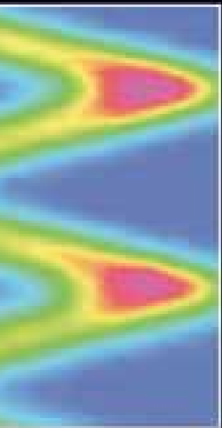
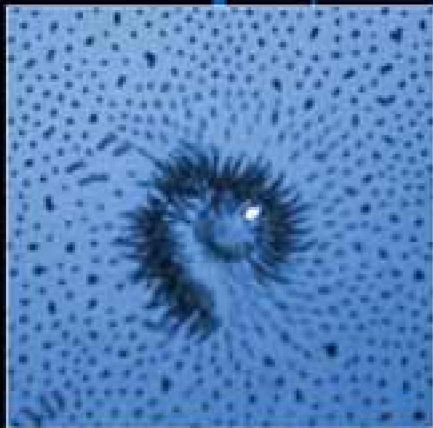
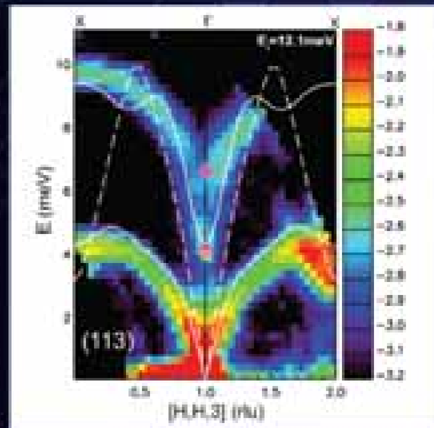
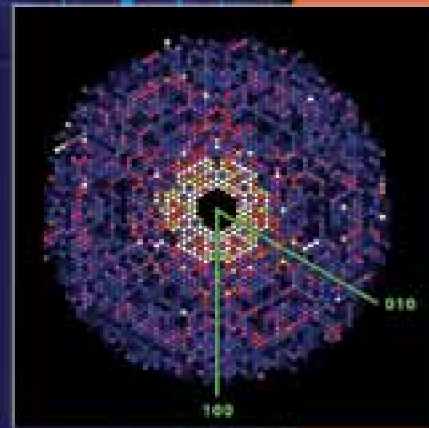








2011

Basic Energy Sciences 2011 Summary Report

U.S. DEPARTMENT OF ENERGY | Office of Science

Cover Images

Front, from right: (1) Researchers obtained these diffraction patterns from more than 15,000 protein nanocrystals using ultrafast, ultraintense x-rays at the Linac Coherent Light Source (see p. 25). (2) Neutron scattering data gathered at the Spallation Neutron Source provide insights into nanoscale processes that control thermal conductivity in lead telluride (see p. 35). (3) Microparticles, energized and directed by a magnetic field, assemble into a star-like structure and capture a targeted particle (see p. 17). (4) These simulation results from the University of California–Los Angeles Neptune accelerator facility are part of research that led to the development of a diagnostic tool for optimizing electron beams to produce subfemtosecond x-ray pulses (see p. 37).

Back, from right: (5) The recently developed proton exchange membrane electrolyzer, shown in cross-section here, generates hydrogen and oxygen from water vapor instead of liquid water (see p. 46). (6) This transmission electron microscope image shows a breakthrough hydrogen-storing material consisting of magnesium nanoparticles embedded in an organic polymer matrix permeable only to H_2 (see p. 36). (7) A newly engineered solar thermoelectric generator can convert sunlight to electricity eight times more efficiently than previous such devices (see p. 41).

Suggested citation for this report: U.S. DOE 2011. *Basic Energy Sciences 2011 Summary Report.* U.S. Department of Energy Office of Science. science.energy.gov/bes/news-and-resources/reports/.

Basic Energy Sciences 2011 Summary Report

U.S. DEPARTMENT OF ENERGY | Office of Science

Table of Contents

Acronyms list and image information are on inside back cover.

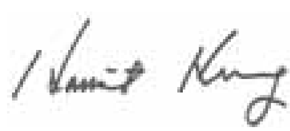
Director's Letter

On behalf of the Department of Energy and the dedicated staff in the Office of Basic Energy Sciences (BES), I am delighted to present this BES 2011 Summary Report. The nature and impact of the research and scientific user facilities that the BES program supports are described here not only for the scientific community, but also for the American public whose tax dollars we are entrusted to invest. To receive federal funding, it is imperative that scientists explain clearly what they do, why they do it, and why it matters in the context of everyday life. This report is one of several mechanisms by which BES communicates the important accomplishments of the scientific research that we support.

