

Synopses of the Department of Energy Energy Frontier Research Centers (EFRCs)

EFR Center for Bio-Inspired Solar Fuel Production

Devons Gust, Director

Arizona State University

Objective: To adapt the fundamental principles of natural photosynthesis to the man-made production of hydrogen or other fuels from sunlight.

A multidisciplinary team will research artificial photosynthetic antennas and reaction centers that absorb light efficiently and convert it to electrochemical energy, a water oxidation catalyst based on that found in photosynthesis and assembled in a way that mimics the process used by nature, and an electron accumulator and proton reduction catalyst based on natural hydrogenase enzymes. The antennas and reaction centers will be designed using the techniques of organic chemistry. The catalysts will be developed using peptide engineering methods. These components will be structurally organized using concepts from materials science, nanotechnology and nucleic acid engineering.

Center for Interface Science: Hybrid Solar-Electric Materials (CIS:HSEM)

Neal R. Armstrong, Director

University of Arizona

Objective: To enhance the conversion of solar energy to electricity using hybrid organic-inorganic materials.

This EFRC will focus on fundamental interfacial problems in solar electric energy conversion to obtain a predictive and molecular level understanding of electron flow through the interfaces of organic materials with metals, semiconductors, and other organic substances. A unique set of surface analytical techniques will be employed to relate the properties of solar light absorption, charge separation, and charge transport at these interfaces with the molecular structure at the nanometer length scale. This center plans collaborations with scientists at the Georgia Institute of Technology, Princeton University, the University of Washington, and the National Renewable Energy Laboratory, and Sandia National Laboratories.

Light-Material Interactions in Energy Conversion

Harry Atwater, Director

California Institute of Technology

Objective: To tailor the properties of advanced materials to control the flow of solar energy and heat.

Research in this EFRC will be organized into four thrust areas aimed at understanding and controlling fundamental material properties that can dramatically improve the collection, absorption, emission and focusing of light in matter, enabling efficient light conversion to electrical energy in photovoltaic solar cells and to chemical energy through solar-driven fuel generation. The science includes up-conversion of low-energy photons for more efficient photovoltaic and photo-electrochemical conversion efficiency, the use of plasmonic nanostructures to more efficiently couple light into and out of ultrathin absorber layers, the use of metamaterials to steer, slow, and focus light, and self assembly of nanostructured materials for light absorption. This EFRC includes planned collaborations with scientists at Lawrence Berkeley National Laboratory and the University of Illinois, and some of the work will be done at the Molecular Foundry at Lawrence Berkeley National Laboratory.

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Center for Nanoscale Control of Geologic CO₂ Donald DePaolo, Director Lawrence Berkeley National Laboratory

Objective: To establish the scientific foundations for the geological storage of carbon dioxide.

The objective this EFRC is to enhance the scientific foundation of how subsurface fluids and rocks interact as they are moved away, sometimes far away, from equilibrium by technological applications. The immediate application of interest is the problem of geological storage of carbon dioxide related to reducing greenhouse gases released to the atmosphere from stationary power sources, but long term benefits are expected for predicting the performance of any subsurface storage application for long periods of time. The EFRC includes planned collaborations with scientists at Lawrence Livermore National Laboratory, Oak Ridge National Laboratory, Massachusetts Institute of Technology, and the University of California-Davis. The EFRC will utilize the Advanced Light Source, Molecular Foundry, and National Energy Research Scientific Computing Center at Lawrence Berkeley National Laboratory and the Spallation Neutron Source Oak Ridge National Laboratory.

Center on Nanostructuring for Efficient Energy Conversion Fritz Prinz, Director Stanford University

Objective: To design, create, and characterize materials at the nanoscale for a wide variety of energy applications.

The EFRC will undertake fundamental scientific study and development of nanostructured materials targeted to provide the basis of new active materials components for a wide range of future energy applications. These materials will form the functional elements leading to next generation devices for electrical energy storage (batteries, capacitors), the conversion of solar and electrical energy into fuels, hydrogen and solid oxide fuel cells, and solid state lighting with the associated reduction of CO₂ emissions. This EFRC will utilize a combination of techniques in developing new complex hybrid materials, employing advanced characterization methods and theoretical modeling in the research aimed at ultra small functional nanostructures with enhanced surface properties necessary to accelerate and address future needs for energy conversion, storage and transport. The EFRC plans collaborations with scientists at the Carnegie Institution, HRL Laboratories, and the Technical University of Denmark.

Center for Gas Separations Relevant to Clean Energy Technologies Berend Smit, Director University of California, Berkeley

Objective: To design and synthesize new forms of matter with tailored properties for gas separations in applications including carbon capture and sequestration.

This EFRC will address the challenge associated with the design and synthesis of revolutionary new forms of matter with tailored properties for gas separations. New classes of materials will be developed to affect gas separations with an unprecedented level of molecular control. Guided by modern characterization and computational methods, further refinement of designs will enable chemical control for efficient gas separations that are essential to the development of clean energy technologies. This EFRC includes planned collaborations with scientists at the Lawrence Berkeley National Laboratory, Texas A&M University, the University of California - Los Angeles, the University of Amsterdam, and the Norwegian University of Science and Technology.

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Molecularly Assembled Material Architectures for Solar Energy Production, Storage, and Carbon Capture

Vidvuds Ozolins, Director

University of California, Los Angeles

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

The objective of this EFRC will be achieved through a combination of theoretical modeling, computer simulation, materials synthesis, and experimental measurements on materials that enhance performance and are economically viable on a large scale. The EFRC plans collaborations with scientists at the National Renewable Energy Laboratory, Eastern Washington University, the University of Kansas, and the University of California-Davis.

Center on Materials for Energy Efficiency Applications

John Bowers, Director

University of California, Santa Barbara

Objective: 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.

The research in this EFRC is comprised of fundamental studies involving synthesis and characterization of a variety of materials: organic, inorganic, nanostructured and bio-inspired materials for solar energy conversion; nanostructured thermoelectric materials for heat transport; and gallium-nitride-based materials for solid-state lighting. This EFRC includes planned collaboration with scientists at the National Renewable Energy Laboratory, Los Alamos National Laboratory, the University of California Santa Cruz, and the University of Michigan.

Emerging Materials for Solar Energy Conversion and Solid State Lighting

Paul Daniel Dapkus, Director

University of Southern California

Objective: To simultaneously explore the light absorbing and emitting properties of hybrid inorganic-organic materials for solar energy conversion and solid-state lighting.

This EFRC seeks to devise novel nanostructured materials to serve as active elements in hybrid inorganic/organic systems for both visible light sources and solar electric energy converters. Scientists will perform research on organic materials and thin layer semiconductor nanostructures and will exploit the opportunities that result from the parallel study of these complementary systems of light emission and light absorption. Collaborations are planned with scientists from the University of Illinois, the University of Michigan, and the University of Virginia.

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Center for Inverse Design **Alex Zunger, Director** **National Renewable Energy Laboratory**

Objective: 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.

This EFRC will use theory and computation to identify materials and device structures expressly designed for energy conversion instead of relying on trial-and-error methods of materials synthesis and physical characterization, which are then followed by theoretical analysis. In this inverse process, the EFRC will exploit a combination of novel theoretical methods and the immense power of modern computational capabilities. The EFRC includes collaborations with scientists at Northwestern University, Stanford University, and Oregon State University and will utilize the Stanford Synchrotron Radiation Lightsource at the SLAC National Accelerator Laboratory.

