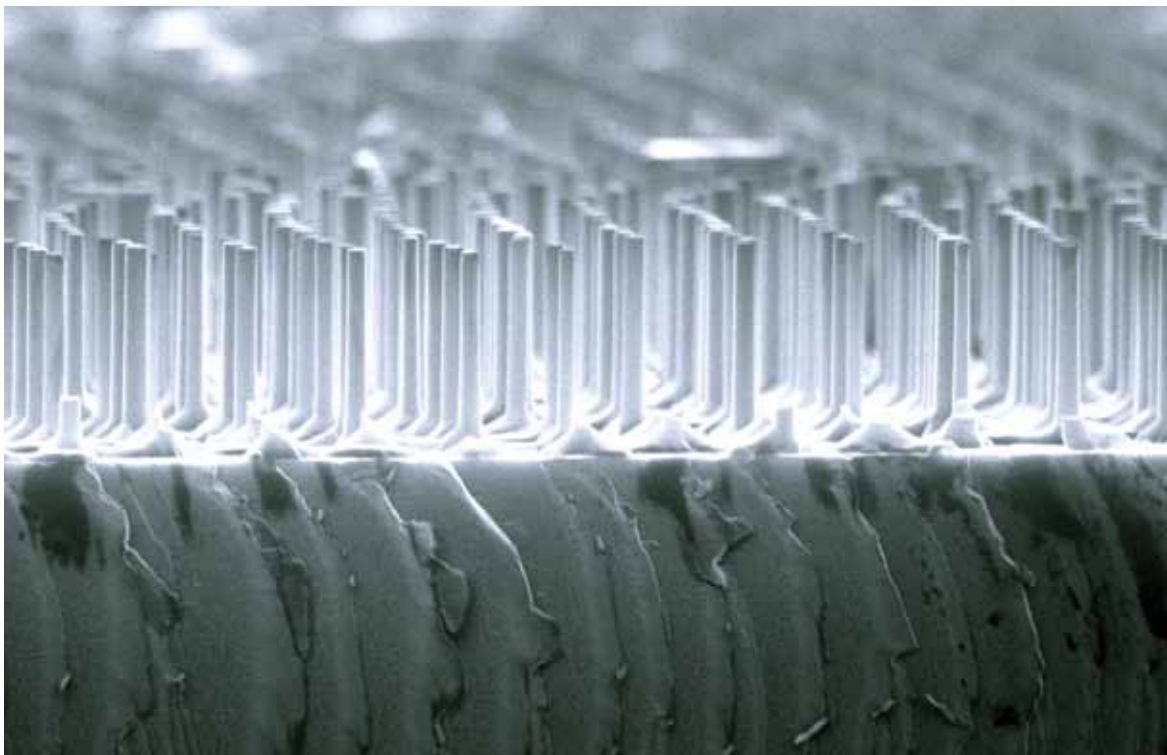
Sandia National Laboratories

Partner Institutions

California Institute of Technology
Los Alamos National Laboratory
University of Massachusetts, Lowell
University of New Mexico
Northwestern University
Philips Lumileds Lighting
Rensselaer Polytechnic Institute

Research Topics

solar photovoltaics, solid state lighting,
defects, charge transport, rare earth
elements, inorganic materials, semi-
conductors



ABOVE: A gallium nitride nanowire forms a flashlight-shaped LED with dimensions about one thousand times smaller than a human hair.

TOP: An ordered gallium nitride array fabricated on sapphire wafers by a two-step etching process. Nanowires may form the foundation for future-generation LEDs due to their unique properties.

Mission

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

Achievements

While today's solid-state lighting devices are based on planar thin-film structures, altogether new material architectures may lead to white-lighting sources with even higher performance—and greater energy savings. Scientists at the SSLs center at Sandia National Laboratories have developed a new technique for fabricating periodic, large-area arrays of “nanowires” made of gallium nitride, the semiconductor material used in white, blue, and green light-emitting diodes, or LEDs. Using high-resolution electron microscopy, the researchers found that the nanowires are largely free of the crystal defects that limit the performance of current-generation LEDs. Nanowire LED structures created using this technique also showed greatly enhanced brightness, as the unique nanowire geometry allows for highly efficient light transfer out of the device.

Center for Electrocatalysis, Transport Phenomena, and Materials for Innovative Energy Storage (CETM)

Director

Grigori Soloveichik

Lead Institution

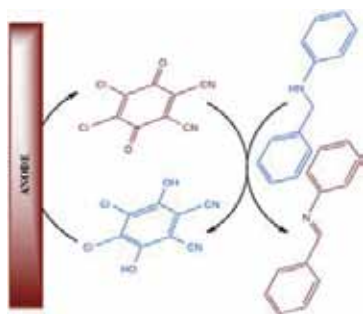
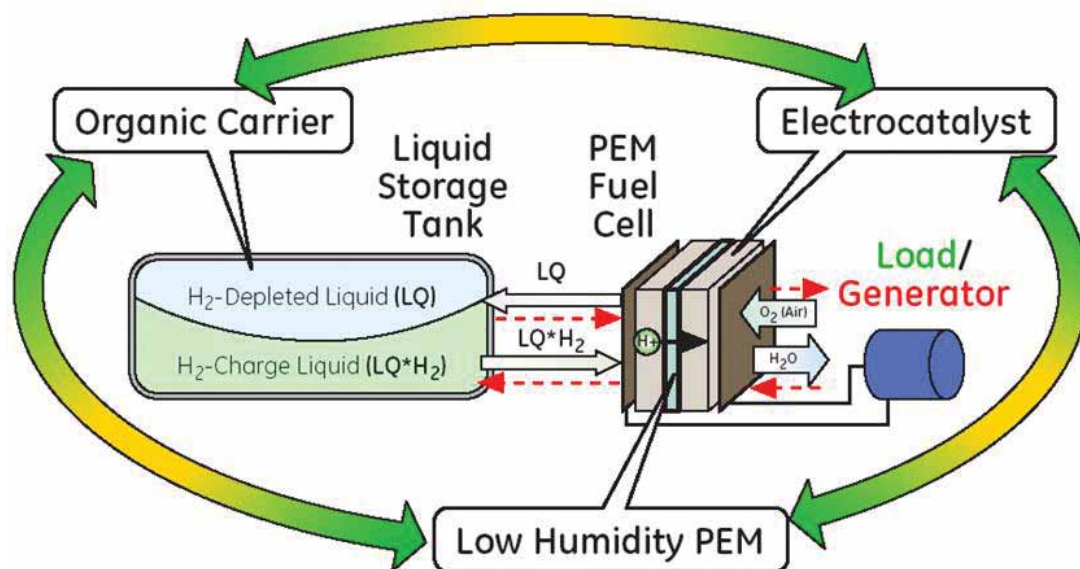
General Electric Global Research

Partner Institutions

Lawrence Berkeley National
Laboratory
Stanford University
Yale University

Research Topics

catalysis, electrical energy storage,
membranes, hydrogen, interfaces,
charge transport, organic materials,
polymers



ABOVE: Illustration of the reaction pathway for organic-catalyst-mediated fuel electrodehydrogenation. The hydrogen is stored in a liquid fuel by bonding it chemically to an organic molecule that can exist in both hydrogenated (blue) and dehydrogenated (red) states.

TOP: Conceptual design of an organic liquid-fuel cell/flow battery and key enabling technologies including an organic carrier (liquid fuel), electrocatalyst, and low humidity proton exchange membrane (PEM).

Mission

To develop the fundamental basis for an entirely new high-density energy storage system that combines the best properties of a fuel cell and a flow battery.

Achievements

Researchers at the multi-institutional CETM have used theoretical and experimental methods to obtain a fundamental understanding of liquid fuel and catalyst structure-property relationships in virtual hydrogen storage systems. These systems do not directly use hydrogen gas; rather, the hydrogen is chemically bonded in the liquid organic fuel. When needed, protons (H^+) and electrons, the charge carriers in the fuel cell, are directly extracted from the organic fuel. Knowledge of catalyst structure-property relationships has led to the discovery of the first example of an organic electrocatalytic system that uses a liquid fuel. A second recent notable achievement is the understanding of fuel requirements to maximize power output of an organic fuel cell. These breakthroughs will enable the widespread implementation of fuel cells in energy storage applications ranging from transportation to adoption of renewable energy sources.

Center for Emergent Superconductivity (CES)

Director

J. C. Séamus Davis

Lead Institution

Brookhaven National Laboratory

Partner Institutions

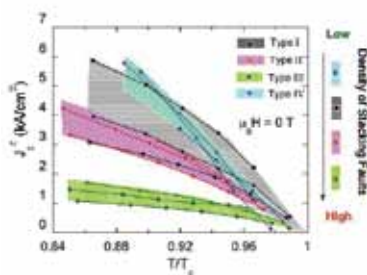
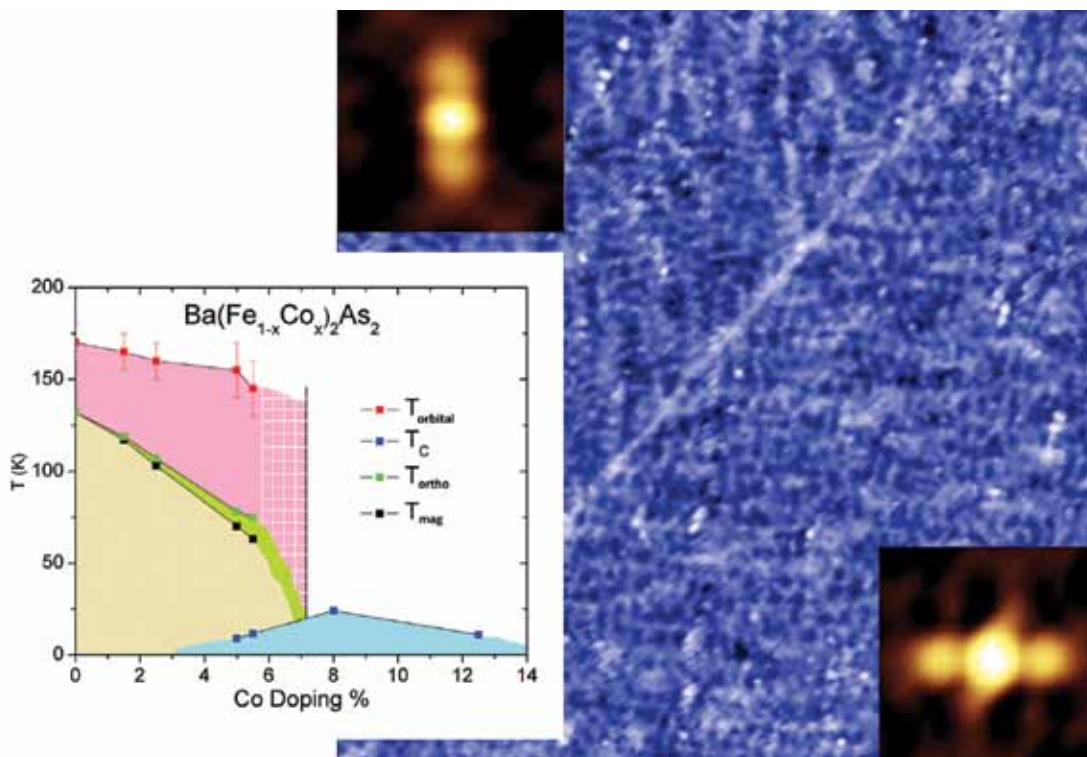
Argonne National Laboratory

University of Illinois, Urbana–

Champaign

Research Topics

electrical energy storage, superconductivity, smart grid, defects, inorganic materials



ABOVE: Critical supercurrent anisotropy in commercial copper oxide superconducting tapes: Perpendicular critical current (J_c^c) vs. temperature (T/T_c) strongly depends on the concentration of stacking fault defects. **TOP:** Electronic anisotropy in Fe-based high temperature superconductors: symmetry-breaking orbital order appears at high temperature (pink region) and spontaneous nanoscale electronic inhomogeneity revealed by STM (blue image) at low temperature.

Mission

To discover new high-temperature superconductors and improve the performance of known superconductors by understanding the fundamental physics of superconductivity.

Achievements

CES elucidated the highly anisotropic behavior at both the macroscopic and microscopic levels in two classes of high temperature superconductors, namely the copper-based and the recently discovered iron-based superconductors. Working with American Superconductor, CES scientists showed that commercial superconducting cuprate wires can exhibit surprisingly large variations in critical current in different directions, up to a factor of 2000 depending on microstructure. The low current direction can limit the current carried by cables wound from these wires, a primary figure of merit for power grid applications. The iron-based superconductors do not show such variations in critical current. However, at the microscopic level they exhibit a new type of electronic ordering that leads into nanoscale variations in the electronic heterogeneity at low temperatures. This may play a role in the very high critical currents of these materials. These different manifestations of anisotropy are central to applications of these new classes of superconductors.

Energy Materials Center at Cornell (emc²)

Director

Héctor D. Abruña

Lead Institution

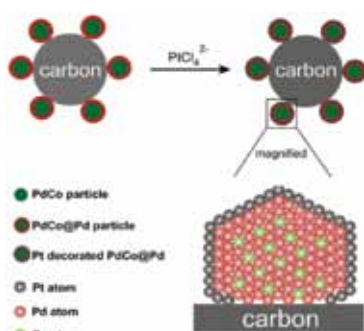
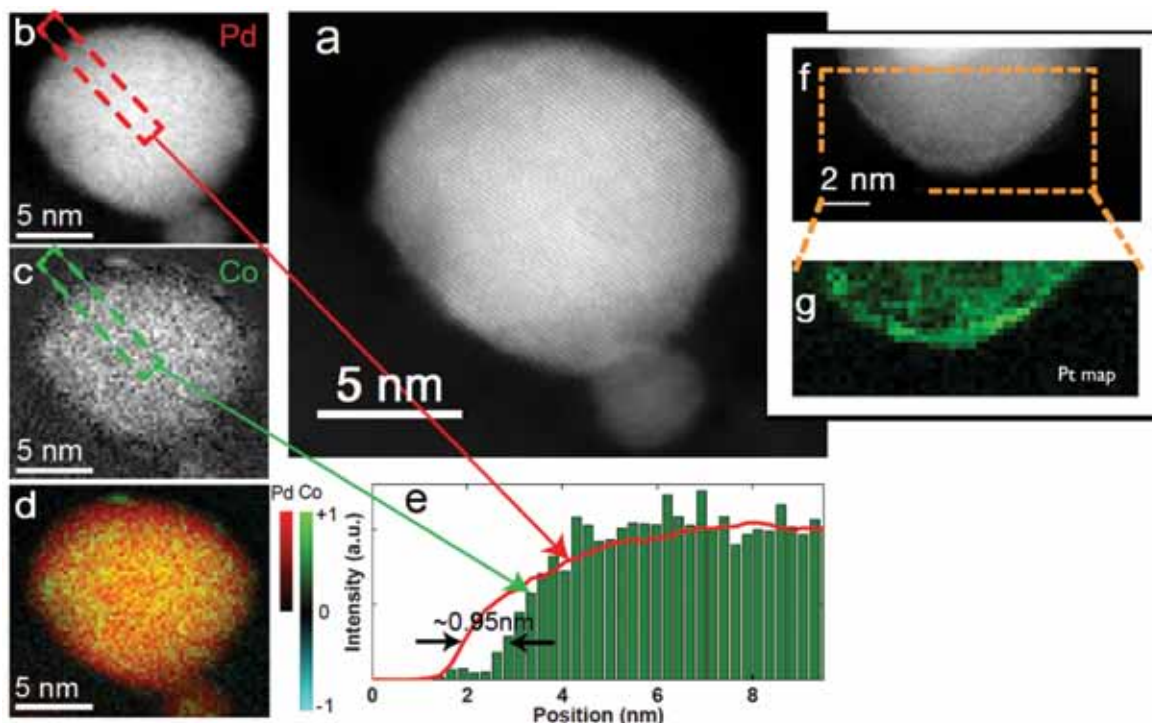
Cornell University