Center for Energy Frontier Research in Extreme Environments (Efree) **Mao Ho-Kwang, Director** **Carnegie Institution of Washington**

Objective: To accelerate the discovery of energy-relevant materials that can tolerate transient extremes in pressure and temperature.

This EFRC will also explore what happens to such materials when they are returned to ambient conditions and investigate the mechanisms of high-pressure and high-temperature material failure. Studies are planned on metals; superconducting, electronic, and magnetic materials; hydrogen and hydrogen-bearing materials; novel molecular and covalent compounds; catalysts; and nanophase, composite, and geological materials. The Efree EFRC includes planned collaborations with scientists at nine U.S. universities and six DOE national laboratories. Efree researchers will carry out novel materials synthesis, state-of-the-art high pressure-temperature materials characterization with neutron, laser, synchrotron x-ray, and micro-nano analysis probes, and theoretical studies at Carnegie laboratories, universities, and synchrotron and neutron scattering facilities within DOE national laboratories.

Rational Design of Innovative Catalytic Technologies for Biomass Derivative Utilization **Dionisios Vlachos, Director** **University of Delaware**

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

Heterogeneous catalysts designed specifically for the energy- and atom-efficient conversion of complex biomass molecules and materials will be the core knowledge to be pursued in this EFRC. Scientists in the EFRC will launch a first-principles attack on the key chemical and materials challenges associated with biomass conversion and will devise novel analytical techniques to acquire atomistic, molecular and dynamic level information from these systems. The EFRC will emphasize multi-scale modeling to treat the natural material complexity; the discovery of processes designed to manipulate complex mixtures and their reactivity, and the development of new analytical methods for characterization of reacting media. The EFRC plans collaborations with scientists at Lehigh University, California Institute of Technology, and the Universities of Massachusetts, Minnesota, Pennsylvania, Southern California, and Stony Brook.

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It will also utilize the National Synchrotron Light Source at Brookhaven National Laboratory and several Office of Science computational facilities.

Center for Materials Science of Nuclear Fuel

Dieter Wolf, Director

Idaho National Laboratory

Objective: To develop predictive computational models, validated by experiments, for the thermal and mechanical behavior of analogues to nuclear fuel.

The research in this EFRC is focused specifically on providing a better mechanistic understanding of the effects of irradiation on UO₂ and Mo. The research would help bridge gaps between *ab initio* and molecular dynamics simulations through computation benchmarked with experimental characterization following proton, ion, and neutron irradiation. The understanding developed would advance design capability for future nuclear fuel systems. This EFRC includes planned collaborations with scientists at the Colorado School of Mines, Florida State University, North Carolina State University, the University of Florida, Washington State University, the University of Wisconsin, and Oak Ridge National Laboratory.

Institute for Atom-Efficient Chemical Transformations (IACT)

Christopher Marshall, Director

Argonne National Laboratory

Objective: To discover, understand, and control efficient chemical pathways for the conversion of coal and biomass into chemicals and fuels.

Modern experimental and computational techniques will be used to address the computational design and the atomic level characterization of working catalysts for complex molecular mixtures modeled after coal and biomass. Bio-inspired catalysts will be synthesized and evolved for the selective disassociation of oxygen from model mixtures, selective hydrogenation of oxygen functional groups, and controlled carbon-carbon linking. Complex, multifunctional catalysts that behave predictably under reaction conditions at relatively high temperature and in solvents will be developed to uncover detailed structure-reactivity relationships. The IACT plans collaborations with researchers from Argonne National Laboratory, Northwestern University, Purdue University, and University of Wisconsin-Madison. IACT will make use of the Advanced Photon Source at Argonne National Laboratory and several Office of Science computational facilities.

Center for Electrical Energy Storage: Tailored Interfaces

Michael Thackeray, Director

Argonne National Laboratory

Objective: To understand complex phenomena in electrochemical reactions critical to advanced electrical energy storage.

This EFRC will explore the scientific challenges that limit the progress and application of electrical energy storage technologies for energy generated by alternative sources (wind, solar, geothermal, and marine), as well as for transportation (hybrid and all-electric vehicles), medicine, defense and aerospace, telecommunications, and consumer products. The overarching goal of the EFRC is to acquire a fundamental understanding of highly complex phenomena at electrode/electrolyte interfaces that control electrochemical reactions and processes in electrical energy storage devices. The EFRC includes planned collaborations with scientists at

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Northwestern University and the University of Illinois at Urbana-Champaign and will utilize the Center for Nanoscale Materials, the Advanced Photon Source, and the Argonne Leadership Class Computing Facility at Argonne National Laboratory.

Argonne-Northwestern Solar Energy Research (ANSER) Center

Michael R. Wasielewski, Director
Northwestern University

Objective: To revolutionize the design, synthesis, and control of molecules, materials, and processes in order to dramatically improve conversion of sunlight into electricity and fuels.

The research in this EFRC addresses the basic solar energy conversion steps of charge photo-generation, separation, recombination, as well as charge and energy transfer among molecules, across interfaces, and through nanostructured architectures. The center will focus on the science needed to create integrated molecular systems for artificial photosynthesis, to control interfacial processes critical in organic photovoltaics, and to enable three-dimensional nanostructured materials organization for solar fuels and hybrid photovoltaics. The EFRC includes planned collaborations with scientists at Argonne National Laboratory, where the Advanced Photon Source and the Center for Nanophase Materials will play an important role, as well as the University of Chicago, the University of Illinois, and Yale University.

Center for Integrated Training in Far-From-Equilibrium and Adaptive Materials (CITFAM)

Bartosz Grzybowski, Director
Northwestern University

Objective: To synthesize, characterize, and understand new classes of materials under conditions far from equilibrium relevant to solar energy conversion, storage of electricity and hydrogen, and catalysis.

This EFRC combines new research on non-equilibrium systems with nanoscale materials science to achieve its objective. The combination of theory, simulations and experimentation will allow this EFRC to develop materials that are not only structurally robust, but also have the ability to change and optimize their own performance in response to environmental stimuli. The EFRC plans collaborations with scientists at the University of Michigan and Harvard University.

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

Maureen McCann, Director
Purdue University

Objective: To use fundamental knowledge about the interactions between catalysts and plant cell walls to design improved processes for the conversion of biomass to energy, fuels, or chemicals.

This EFRC will combine expertise in biology, chemistry, and engineering to increase much needed knowledge of catalysis pertaining to plant cell wall chemistry. The EFRC includes planned collaborations with scientists at the University of Tennessee for development of “hybrid” catalysts and catalytic conversion of renewable materials; with National Renewable Energy Laboratory for advanced, high resolution biomass imaging technology and computational modeling; and with researchers at the Argonne National Laboratory for advanced scattering and imaging techniques using the Advanced Photon Source. Additional scattering experiments using the Spallation Neutron Source at Oak Ridge National Laboratory are also planned.

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Materials Science of Actinides

Peter C. Burns, Director
University of Notre Dame

Objective: 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.

All nuclear fuels contain actinide materials; the research of this EFRC is expected to lead to better fundamental understanding, as well as control of, chemical and physical processes that occur in the extreme environments within the nuclear fuel cycle: nuclear fuels during and after irradiation in a nuclear reactor; recycling of used nuclear fuel to create a “green” closed nuclear fuel cycle; and the behavior of radioactive materials in nuclear waste repositories. This EFRC includes planned collaborations with scientists at the University of Michigan and the University of California-Davis; Pacific Northwest National Laboratory including the Environmental Molecular Sciences Laboratory, Savannah River National Laboratory, and Sandia National Laboratories. The EFRC will make use of the National Synchrotron Light Source at Brookhaven National Laboratory, the Advanced Photon Source at Argonne National Laboratory, and the Spallation Neutron Source at Oak Ridge National Laboratory.

Computational Catalysis and Atomic-Level Synthesis of Materials: Building Effective Catalysts from First Principles

James Spivey, Director
Louisiana State University

Objective: To develop computational tools to accurately model catalytic reactions and thereby provide the basis for the design of new catalysts.

The research in this EFRC will use recently developed tools to accurately simulate a catalytic reaction purely by computation, from first principles, and thus provide a different way to develop new materials other than by experimental trial and error. Scientists in this EFRC plan to carry out reactions computationally, postulate exact catalysts, synthesize them precisely, and fully characterize their performance. The EFRC plans collaborations with scientists at Tulane University, Oak Ridge National Laboratory, Texas A&M University, the University of Florida, Clemson University, Georgia Tech, the University of Utrecht, Grambling University, Louisiana Tech, and Penn State University. The EFRC will utilize the Center for Nanophase Materials Sciences at Oak Ridge National Laboratory, the Advanced Light Source at Lawrence Berkeley National Laboratory, the Advanced Photon Source at Argonne National Laboratory, and the Center for Integrated Nanotechnologies at Los Alamos and Sandia National Laboratories.

Solid-State Solar-Thermal Energy Conversion Center

Gang Chen, Director
Massachusetts Institute of Technology

Objective: To create novel, solid-state materials for the conversion of sunlight and heat into electricity.

This EFRC aims to advance our fundamental scientific understanding of thermoelectric and thermo-photovoltaic materials and to develop novel materials and devices to harvest energy from the sun and terrestrial heat sources. The multidisciplinary effort integrates theory and experiment to study the fundamentals of photon, phonon and charge carrier interactions in thermoelectric

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materials and will also utilize photonic crystals and metamaterials to convert the solar energy spectrum, in an attempt to provide an ideal match to the bandgap of photovoltaic materials. This EFRC includes planned collaborations with scientists at Boston College and Oak Ridge National Laboratory, and will encompass novel materials synthesis, phonon and electron spectroscopies, multi-scale modeling and simulation, and will utilize scanning transmission electron microscopy imaging facilities, neutron spectrometers at the High-Flux Isotope Reactor and the Spallation Neutron Source of the Oak Ridge National Laboratory and ultraviolet photoelectron spectroscopy at the National Synchrotron Light Source at Brookhaven National Laboratory.

Center for Excitonics

Marc A. Baldo, Director

Massachusetts Institute of Technology

Objective: 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.

With photosynthesis as an inspiration and guide, this EFRC will achieve its objective through a combination of theory, modeling, materials synthesis, and characterization. The planned research has the following goals: understand the effects of environment and coherence on exciton transport in complex nanostructures; explore and characterize novel excitonic states, including hybrid organic-inorganic excitons, strongly coupled exciton-polaritons and exciton plasmon polaritons; and perform spectroscopic studies of exciton formation, dissociation, fission, and annihilation. This EFRC includes planned collaborations with scientists at Harvard University and Brookhaven National Laboratory, and some of the work will be done using the Center for Functional Nanomaterials at Brookhaven.

Polymer-Based Materials for Harvesting Solar Energy

Thomas Russell, Director

University of Massachusetts

Objective: To use novel, self-assembled polymer materials in systems for the conversion of sunlight into electricity.

The goal of this EFRC will be achieved through a fundamental understanding of polymer materials, the theory and modeling of non-equilibrium structures, and an innovative research program with polymer nanostructures. This effort will combine extensive expertise in the preparation of polymeric materials with x-ray and neutron scattering for characterization of the nanometer dimension polymer structures. This EFRC includes planned collaborations with scientists from institutions in Korea, Japan, and Germany and with the National Renewable Energy Laboratory, the University of Pittsburgh and Pennsylvania State University. It will perform neutron scattering at the High Flux Isotope Reactor and Spallation Neutron Source at Oak Ridge National Laboratory.

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Science of Precision Multifunctional Nanostructures for Electrical Energy Storage **Gary Rubloff, Director** **University of Maryland**

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

Nano-structured electrodes offer vastly greater surface area and smaller path lengths for motion of electrons and ions, increasing the rate at which charges can be moved and stored, leading to much increased power and energy density and faster charging. By using materials in precisely built nanostructures, energy storage devices will hold more energy, will charge or deliver electricity faster, and remain stable for longer lifetimes, while reducing space and weight. This EFRC includes the planned collaborations with scientists from the University of Florida, Yale University, the University of California, Irvine, Sandia National Laboratories, and Los Alamos National Laboratory, including the Center for Integrated Nanotechnologies at Los Alamos and Sandia.

Revolutionary Materials for Solid State Energy Conversion: A DOE Energy Frontier Research Center **Donald Morelli, Director** **Michigan State University**

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

This EFRC will achieve its objective through the novel design, synthesis, and characterization of thermoelectric materials. The effort will focus on lowering the thermal conductivity and manipulating the electronic density of states to improve the electrical conductivity in broad range of materials, including nanostructured composites, spinodal-decomposed materials, self-assembled nanostructures, disordered inhomogeneous bulk systems, and semiconductors with resonant levels. The EFRC includes planned collaborations with scientists at Northwestern University, Ohio State University, University of Michigan, University of California-Los Angeles, Wayne State University, and Oak Ridge National Laboratory.

Solar Energy Conversion in Complex Materials (SECCM) **Peter Green, Director** **University of Michigan**

Objective: 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.

An integrated theoretical, experimental and computational approach will be taken in this EFRC to understand how multiple interfaces and high surface areas in these two means of energy conversion affect charge transport and heat conduction. This research effort plans to make use of the expertise in theory, computation, materials growth and synthesis, ultrafast optical sciences, and materials characterization.

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Center for Advanced Biofuels Systems (CABS)

Richard Sayre, Director

Donald Danforth Plant Science Center

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

CABS will focus its efforts on the model algae *Chlamydomonas* and the oilseed plant *Camellina*. Metabolic networks will be modified to increase lipid and thus “bio-oil” synthesis, and new metabolic pathways will be designed for production of hydrocarbons from sunlight. Utilizing the skills of plant biochemists, biophysicists, and computational biologists, this innovative center will integrate all aspects of metabolism, from the early events in photosynthesis to the synthesis and accumulation of oils and biofuel precursors. This EFRC may lead to a transformational channeling of solar energy through carbon metabolism and, ultimately, into biofuels and includes planned collaborations with scientists at University of Nebraska, University of Missouri-St. Louis, University of Arizona, and Michigan State University.

Photosynthetic Antenna Research Center (PARC)

Robert Blankenship, Director

Washington University, St. Louis

Objective: To understand the basic scientific principles that underpin the efficient functioning of the natural photosynthetic antenna system as a basis for man-made systems to convert sunlight into fuels.