Partner Institution

Lawrence Berkeley National
Laboratory

Research Topics

catalysis, electrical energy storage,
defects, membranes, hydrogen,
interfaces, matter by design, charge
transport, organic materials, inorganic
materials, polymers, semiconductors,
oxides



ABOVE: Cartoon showing composition of Pt on PdCo@Pd core-shell nanoparticles. **TOP:** STEM image of a PdCo@Pd core-shell nanoparticle (a) and EELS of the same particle highlighting the location of (b) Pd, (c) Co, and (d) Pd and Co atoms relative to each other. EELS line profile of the nanoparticle reveals the Pd shell at 2-3 nm (e). STEM image of Pt-modified PdCo@Pd particle (f) showing the thin Pt covering (EELS image, g).

Mission

To advance the science of energy conversion and storage by understanding and exploiting fundamental properties of active materials and their interfaces.

Achievements

Research at emc² focuses on the synthesis, modeling and characterization of advanced materials to overcome key challenges in fuel cell and battery technologies. For example, the oxygen reduction reaction (ORR) is one of the main obstacles to increasing the efficiency and power of fuel cells. Researchers at emc² have developed a simple synthesis method to prepare carbon-supported palladium-cobalt (Pd/Co) nanoparticles coated with a thin layer of pure palladium for use as ORR catalysts. Depositing a single layer of platinum via a spontaneous displacement reaction significantly enhanced the stability and electrocatalytic activity of these nanoparticles. High resolution scanning transmission electron microscopy (STEM) and electron energy loss spectroscopy (EELS) are used by emc² to characterize their core-shell nanoparticles. Both the synthesis and the platinum deposition methods are suitable for large-scale production yielding a highly active catalyst for fuel cell cathodes with significantly lower platinum (Pt) content and much lower cost.

Northeastern Center for Chemical Energy Storage (NECCES)

Director

Clare P. Grey
Stan Whittingham (as of June 2011)

Lead Institution

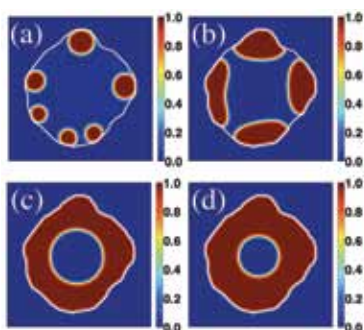
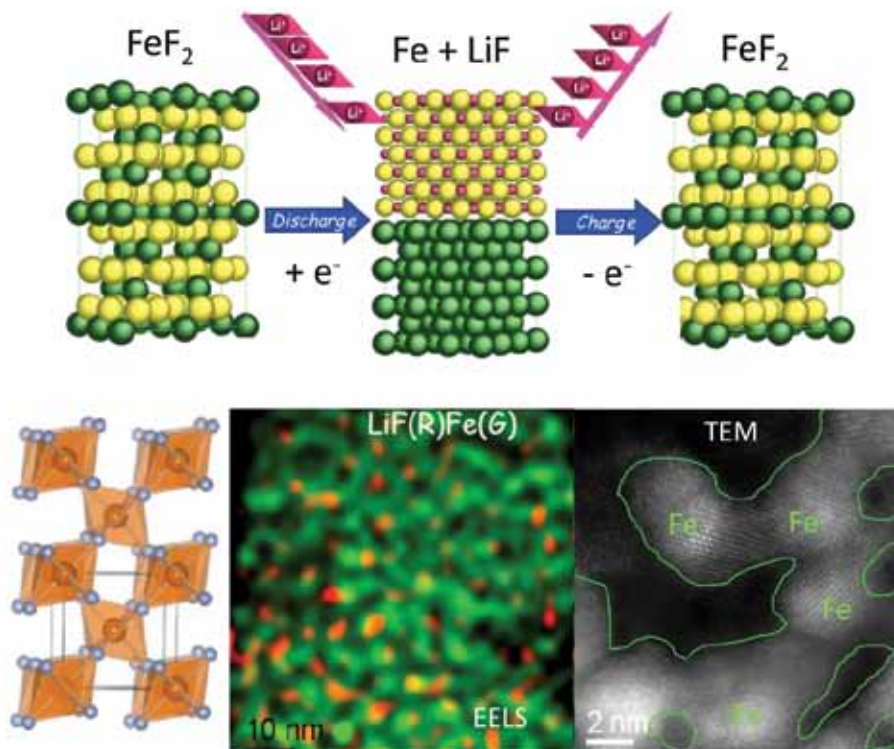
Stony Brook University

Partner Institutions

Argonne National Laboratory
Binghamton University
Brookhaven National Laboratory
University of California, San Diego
Lawrence Berkeley National Laboratory
Massachusetts Institute of Technology
University of Michigan
Rutgers University

Research Topics

electrical energy storage, defects,
interfaces, matter by design, charge
transport, inorganic materials, oxides



ABOVE: Simulations show how lithium is inserted into individual particles as a function of diffusion rates and particle sizes and shapes. **TOP:** The electrode material iron fluoride converts to a mixture of a lithium fluoride salt and small nanoparticles of metallic iron (upper image) on reacting with lithium. The iron nanoparticles form a connected, three-dimensional conducting matrix (lower pictures), covered by lithium fluoride, an insulating salt

Mission

To understand how fundamental chemical reactions occur at electrodes and to use this knowledge to design new chemical energy storage systems.

Achievements

Developing the next generation of rechargeable batteries requires a better understanding of how the different components in the battery function during charging and discharging. Research at NECCES focuses on identifying the critical mechanisms required for improved function—for example in rate and capacity—of electrode materials. Researchers study two classes of materials: conversion materials (upper image) and intercalation (image at left). Conversion reactions involve the reversible structural transformation of the original material into a nanocomposite. Using a combination of state-of-art instrumentation at universities and national laboratories, NECCES scientists have shown that a major reason for the excellent reversibility of the high-capacity electrode material iron fluoride involves the formation (on reaction with lithium) of a continuous conductive pathway of iron nanoparticles, covered by the insulating salt lithium fluoride. The conductive pathway allows electrons to be removed and inserted into the composite.