PARC proposes a program in basic scientific research aimed at understanding the principles of light harvesting and energy funneling as applied to natural photosynthetic, bio-hybrid and bio-inspired antenna systems. The goal of this work is to elucidate the basic scientific principles that underlie the efficient functioning of natural photosynthetic antenna systems and how those principles can be translated into concepts that will form the basis for next-generation systems for solar energy conversion. This will be accomplished using structural techniques such as neutron scattering and diffraction at the Spallation Neutron Source and the High Flux Isotope Reactor at Oak Ridge National Laboratory, and advanced microscopy at the Center for Integrated Nanotechnology at Los Alamos and Sandia National Laboratories. PARC includes planned collaborations with scientists at the Donald Danforth Plant Science Center, Los Alamos National Laboratory, North Carolina State University, Oak Ridge National Laboratory, Sandia National Laboratories, the University of California-Riverside, the University of Glasgow (UK), the University of Pennsylvania, and the University of Sheffield (UK).

Solar Fuels and Next Generation Photovoltaics

Thomas J. Meyer, Director

University of North Carolina at Chapel Hill

Objective: To synthesize new molecular catalysts and light absorbers and integrate them into nanoscale architectures for improved generation of fuels and electricity from sunlight.

This EFRC will pursue fundamental scientific research needed to synthesize new molecular catalysts and light absorbers, and to design novel materials and nanoscale architectures, that can enable low-cost and efficient solar fuels from artificial photosynthesis and solar electricity from next generation photovoltaics. Advanced experimental and theoretical methods will be developed to investigate photocatalytic components and their integration in hybrid interfacial systems for production of hydrogen and hydrocarbon fuels, and to investigate polymeric photovoltaics, hybrid

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composite systems with quantum-confined nanostructures, and nanoscale photonic architectures to enhance light capture. The EFRC includes planned collaborations with scientists at Duke University, University of Florida, North Carolina Central University, and North Carolina State University.

Energy Frontier Research Center for Combustion Science Chung K. Law, Director Princeton University

Objective: To develop a suite of predictive combustion modeling capabilities for the chemical design and utilization of non-petroleum based fuels in transportation.

This EFRC plans to construct accurate combustion models by the use of three dimensional representations of the interacting chemistry functional groups, coupled with quantum chemical predictions of reaction rate coefficients, and to validate these models by comparisons with experimental data from a variety of measurements on gas-phase reactions. The EFRC will significantly impact the combustion community by developing a suite of predictive high-fidelity simulation and combustion modeling capabilities for designing novel non-petroleum based fuels for advanced transportation engines, which will be characterized and validated by experiments at molecular and macroscopic scales. The EFRC includes planned collaborations with scientists at Case Western Reserve University, Cornell University, Massachusetts Institute of Technology, the University of Minnesota, the University of Southern California, the Combustion Research Facility at Sandia National Laboratory, and Stanford University. It will utilize the Advanced Light Source at Lawrence Berkeley National Laboratory.

The Center for Advanced Solar Photophysics Victor Klimov, Director Los Alamos National Laboratory

Objective: 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.

The purpose of this EFRC is to develop novel physics, materials, and architectures for harvesting solar light and converting it into electrical charges with efficiencies at or above equilibrium thermodynamic limits. Experts in nanoscience will create novel spherical and planar architectures of nanometer dimension for manipulation of solar light absorption and electron transport and collection for use in solar electricity and fuel production. Significant synergy in this program is provided through planned collaborations with the National Renewable Energy Laboratory, the University of Minnesota, the University of North Carolina, the University of California-Irvine, Rice University, the Colorado School of Mines, and the University of Colorado.

Extreme Environment-Tolerant Materials via Atomic Scale Design of Interfaces Michael Nastasi, Director Los Alamos National Laboratory

Objective: 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.

This EFRC recognizes that the challenge to developing materials with radically extended performance limits at irradiation and mechanical extremes will require designing and perfecting atom- and energy efficient synthesis of revolutionary new materials that maintain their desired

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properties while being driven very far from equilibrium. To address these issues, the EFRC will develop a fundamental understanding of how atomic structure and energetics of interfaces contribute to defect and damage evolution in materials, and use this information to design nanostructured materials with tailored response at irradiation and mechanical extremes. This EFRC includes planned collaborations with scientists at the Massachusetts Institute of Technology, Lawrence Livermore National Laboratory and the University of Illinois. The EFRC will utilize the Center for Integrated Nanotechnologies at Los Alamos and Sandia National Laboratories and the Electron Microscopy Center at Argonne National Laboratory.

EFRC for Solid State Lighting Science

Jerry Simmons, Director

Sandia National Laboratories

Objective: To study energy conversion in tailored nanostructures as a basis for dramatically improved solid-state lighting.

The work in this EFRC is grouped into three thrust areas: investigation of energy conversion processes in low-dimensional nanostructures including luminescent nanowires, nanodots, and hybrid structures; study of energy conversion processes in photonic structures with characteristic length scales that are shorter than the wavelength of the radiation used; and exploration of the fundamental relationship between defects and luminescent properties in compound semiconductors with wide band-gaps. This EFRC includes planned collaborations with scientists at Rensselaer Polytechnic Institute, the University of New Mexico, California Institute of Technology, Los Alamos National Laboratory, Yale University, Northwestern University, the University of Massachusetts-Lowell, and Philips Lumileds Lighting. The EFRC will also make use of nanoscience-related capabilities of the Center for Integrated Nanotechnologies, jointly operated by Los Alamos and Sandia National Laboratories.

Center for Emergent Superconductivity

J.C. Seamus Davis, Director

Brookhaven National Laboratory

Objective: By understanding the fundamental physics of superconductivity, to discover new high-temperature superconductors and improve the performance of known superconductors.

This EFRC aims to discover new superconductors with higher critical temperatures, critical currents and isotropy, and to improve the performance of known superconductors while seeking an understanding of the physics that controls their critical temperature, critical current, and overall performance. The EFRC will execute combined experimental and theoretical investigations of known high-temperature superconductors in an attempt to elucidate the mechanism of superconductivity. This understanding will be used to propose viable and realistic new materials systems to investigate, to develop new ways to control the behavior of vortex matter, and to direct the discovery of new or improved families of superconducting materials with higher critical temperatures and critical currents. The EFRC includes planned collaborations with scientists at Argonne National Laboratory and University of Illinois and will perform neutron scattering experiments at the Spallation Neutron Source at Oak Ridge National Laboratory and angle-resolved photoemission experiments at the National Synchrotron Light Source at Brookhaven National Laboratory and the Advanced Photon Source at Argonne National Laboratory.

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Re-Defining Photovoltaic Efficiency Through Molecule-Scale Control

James Yardley

Columbia University

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

This EFRC brings together a team of theoretical, computational and experimental experts on nanoparticles to address the fundamental scientific challenges in nanoscale materials, complex layered structures, and interconnection schemes. Knowledge from these fundamental studies will significantly improve solar energy conversion in organic molecular systems. The EFRC plans collaborations with solar-energy experts from University of Minnesota, Purdue University, University of Arkansas, Brookhaven National Laboratory including the Center for Functional Nanomaterials, and General Electric.

Nanostructured Interfaces for Energy Generation, Conversion, and Storage

Hector Abruña, Director

Cornell University

Objective: To understand and control the nature, structure, and dynamics of reactions at electrodes in fuel cells, batteries, solar photovoltaics, and catalysts.

This EFRC will concentrate on the overriding theme of understanding the nature, structure, and dynamics of interfaces on energy generation, conversion and storage. Reactions at electrodes in fuel cells, charging and discharging reactions in lithium ion batteries, charge generation in photovoltaic and photo-electrochemical devices, and numerous catalytic systems all depend critically on the nature and structure of interfaces between materials and different states of matter. The center will integrate the synthesis of model systems with atomic level control, and explore electronically conducting polymers in contact with metal electrodes. In addition, fundamental theory and computations, combined with the development of tools that will provide *in-situ* spatiotemporal characterization, will differentiate the fundamental properties of the best materials over the range of intended operating conditions. These investigations will dramatically accelerate the development of energy generation, conversion and storage technologies and thus, the evolution of the entire energy landscape. This EFRC includes a planned collaboration with scientists at Lawrence Berkeley National Laboratory.

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

Grigorii Soloveichik, Director

General Electric Global Research

Objective: To explore the fundamental chemistry needed for an entirely new approach to energy storage that combines the best properties of a fuel cell and a flow battery.

The focus of this EFRC is to explore the fundamental chemistry of electrocatalysis and ionic transport required for an entirely new approach to energy storage through the use of an organic carrier as reversible 'virtual hydrogen storage'. This fundamental knowledge base will enable the technology development of an innovative high-density energy storage and conversion system combining the best properties of a fuel cell and a flow battery for stationary and mobile applications. The EFRC includes planned collaborations with scientists at Yale University, Stanford University and Lawrence Berkeley National Laboratory.

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Northeastern Chemical Energy Storage Center (NOCESC)

Clare P. Grey, Director

State University of New York, Stony Brook

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

This EFRC seeks a fundamental understanding of how electrode reactions occur, and how they can be tailored by appropriate electrode design, so that critical structural and physical properties that are vital to improving battery performance can be identified and used to design new battery systems. The NOCESC will also develop advanced *in-situ* diagnostic methods for chemical energy storage systems that combine multiple experimental approaches, such as spectroscopy and imaging. The EFRC includes planned collaboration with scientists from Rutgers University, SUNY-Binghamton, the Massachusetts Institute of Technology, Lawrence Berkeley National Laboratory, the University of Michigan, Argonne National Laboratory including the Advanced Photon Source, Brookhaven National Laboratory including the National Synchrotron Light Source and the Center for Functional Nanomaterials, and the University of Florida.

Center for Lignocellulose Structure and Function

Daniel Cosgrove, Director

Pennsylvania State University

Objective: To dramatically increase our fundamental knowledge of the physical structure of bio-polymers in plant cell walls to provide a basis for improved methods for converting biomass into fuels.

To achieve its objective, this EFRC will study the physical structure of lignocellulose at the nanoscale level and the rules and principles by which lignocellulose is created. An interdisciplinary team that includes plant and microbial molecular biologists, chemists, physicists, material scientists, engineers and computational modelers will utilize advanced, cutting-edge approaches and methodology to bring about desperately needed advances in the fundamental understanding of the “rules of assembly” of plant cell wall. Specifically, the focus will be placed on understanding the cellulose synthesis, lignocellulose assembly, and the relationship between nanoscale structure and macroscale properties such as porosity and mechanics of the plant cell wall. This EFRC has strong potential for transforming bioenergy and materials sciences through combined molecular, genetic, and nano-materials engineering approaches and includes planned collaborations with scientists at North Carolina State University and Virginia Polytechnic Institute and State University.

Science Based Nano-Structure Design and Synthesis of Heterogeneous Functional Materials for Energy Systems

Kenneth Reifsnider, Director

University of South Carolina

Objective: To build a scientific basis for bridging the gap between making nano-structured materials and understanding how they function in a variety of energy applications.

This EFRC will focus specifically on nanostructured heterogeneous functional materials (NSHFMs) and how they work as described by multi-scale theoretical models and experimental results. NSHFMs are literally disruptive material concepts, in the sense that they have quickly replaced homogeneous materials in a host of energy-centric devices that make electrochemistry, fuel synthesis, chemical refinement, hydrogen storage, heat storage, and other essential processes

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possible. The objective of the work is to establish the associated control science to enable simulation-based design and creation of nano-synthesis concepts and processes that control the nano-structural configurations and interfaces (physics, chemistry and geometry) of the active phases. This EFRC includes planned collaborations with scientists at the Georgia Institute of Technology, North Carolina State University, Princeton University, University of Pennsylvania, University of Utah, University of California-Santa Barbara, University of Connecticut, Pacific Northwest National Laboratory, Oak Ridge National Laboratory, Savannah River National Laboratory and the Advanced Photon Source at Argonne National Laboratory.

Energy Frontier Center for Defect Physics in Structural Materials (CDP)

Malcolm Stocks, Director

Oak Ridge National Laboratory

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

The three thrusts in this EFRC are: experimental observation of cascade dynamics using very short X-ray pulses; measurement of local stresses near dislocations and their interactions with defects; and, quantum Monte Carlo calculations of the magnetic equation of state for 3d-transition metals coupled with molecular dynamics simulations of nuclear and spin degrees of freedom for the same metals and alloy systems. The EFRC will enable first measurements of defect evolution in primary radiation damage formation, including the initial picoseconds that set the stage for later defect evolution. This experimental information and closely coupled advanced models are essential to explain how structural materials react to extreme radiation environments. This EFRC includes planned collaborations with scientists at the University of Tennessee, the University of Illinois, Ohio State University, Brown University, the University of California-Berkeley, North Carolina State University, and Lawrence Livermore National Laboratory. Experiments are planned for the Advanced Photon Source at Argonne National Laboratory and the Linac Coherent Light Source at the SLAC National Accelerator Laboratory.

Fluid Interface Reactions, Structures and Transport (FIRST) Center

David Wesolowski, Director

Oak Ridge National Laboratory

Objective: To provide basic scientific understanding of phenomena that occur at interfaces in electrical energy storage, conversion of sunlight into fuels, geological sequestration of carbon dioxide, and other advanced energy systems.

This EFRC will achieve its objective through unprecedented molecular resolution at fluid-solid interfaces made feasible by the utilization of a unique combination of experimental and computational capabilities: neutron scattering at the Spallation Neutron Source and High Flux Isotope Reactor at ORNL; extensive materials synthesis and characterization capabilities at the Center for Nanophase Materials Science at ORNL and the Advanced Photon Source at ANL; and computational simulations on leadership-class computing facilities at the National Center for Computational Sciences at ORNL. The EFRC includes planned collaborations with scientists at Argonne National Laboratory, Northwestern University, Drexel University, the University of Tennessee, the University of North Carolina, and the University of Virginia.

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Frontiers of Subsurface Energy Security

Gary Pope, Director

University of Texas, Austin

Objective: To harness recent theoretical and experimental advances to explain the transport of native and injected fluids, particularly carbon dioxide, in geological systems over multiple length scales.