Re-Defining Photovoltaic Efficiency Through Molecular Scale Control (RPEMSC)

Director

James Yardley

Lead Institution

Columbia University

Partner Institutions

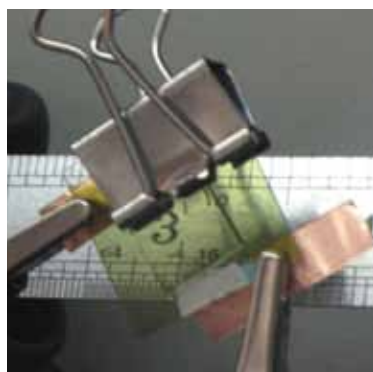
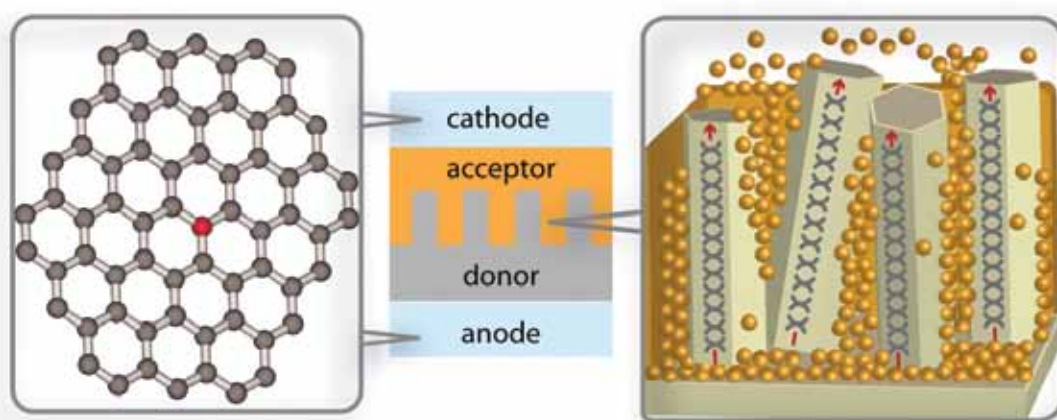
Brookhaven National Laboratory

Purdue University

University of Texas at Austin

Research Topics

solar photovoltaics, interfaces, matter by design, charge transport, organic materials, inorganic materials, polymers, semiconductors



ABOVE: Transparent, flexible organic solar cell with graphene electrodes.

TOP: Schematic of a nanostructured solar cell. RPEMSC researchers are exploiting self-assembly of molecular partners and the tunability of graphene electronic properties through doping to create nanostructured solar cells with improved functional performance.

Mission

To develop the enabling science needed to realize breakthroughs in the efficient conversion of sunlight into electricity in nanometer sized thin films.

Achievements

Researchers at the RPEMSC are leveraging accomplishments in organic photovoltaic (OPV) research to produce a next-generation solar cell, visualized schematically above. Scientists have designed shape-complementary molecules that self-assemble into a nanostructured photoactive region with well-defined interfaces (right). Researchers can directly grow vertical nanocrystals on graphene, an inexpensive, transparent material and a promising candidate for future electrodes in solar cells. Fabrication of graphene anodes, which requires graphene generated with an excess of electrons, is accessible by replacing a carbon (grey) atom with nitrogen (red) (left). Graphene can also be used as an OPV cathode through a process known as “contact doping,” in which contact with an electron donor layer enables charge transfer. These achievements point the way to the construction of transparent, light-weight all-carbon solar cells, and show that controlling device components at the molecular scale can make possible new architectures that redefine conventional solar-cell efficiency.

Solar Fuels and Next Generation Photovoltaics (UNC)

Director

Thomas J. Meyer

Lead Institution

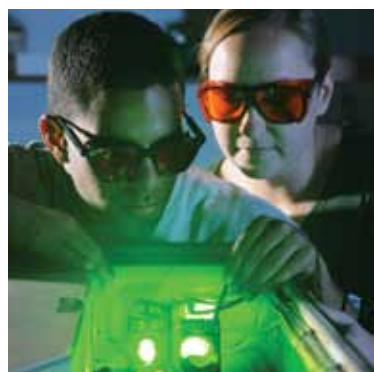
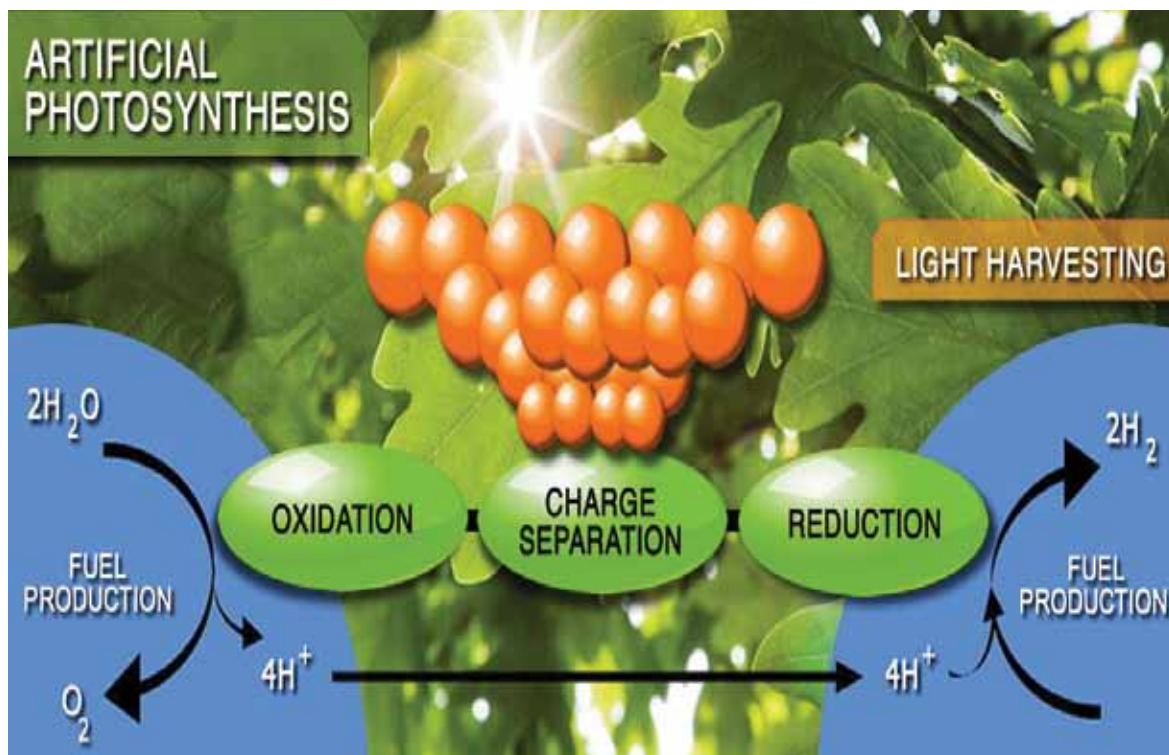
University of North Carolina at
Chapel Hill

Partner Institutions

Duke University
North Carolina State University
North Carolina Central University
University of Florida
Research Triangle Institute

Research Topics

catalysis, solar photovoltaics, solar fuels, photosynthesis, electrical energy storage, hydrogen, interfaces, charge transport, organic materials, inorganic materials, polymers, semiconductors, oxides



ABOVE: Graduate students conduct an experiment in the UNC EFRC Laser Facility. **TOP:** The UNC EFRC is conducting research on capturing sunlight and using it to drive solar fuel reactions or photovoltaic devices. The Center's efforts range from basic research on fundamental processes to integrating components into sub-systems and sub-systems into prototype devices.

Mission

To 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 and electricity.

Achievements

UNC EFRC conducts research on harnessing sunlight to drive solar fuel reactions in photoelectrochemical cells or to produce electricity in next generation photovoltaics. Highly integrated teams conduct research in a multidisciplinary environment. Research in solar fuels is based on a modular approach that integrates multiple functions from light absorption to catalysis in assemblies on electrode surfaces. Significant progress has been made in identifying new approaches to water oxidation, an important solar fuel reaction, and in reducing carbon dioxide to high-energy solar fuels both in solution and at interfaces. Researchers have developed new organic-inorganic hybrid materials that integrate catalysts and light-harvesting assemblies and these have been incorporated into prototypical devices.

Center for Lignocellulose Structure and Formation (CLSF)

Director

Daniel Cosgrove

Lead Institution

Pennsylvania State University

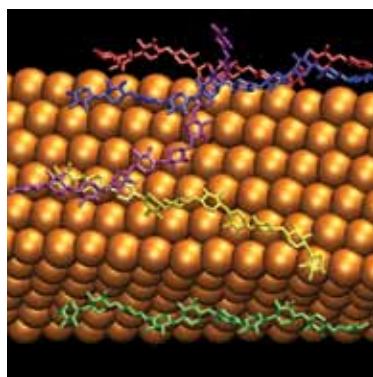
Partner Institutions

North Carolina State University

Virginia Tech University

Research Topics

biofuels, membranes, interfaces,
matter by design, high performance
computing, organic materials



ABOVE: Simulation of interactions between cellulose microfibrils (orange) and xylan chains (various colors) reveal the fundamental mechanics of wall cohesiveness, recalcitrance to enzymes and lignocellulose organization.

TOP: Left: Molecular model of cellulose synthase embedded in membrane. Many synthases form a complex (bottom right) that makes a crystalline ribbon, called a microfibril. Microfibrils are woven together in the cell wall (top) of plants.

Mission

To dramatically increase our fundamental knowledge of the formation and physical interactions of bio-polymer networks in plant cell walls to provide a basis for improved methods for converting biomass into fuels.

Achievements

Protein modelers in CLSF are using computational methods to solve the structure of cellulose synthase, the enzyme that polymerizes sugars to make cellulose. CLSF biochemists are isolating cellulose synthase complexes from plants to elucidate how they work and cell biologists are using advanced imaging techniques to visualize the synthase complexes to study their formation, movement and turnover. At a second level, biologists, spectroscopists, engineers and molecular modelers are working together to identify how cellulose interacts with itself and with matrix polymers to form a cohesive nanocomposite that is remarkably “recalcitrant,” or difficult to crack open, for economical conversion to a transportation fuel. Researchers at CLSF are also developing new spectroscopic methods to assess cellulose crystallinity and its interaction with other polymers in the cell wall.

Heterogeneous Functional Materials Center (HeteroFoaM)

Director

Kenneth Reifsnider

Lead Institution

University of South Carolina

Partner Institutions

University of California, Santa Barbara

University of Connecticut

Georgia Institute of Technology

Princeton University

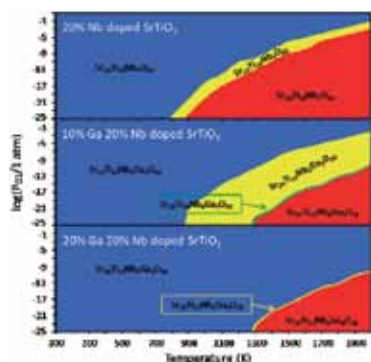
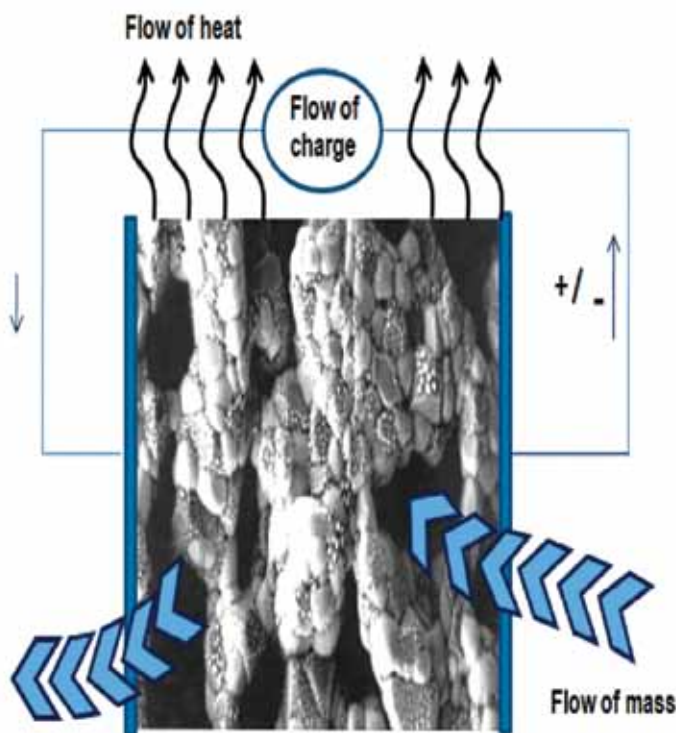
Rochester Institute of Technology

Savannah River National Laboratory

University of Utah

Research Topics

electrical energy storage, membranes, interfaces, matter by design, charge transport, inorganic materials, semiconductors, oxides



ABOVE: The introduction of gallium (Ga) and niobium (Nb) influences the ionic and electronic conductivity of strontium titanate (SrTiO_3) materials as show in these *ab initio* thermodynamic studies. **TOP:** First principles calculations of balance of mass, momentum, energy, and charge in local 3-D morphologies enable the design of new heterogeneous functional materials for energy storage and conversion applications.

Mission

To create control science to build a bridge between synthesis and modeling by understanding, modeling, designing, and synthesizing heterogeneous functional materials from the atomistic to nano-scale to macro-scale for energy storage and conversion systems such as fuel cells, batteries, supercapacitors, electrolyzers, and solid membranes.

Achievements

Heterogeneous functional materials are commonplace in nature—from biological to geological systems. Their properties and functionality are intricately related to their structure, composition, morphology and feature size. HeteroFoaM research focuses on the design and synthesis of heterogeneous functional materials for chemical and energy transformation processes. Recent achievements include enhanced understanding of the effects of nano- to macro-scale morphologies on energy conversion and storage devices such as fuel cells, hydrogen generators, capacitors, batteries and separation membranes. An integrated approach combines atomistic to continuum modeling, multiscale design, synthesis and processing of materials, and *in situ* characterization using various spectroscopic and microscopic techniques in two and three dimensions.