Specifically, this EFRC will study reactive transport in geologic systems over length scales from nanometers to those of geological basins. The interdisciplinary team combines expertise in geologic basin analysis, petroleum-reservoir-scale engineering, and fine-scale geophysical and geochemical modeling. The project will incorporate intricate coupled physical and chemical processes related to flow and transport of native and injected fluids in a range of significant geological environments. The long-term benefits from this improved understanding will extend far beyond the current focus on storage of greenhouse gases to reduce atmospheric emissions to understanding the stability of geological systems and materials that are far-from-equilibrium for long periods of time. This EFRC is a collaboration with Sandia National Laboratories and will utilize that laboratory's Center for Integrated Nanotechnologies (jointly operated with Los Alamos National Laboratory) and computational capabilities.

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

Paul Barbara, Director

University of Texas, Austin

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

This EFRC will establish a fundamental research program that will lead to a molecular-level understanding of the critical interfacial charge separation and charge transfer processes which underpin the function of highly promising and innovative nanostructured molecular materials for organic photovoltaic (OPV) and electrical-energy-storage (EES) energy applications. The team of scientists will utilize powerful imaging and single-particle spectroscopies to make correlated measurements of structure and charge separation-transfer processes on the molecular scale in the study of interfacial prototypes varying in complexity from well-defined epitaxial crystals and interfaces, through isolated crystals and interfaces, and on to actual OPV and EES devices. The EFRC includes planned collaborations with scientists at Sandia National Laboratories.

Center for Catalytic Hydrocarbon Functionalization

Brent T. Gunnoe, Director

University of Virginia

Objective: To develop novel catalysts and manipulate their reactivity for the efficient conversion of hydrocarbon gases into liquid fuels.

This EFRC will focus specifically on novel catalysts for the conversion hydrocarbon gases to more useful liquids through the controlled addition of oxygen. The research team will seek to attain an unprecedented level of molecular understanding and control over catalytic steps involving metal-mediated activation and cleavage of the C-H bond, coordination and activation of the oxygen-delivery reagents, C-O bond formation, dissociation of the liquid fuel product, and the inhibition of any further deleterious reaction. The EFRC includes planned collaborations with

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scientists at the California Institute of Technology, Princeton University, the University of California - Berkeley, the University of Maryland, Iowa State University, the University of North Carolina, North Texas University, Yale University, and Scripps Research Institute – Florida.

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

Objective: To develop a comprehensive understanding of how chemical and electrical energy contained in fuels is exchanged, stored and released.

Electrocatalytic processes that involve multi-proton, multi-electron redox reactions will be the core subject of basic study for this EFRC. These reactions are relevant to solar energy storage, fuel cells, and biological transduction systems. The ultimate vision of the EFRC is to achieve the ability to design molecular electrocatalysts from first-principle methods and then control the molecular flow of protons with uniquely developed proton relays. The EFRC will involve scientists at the University of Washington, Pennsylvania State University, and the University of Wyoming, coordinating activities in synthetic inorganic catalysis, electrochemistry, and various types of spectroscopic and theoretical methods.

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Institution	Location	State	EFRC Name	EFRC Director	EFRC Objective
Arizona State University*	Tempe	AZ	EFR Center for Bio-Inspired Solar Fuel Production	Gust, J. Devens	Adapt the fundamental principles of natural photosynthesis to the man-made production of hydrogen or other fuels from sunlight.
University of Arizona*	Tuscon	AZ	Center for Interface Science: Hybrid Solar-Electric Materials (CIS:HSEM)	Armstrong, Neal R.	Enhance the conversion of solar energy to electricity using hybrid inorganic-organic materials.
California Institute of Technology	Pasadena	CA	Light-Material Interactions in Energy Conversion	Atwater, Harry	Tailor the properties of advanced materials to control the flow of solar energy and heat.
Lawrence Berkeley National Laboratory	Berkeley	CA	Center for Nanoscale Control of Geologic CO ₂	DePaolo, Donald	Establish the scientific foundations for the geological storage of carbon dioxide.
Stanford University	Stanford	CA	Center on Nanostructuring for Efficient Energy Conversion	Prinz, Fritz	Design, create, and characterize materials at the nanoscale for a wide variety of energy applications.
University of California, Berkeley	Berkeley	CA	Center for Gas Separations Relevant to Clean Energy Technologies	Smit, Berend	Design and synthesize new forms of matter with tailored properties for gas separations in applications including carbon capture and sequestration.
University of California, Los Angeles	Los Angeles	CA	Molecularly Assembled Material Architectures for Solar Energy Production, Storage, and Carbon Capture	Ozolins, Vidvuds	Acquire a fundamental understanding and control of nanoscale material architectures for conversion of solar energy to electricity, electrical energy storage, and separating/capturing greenhouse gases.
University of California, Santa Barbara*	Santa Barbara	CA	Center on Materials for Energy Efficiency Applications	Bowers, John	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.
University of Southern California*	Los Angeles	CA	Emerging Materials for Solar Energy Conversion and Solid State Lighting	Dapkus, Paul Daniel	Simultaneously explore the light absorbing and emitting properties of hybrid inorganic-organic materials for solar energy conversion and solid-state lighting.
National Renewable Energy Laboratory	Golden	CO	Center for Inverse Design	Zunger, Alex	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.

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Institution	Location	State	EFRC Name	EFRC Director	EFRC Objective
Carnegie Institute of Washington	Washington	DC	Center for Energy Frontier Research in Extreme Environments (Efree)	Mao, Ho-Kwang	Accelerate the discovery of energy-relevant materials that can tolerate transient extremes in pressure and temperature.
University of Delaware*	Newark	DE	Rational Design of Innovative Catalytic Technologies for Biomass Derivative Utilization	Vlachos, Dionisios	Design and characterize novel catalysts for the efficient conversion of the complex molecules comprising biomass into chemicals and fuels.
Idaho National Laboratory	Idaho Falls	ID	Center for Materials Science of Nuclear Fuel	Wolf, Dieter	Develop predictive computational models, validated by experiments, for the thermal and mechanical behavior of analogues to nuclear fuel.
Argonne National Laboratory	Argonne	IL	Institute for Atom-Efficient Chemical Transformations (IACT)	Marshall, Christopher	Discover, understand, and control efficient chemical pathways for the conversion of coal and biomass into chemicals and fuels.
Argonne National Laboratory	Argonne	IL	Center for Electrical Energy Storage: Tailored Interfaces	Thackeray, Michael	Understand complex phenomena in electrochemical reactions critical to advanced electrical energy storage.
Northwestern University	Evanston	IL	Argonne-Northwestern Solar Energy Research (ANSER) Center	Wasielewski, Michael	Revolutionize the design, synthesis, and control of molecules, materials, and processes in order to dramatically improve conversion of sunlight into electricity and fuels.
Northwestern University*	Evanston	IL	Center for Integrated Training in Far-From-Equilibrium and Adaptive Materials (CITFAM)	Grzybowski, Bartosz	Synthesize, characterize, and understand new classes of materials under conditions far from equilibrium relevant to solar energy conversion, storage of electricity and hydrogen, and catalysis.
Purdue University*	West Lafayette	IN	Center for Direct Catalytic Conversion of Biomass to Biofuels (C3Bio)	McCann, Maureen	Use fundamental knowledge about the interactions between catalysts and plant cell walls to design improved processes for the conversion of biomass to energy, fuels, or chemicals.
University of Notre Dame*	Notre Dame	IN	Materials Science of Actinides	Burns, Peter C.	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.
Louisiana State University	Baton Rouge	LA	Computational Catalysis and Atomic-Level Synthesis of Materials: Building Effective Catalysts from First Principles	Spivey, James	Develop computational tools to accurately model catalytic reactions and thereby provide the basis for the design of new catalysts.