Center for Defect Physics (CDP)

Director

G. Malcolm Stocks

Lead Institution

Oak Ridge National Laboratory

Partner Institutions

Ames Laboratory

Brown University

University of California, Berkeley

Carnegie Mellon University

University of Illinois, Urbana-
Champaign

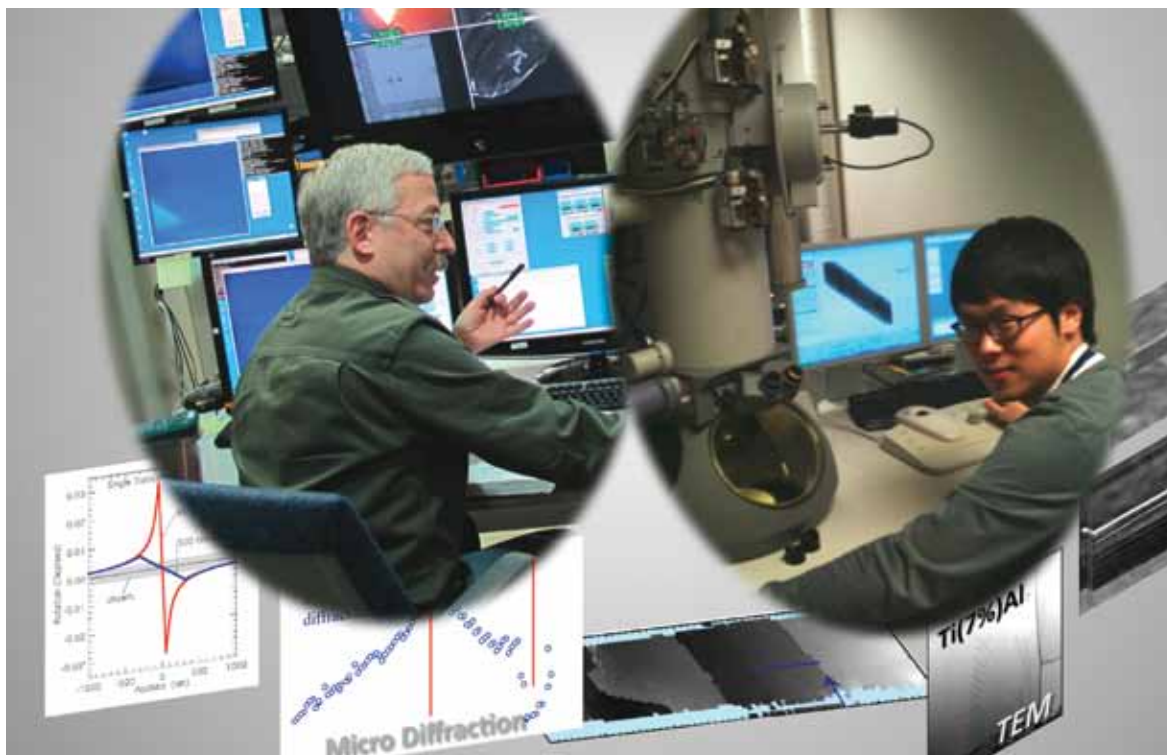
Lawrence Livermore National
Laboratory

Ohio State University

University of Tennessee

Research Topics

nuclear, extreme environment, defects,
interfaces, matter by design, ultrafast
science, high performance computing,
inorganic materials



ABOVE: Submicron x-ray beams map the lattice rotations around dislocation lines identified in the underlying transmission electron microscope, or TEM, image. The dislocations at the large arrow collectively tilt the lattice. The isolated dislocations to the right (medium arrow) produce only localized rotations that generally cancel each other out.

TOP: CDP doctoral student (right) characterizes with TEM a sample for CDP staff (left) to investigate with submicron x-ray microscopy.

Mission

To enhance our fundamental understanding of defects, defect interactions, and defect dynamics that determine the performance of structural materials in extreme environments.

Achievements

Understanding the properties of defects is key to developing new materials for extreme environments. Defects in metals range in size from missing or out-of-place atoms to more extended defects such as dislocations and grain boundaries containing lines or planes of out-of-place atoms. Research at CDP combines experimental and theoretical techniques to study the formation, evolution and interactions of defects using temporally- and spatially-resolved techniques that are only now becoming available. Recent progress includes the ability of ~300-nm resolution x-ray micro-diffraction to measure micro-rotations and locate single dislocations and dislocation arrays identified by electron microscopy in a thin titanium-aluminum alloy crystal. X-ray optics currently under development in collaboration with the Advanced Photon Source at Argonne National Laboratory will allow researchers to measure the response of single dislocations to internal defects and external stress fields with sub-100 nanometer resolution.

Fluid Interface Reactions, Structures and Transport Center (FIRST)

Director

David J. Wesolowski

Lead Institution

Oak Ridge National Laboratory

Partner Institutions

Argonne National Laboratory

Drexel University

Georgia State University

Northwestern University

Pennsylvania State University

Suffolk University

Vanderbilt University

University of Virginia

Research Topics

catalysis, solar fuels, electrical energy

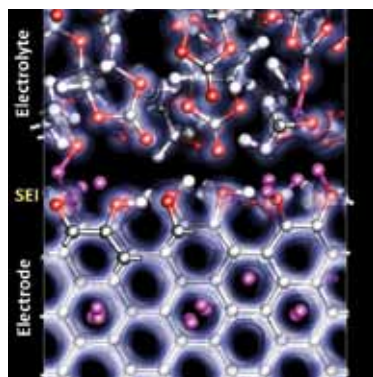
storage, extreme environment,

interfaces, matter by design, charge

transport, high performance

computing, inorganic materials,

semiconductors, oxides



ABOVE: FIRST's computer cluster is used to simulate reactions at fluid-solid interfaces, such as solid-electrolyte interphase formation at lithium-ion battery anodes (lithium-purple, oxygen-red, carbon-grey, hydrogen-white). **TOP:** Ray Unocic leads a team at Oak Ridge National Laboratory developing transmission electron microscopy to enable live-action observations of electrode/electrolyte interactions for advanced electrical energy storage and catalysis.

Mission

To develop quantitative and predictive models of the unique nanoscale environment at fluid-solid interfaces that will enable transformational advances in electrical energy storage and heterogeneous catalysis for solar fuels.

Achievements

The properties of fluids—their structures, diffusion dynamics, chemical reactivity—are profoundly altered in the nanoscale region near solid surfaces. Charge and mass transport and reactions at such interfaces critically control the performance of energy-relevant systems such as batteries, supercapacitors, and heterogeneous catalysts for the production of solar fuels. The FIRST Center integrates the synthesis of new materials (electrodes, electrolytes); neutron, x-ray and other probes of molecular properties at interfaces; and multiscale molecular modeling to understand and predict the performance of next-generation energy systems. Recent achievements include the development of electrochemical strain microscopy, for tracking lithium-ion transport and intercalation in batteries; coupling neutron scattering and computational models of the dynamics of ionic liquid transport in nanoporous electrodes; and fabrication of microsupercapacitors made from onion-like carbon nanoparticles that exhibit ultra-high electrical power densities.

Center for Frontiers of Subsurface Energy Security (CFSES)

Director

Gary A. Pope

Lead Institution

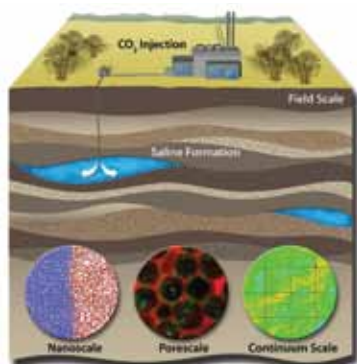
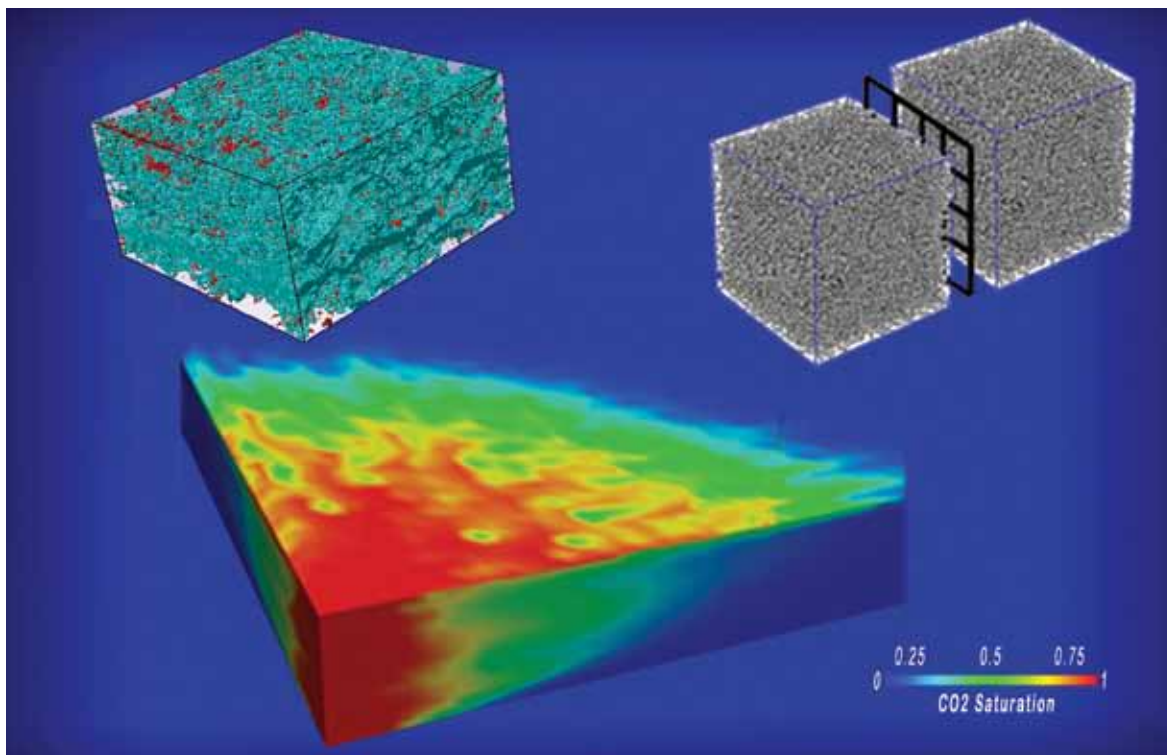
University of Texas at Austin

Partner Institution

Sandia National Laboratories

Research Topics

nuclear, extreme environment, high performance computing, carbon sequestration, interfaces, inorganic materials



ABOVE: CFSES is integrating multi-disciplinary scientific research from the molecular to field scale to assure safe, secure and economical underground storage of CO₂. **TOP:** CFSES combines experimental data (top left) with state-of-the-art simulations (top right) to create tools that will help determine what will happen when CO₂ is injected underground (bottom).

Mission

To pursue the scientific understanding of multiscale, multiphysics processes and to ensure safe and economically feasible storage of carbon dioxide and other byproducts of energy production without harming the environment.

Achievements

CFSES integrates multiscale experimental data and modeling results to create new approaches and models to understand the geological complexity, variability and uncertainty of processes involved in the underground storage of CO₂. Researchers measured the rate of CO₂ dissolving inside a pore, the impact of mineral surfaces on bacterial survival, and the influence of biofilm formation on the movement of CO₂. In addition, they collected field data that demonstrated carbonate cementation obstructs permeability at the pore scale but not leakage pathways at the field scale. They have developed approaches for incorporating detailed smaller-scale information into larger-scale models and for coupling of hydrological and mechanical processes to forecast fracture growth. While building scientific leadership through the active involvement of students and post-docs, CFSES developed more accurate and quick modeling tools for large-scale CO₂ storage predictions.

Understanding Charge Separation and Transfer at Interfaces in Energy Materials (CST)

Director

Xiaoyang Zhu

Lead Institution

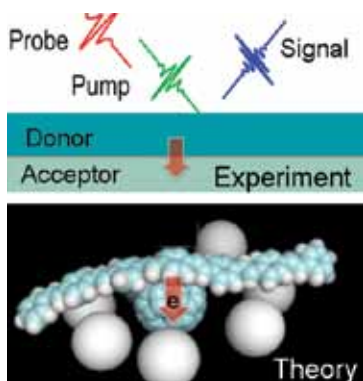
University of Texas at Austin

Partner Institution

Sandia National Laboratories

Research Topics

solar photovoltaics, electrical energy storage, defects, interfaces, matter by design, charge transport, ultrafast science, organic materials, inorganic materials, polymers, semiconductors, oxides



ABOVE:The CST uses newly developed experimental techniques, including interface-specific laser spectroscopy, coupled with advanced theoretical methods to answer key questions on charge separation and transfer for solar cell and battery materials. **TOP:** CST postdoctoral fellow Raluca Gearba prepares a nanostructured photovoltaic film to investigate its charge separation and transfer mechanisms.

Mission

To pursue fundamental research on charge transfer processes that underpin the function of highly promising molecular materials for photovoltaic and electrical energy storage applications.

Achievements

An improved fundamental understanding of the charge separation and transfer (CST) processes that occur at interfaces in nanostructured energy materials will lead to breakthroughs in the energy conversion and storage efficiencies of solar cells and next-generation batteries. Toward this goal, the research team uses experimental and theoretical methods developed by CST to elucidate CST mechanisms at the nanoscale and to optimize the design of CST material interfaces. Recent achievements include enhanced control of the arrangement of individual molecules in organic photovoltaic materials; exploration of the relationship between a material's intrinsic interfacial electric field and its CST efficiency; ready synthesis of highly pure polymers for photovoltaic applications; and high-resolution imaging and spectroscopy of phase boundaries that influence lithium-ion battery performance.

Center for Catalytic Hydrocarbon Functionalization (CCHF)