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Institution	Location	State	EFRC Name	EFRC Director	EFRC Objective
Massachusetts Institute of Technology	Cambridge	MA	Solid-State Solar-thermal Energy Conversion Center (S3TEC CENTER)	Chen, Gang	Create novel, solid-state materials for the conversion of sunlight and heat into electricity.
Massachusetts Institute of Technology*	Cambridge	MA	Center for Excitonics	Baldo, Marc	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.
University of Massachusetts*	Amherst	MA	Polymer-Based Materials for Harvesting Solar Energy	Russell, Thomas	Use novel, self-assembled polymer materials in systems for the conversion of sunlight into electricity.
University of Maryland	College Park	MD	Science of Precision Multifunctional Nanostructures for Electrical Energy Storage	Rubloff, Gary	Understand and build nano-structured electrode components as the foundation for new electrical energy storage technologies.
Michigan State University	East Lansing	MI	Revolutionary Materials for Solid State Energy Conversion	Morelli, Donald	Investigate the underlying physical and chemical principles of advanced materials for the conversion of heat into electricity.
University of Michigan*	Ann Arbor	MI	Solar Energy Conversion in Complex Materials (SECCM)	Green, Peter	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.
Donald Danforth Plant Science Center	St. Louis	MO	Center for Advanced Biofuels Systems	Sayre, Richard	Generate the fundamental knowledge required to increase the efficiency of photosynthesis and production of energy-rich molecules in plants.
Washington University, St. Louis	St. Louis	MO	Photosynthetic Antenna Research Center	Blankenship, Robert	Understand the basic scientific principles that underlie the efficient functioning of the natural photosynthetic antenna system as a basis for man-made systems to convert sunlight into fuels.
University of North Carolina*	Chapel Hill	NC	Solar Fuels and Next Generation Photovoltaics	Meyer, Thomas	Synthesize new molecular catalysts and light absorbers and integrate them into nanoscale architectures for improved generation of fuels and electricity from sunlight.
Princeton University	Princeton	NJ	Energy Frontier Research Center for Combustion Science	Law, Chung K.	Develop a suite of predictive combustion modeling capabilities for the chemical design and utilization of non-petroleum based fuels in transportation.
Los Alamos National Laboratory	Los Alamos	NM	The Center for Advanced Solar Photophysics	Klimov, Victor	Capitalize on recent advances in the science of how nanoparticles interact with light to design materials that have vastly greater efficiencies for the conversion of sunlight into electricity.

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Institution	Location	State	EFRC Name	EFRC Director	EFRC Objective
Los Alamos National Laboratory	Los Alamos	NM	Extreme Environment-Tolerant Materials via Atomic Scale Design of Interfaces	Nastasi, Michael	Understand, at the atomic scale, the behavior of materials subject to extreme radiation doses and mechanical stress in order to synthesize new materials that maintain their desired properties under such conditions.
Sandia National Laboratories	Albuquerque	NM	EFRC for Solid State Lighting Science	Simmons, Jerry	Study energy conversion in tailored nanostructures as a basis for dramatically improved solid-state lighting.
Brookhaven National Laboratory	Upton	NY	Center for Emergent Superconductivity	Davis, J.C. Seamus	By understanding the fundamental physics of superconductivity, discover new high-temperature superconductors and improve the performance of known superconductors.
Columbia University*	New York	NY	Re-Defining Photovoltaic Efficiency Through Molecule-Scale Control	Yardley, James	Develop the enabling science needed to realize breakthroughs in the efficient conversion of sunlight into electricity in nanometer sized thin films.
Cornell University*	Ithaca	NY	Nanostructured Interfaces for Energy Generation, Conversion, and Storage	Abruna, Hector	Understand and control the nature, structure, and dynamics of reactions at electrodes in fuel cells, batteries, solar photovoltaics, and catalysts.
General Electric Global Research	Niskayuna	NY	Center for Electrocatalysis, Transport Phenomena and Materials for Innovative Energy Storage	Soloveichik, Grigori	Explore the fundamental chemistry needed for an entirely new approach to energy storage that combines the best properties of a fuel cell and a flow battery.
State University of New York, Stony Brook	Stony Brook	NY	Northeastern Chemical Energy Storage Center (NOCESC)	Grey, Clare P.	Understand how fundamental chemical reactions occur at electrodes and use that knowledge to tailor new electrodes to improve the performance of existing batteries or to design entirely new ones.
Pennsylvania State University*	University Park	PA	Center for Lignocellulose Structure and Formation	Cosgrove, Daniel	Dramatically increase our fundamental knowledge of the physical structure of bio-polymers in plant cell walls to provide a basis for improved methods for converting biomass into fuels.
University of South Carolina	Columbia	SC	Science Based Nano-Structure Design and Synthesis of Heterogeneous Functional Materials for Energy Systems	Reifsnider, Kenneth	Build a scientific basis for bridging the gap between making nano-structured materials and understanding how they function in a variety of energy applications.

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Institution	Location	State	EFRC Name	EFRC Director	EFRC Objective
Oak Ridge National Laboratory	Oak Ridge	TN	Energy Frontier Center for Defect Physics in Structural Materials (CDP)	Stocks, G. Malcolm	Enhance our fundamental understanding of defects, defect interactions, and defect dynamics that determine the performance of structural alloys in extreme radiation environments.
Oak Ridge National Laboratory	Oak Ridge	TN	Fluid Interface Reactions, Structures and Transport (FIRST) Center	Wesolowski, David	Provide basic scientific understanding of phenomena that occur at interfaces in electrical energy storage, conversion of sunlight into fuels, geological sequestration of carbon dioxide, and other advanced energy systems.
University of Texas, Austin	Austin	TX	Frontiers of Subsurface Energy Security	Pope, Gary A.	Harness recent theoretical and experimental advances to explain the transport of native and injected fluids, particularly carbon dioxide, in geological systems over multiple length scales.
University of Texas, Austin*	Austin	TX	Understanding Charge Separation and Transfer at Interfaces in Energy Materials and Devices (CST)	Barbara, Paul	Pursue fundamental research on charge transfer processes that underpin the function of highly promising molecular materials for photovoltaic and electrical energy storage applications.
University of Virginia	Charlottesville	VA	Center for Catalytic Hydrocarbon Functionalization	Gunnoe, T. Brent	Develop novel catalysts and manipulate their reactivity for the efficient conversion of hydrocarbon gases into liquid fuels.
Pacific Northwest National Laboratory	Richland	WA	Center for Molecular Electrocatalysis	Bullock, R. Morris	Develop a comprehensive understanding of how chemical and electrical energy contained in fuels is exchanged, stored and released.

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EFRC Fact Sheet

- **DOE Energy Frontier Research Centers (EFRCs)** The EFRCs are a means to enlist the talents and skills of the very best American scientists and engineers to address current fundamental scientific roadblocks to U.S. energy security (<http://www.sc.doe.gov/bes/EFRC.html>).
- The EFRCs will address energy and science “grand challenges” in a broad range of research areas; these “grand challenges” have been defined through a series of more than one dozen technical workshops conducted by the U.S. Department of Energy’s (DOE) Office of Science over the past five years.
- Since 2003, the Basic Energy Sciences program within the Office of Science has organized numerous workshops (<http://www.sc.doe.gov/bes/reports/list.html>) in coordination with the Department’s technology offices to explore significant topics in energy production, conversion, storage, transmission, and waste mitigation. These workshop reports have engaged more than 1,500 participants from universities, DOE national laboratories, and industry, and have identified high priority research directions with promise to address the most critical knowledge and technology gaps.
- The 46 EFRCs, to be funded at \$2-5 million per year each for a planned initial five-year period, were selected from a pool of some 260 applications received in response to a Funding Opportunity Announcement (FOA) issued by the DOE Office of Science in 2008.
- Selection was based on a rigorous merit review process utilizing outside panels composed of scientific experts. This process is described in detail in the EFRC FOA.
- Thirty EFRCs are being funded at a total annual cost of \$100 million under the Fiscal Year (FY) 2009 Federal Budget. The Recovery Act provided a further \$277 million, enabling the Office of Science to establish an additional 16 EFRCs and forward-fund them for the full five-year period.
- In total, the EFRC initiative represents a planned DOE commitment of \$777 million over five years, with the \$400 million in out-year funding for the FY 2009 funded Centers subject to future appropriations.
- Of the 46 EFRCs selected, 31 are led by universities, 12 by DOE National Laboratories, two by nonprofit organizations, and one by a corporate research laboratory.
- There are over 110 institutions, from 36 states plus the District of Columbia and 8 foreign countries, participating.
- In all, they will involve nearly 700 senior investigators and employ, on a full- or part-time basis, an estimated 1100 researchers, including postdoctoral associates, graduate students, undergraduate students, and technical staff.
- Roughly a third of these will be supported by Recovery Act funding.
- EFRC researchers will take advantage of new capabilities in nanotechnology, high-intensity light sources, neutron scattering sources, supercomputing, and other advanced instrumentation, much of it developed with DOE Office of Science support over the past decade, in an effort to lay the scientific groundwork for fundamental advances in solar energy, biofuels, transportation, energy efficiency, electricity storage and transmission, clean coal and carbon capture and sequestration, and nuclear energy.

EFRC Awards by Research Category and Institution

The 46 EFRC awards span the full range of energy research challenges described in the BES *Basic Research Needs* (BRN) series of workshop reports while also addressing one or more of the science grand challenges described in the BESAC report, *Directing Matter and Energy: Five Challenge for Science and the Imagination* (<http://www.sc.doe.gov/bes/reports/list.html>). Because many of the EFRCs address multiple energy challenges that are linked by common scientific themes, such as interfacial chemistry for solar energy conversion and electrical energy storage or rational design of materials for multiple potential energy applications, it is most appropriate to sort the EFRCs by the following taxonomy, with the appropriate BRN reports listed in parentheses:

Renewable and Carbon-Neutral Energy (Solar Energy Utilization, Advanced Nuclear Energy Systems, Biofuels, Geological Sequestration of CO₂)

Energy Efficiency (Clean and Efficient Combustion, Solid State Lighting, Superconductivity)

Energy Storage (Hydrogen Research, Electrical Energy Storage)

Crosscutting Science (Catalysis, Materials under Extreme Environments, other)

In addition, the EFRCs span the full range of eligible institutions.

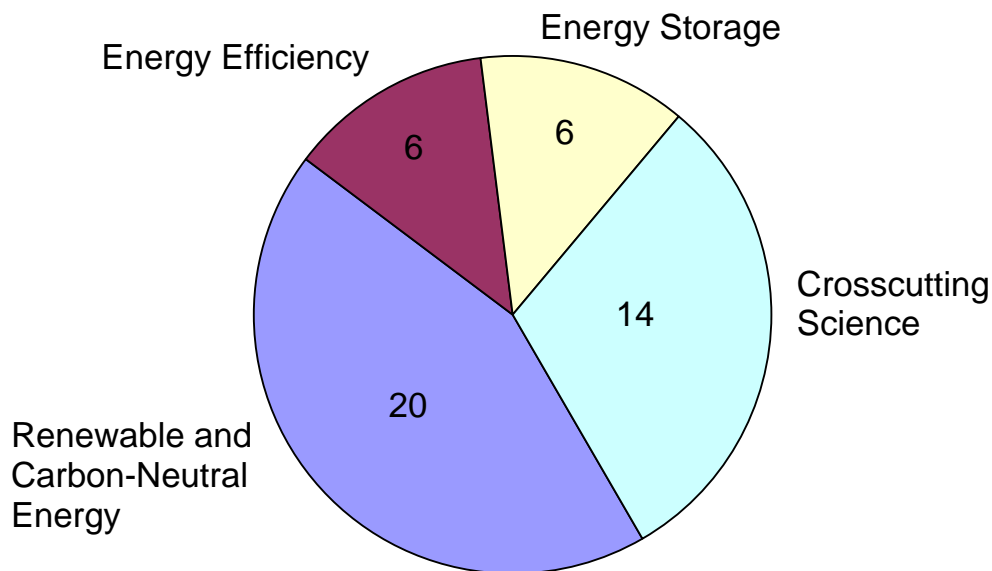


Figure 1. Distribution of EFRC awards by research category.

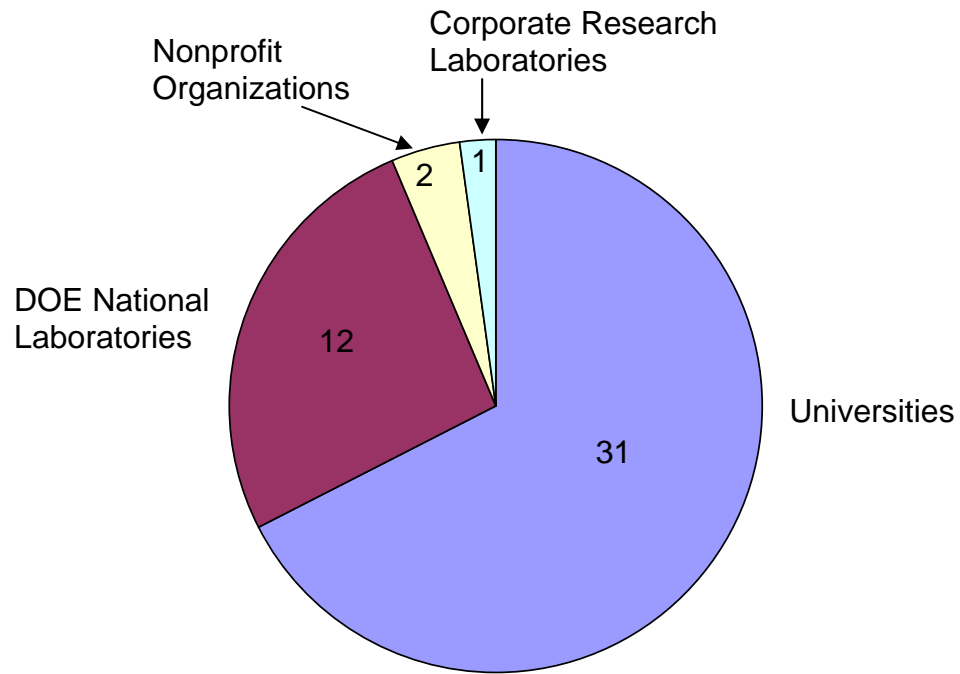


Figure 2. Distribution of EFRC awards by lead institution type.