Director

T. Brent Gunnoe

Lead Institution

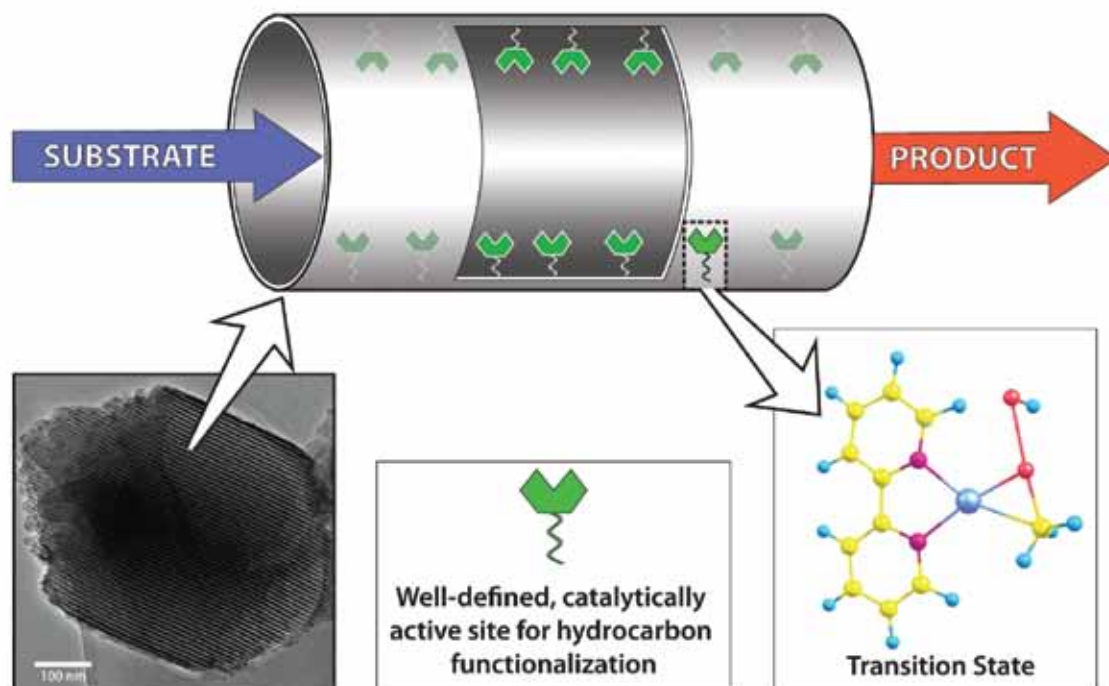
University of Virginia

Partner Institutions

Brigham Young University
California Institute of Technology
Iowa State University
University of Maryland
University of North Carolina
University of North Texas
Princeton University
Scripps Research Institute
Yale University

Research Topics

catalysis, electrical energy storage,
organic materials, inorganic materials,
semiconductors, oxides

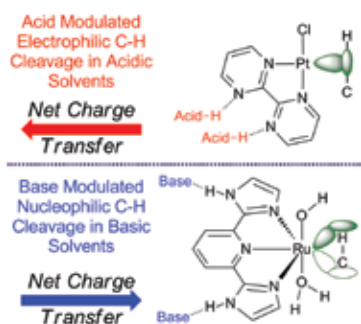


Mission

To develop, validate, and optimize new methods to rearrange the bonds of hydrocarbons, implement enzymatic strategies into synthetic systems, and design optimal environments for catalysts that can be used to reversibly functionalize hydrocarbons.

Achievements

The CCHF is developing methods to produce liquid fuels and electricity from domestic natural gas. Enzymes use hydrophobic and hydrophilic regions to control a substrate's access to a reactive site. CCHF researchers are working on a synthetic analog to enzymes based on mesoporous nanoparticles, whose pore size and polarity can be modulated. Developing homogeneous catalysts that transform natural gas into liquid fuels and tethering them to mesoporous nanoparticle can open new avenues for improved reactivity. In addition, while investigating how solvent influences hydrocarbon functionalization, a CCHF team discovered that basic solvents can promote hydrocarbon activation. Understanding and exploiting reaction environments can lead to entirely new approaches to convert natural gas into liquid fuels or electricity.



ABOVE: Converting natural gas to liquid fuels or electricity requires cleavage of carbon-hydrogen bonds. Depending on the system, either decreasing electron density with acids (red) or increasing electron density with bases (blue) improves reactivity. **TOP:** Well-defined active sites featuring transition metals on mesoporous silica nanoparticles have the potential to increase catalyst stability and generate liquid fuels from natural gas with high selectivity.

Center for Molecular Electrocatalysis (CME)

Director

R. Morris Bullock

Lead Institution

Pacific Northwest National Laboratory

Partner Institutions

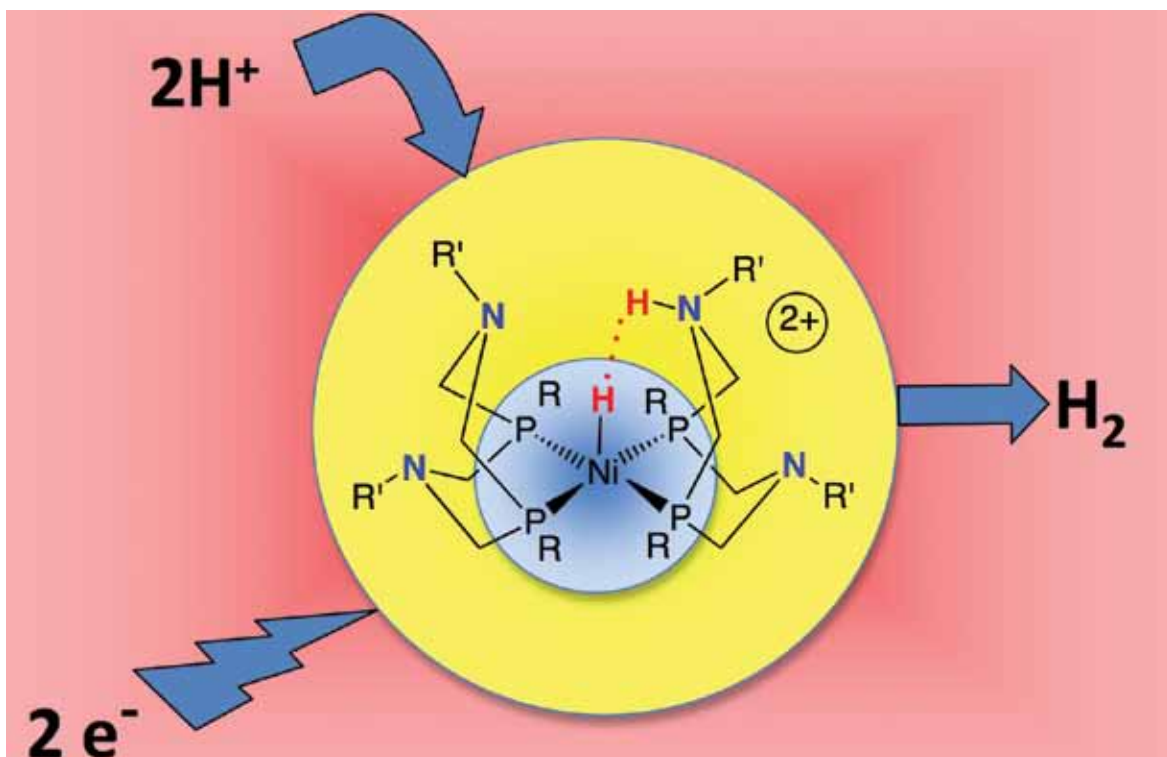
Pennsylvania State University

University of Washington

University of Wyoming

Research Topics

catalysis, electrical energy storage, hydrogen, matter by design, charge transport, organic materials, inorganic materials



ABOVE: Hydrogen bubbles forming on the electrode (black cylinder, right side of photo) in the catalytic production of hydrogen. The nickel catalyst makes the solution color red. **TOP:** Molecular nickel complexes catalyze the production of hydrogen through reduction of two protons by two electrons. Pendant amines (shown as blue nitrogen atoms) function as proton relays to help the reaction proceed quickly.

Mission

To understand, design and develop molecular electrocatalysts for solar fuel production and use.

Achievements

Addressing problems of growing energy demands and escalating carbon emissions will require increased use of non-fossil, sustainable energy sources. The intermittent nature of solar and wind energy calls for reliable systems for storing and delivering the energy—systems where electrocatalysts will play a vital role. Electrocatalysts must efficiently accelerate or catalyze the conversion of energy from electricity into chemical bonds in fuels such as hydrogen—as well as the reverse, converting chemical energy to electrical energy. New molecular catalysts based on inexpensive, earth-abundant nickel, developed in the CME, are the fastest molecular electrocatalysts for both production and use (oxidation) of hydrogen. Key to the design of these catalysts are the pendant amines, nitrogen (N)-containing groups that can bond to a proton, serving as proton relays and accelerating the reaction.

Contacts

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