The introductory overview provides a summary of how BES is organized and how we operate to accomplish our mission of supporting fundamental research to understand, predict, and ultimately control matter and energy, thereby laying the scientific foundation for new energy technologies. The report also presents selected accomplishments from 2011 to illustrate some of the most exciting new scientific advances. Although we cannot describe herein the full technical depth of scientific progress achieved under BES support in the past year, this report should give the reader an indication of the range of scientific discoveries and innovative research funded by BES. Also included are many references to supplementary resources that provide additional details about BES strategic planning, research, and user facilities.

BES core research areas have produced exciting discoveries along a broad spectrum of science: catalysis, superconductivity, magnetism, solar energy conversion, and many more. The Energy Frontier Research Centers (EFRCs) completed their second full year of operation and are vividly demonstrating the power of multidisciplinary teams through scientific advances that simply cannot be accomplished by a single investigator or small research group. Having completed its first full year of operation, the Fuels from Sunlight Energy Innovation Hub is producing important new science and is well on its way to becoming an integrative hub for the solar-fuels research community. Finally, the Linac Coherent Light Source (LCLS)—the world's first x-ray free electron laser—completed its first year of operation. As an unprecedented tool for probing matter, LCLS is producing new science at an extraordinarily rapid pace.

I hope you enjoy reading our report and encourage you to explore the many resources referenced within or contact us directly to learn more about BES and the science we support (science.energy.gov/bes/).



Dr. Harriet Kung

Associate Director of Science
for Basic Energy Sciences

Overview of Basic Energy Sciences

science.energy.gov/bes/

Mission and Research Portfolio

The mission of Basic Energy Sciences (BES) is to support fundamental research to understand, predict, and ultimately control matter and energy at the level of electrons, atoms, and molecules. This research provides the foundation for new energy technologies and supports Department of Energy (DOE) missions in energy, environment, and national security. To accomplish this objective, BES in 2011 invested approximately $700M in some 1,400 core research projects, 46 Energy Frontier Research Centers (EFRCs), and the Fuels from Sunlight Energy Innovation Hub. These investments span diverse sectors across the country, including in 2011 research at more than 170 academic, nonprofit, and industrial institutions in all 50 states and at 14 DOE laboratories. BES also supports world-class, open-access, and complementary scientific user facilities such as intense x-ray sources, neutron scattering centers, electron beam characterization centers, and research centers for nanoscale science. The total annual operating budget of these facilities is about $760M.

BES investments in basic science are critical for providing the technological breakthroughs needed to address the energy challenges facing the United States in the 21st century. Working closely with the research community, BES has developed a research classification that identifies the role its portfolio plays in the progression from basic research to technology maturation and deployment. The figure on p. 3 illustrates this research and development (R&D) continuum and shows that the bulk of BES's portfolio lies in three categories of basic research: grand challenge, discovery, and use-inspired. Grand challenge research addresses the most fundamental questions about matter and energy and challenges and refines the basic understanding of physical and chemical phenomena. Discovery research seeks new understanding of materials or processes related more directly to transformative energy technologies. Use-inspired research, while still addressing fundamental issues, is directed more toward scientific “showstoppers” that limit the development of new energy technologies. These three categories share a common metric—the generation of new scientific knowledge, obtainable through both successful and failed experiments, calculations, and other hypothesis testing.

The path of scientific advancement is neither simple nor straight, and the most remarkable discoveries often arise from the freedom to follow an interesting lead or understand a failure. By contrast, applied research and technology development (shown on the right of the continuum figure) must have practical, achievable targets with specific milestones and deliverables. Failure to meet an applied research goal does not present new opportunities that can be pursued; instead, alternative approaches must be adopted to achieve the milestone and deliver the product. The Fuels from Sunlight Energy Innovation Hub is unique in the BES portfolio because it intentionally integrates both basic and applied research, pushing toward creation of a commercially viable system for generating solar fuels.

From single-investigator studies to large multidisciplinary research centers, BES uses several modalities to adequately address the needs spanning its basic research activities. The university portfolio in the BES core research areas is dominated by single-investigator grants

<table>
<tr><th colspan="3">Basic Research
Grand Challenge Discovery Use-Inspired</th><th colspan="3">Applied Research and Technology Development and Deployment</th></tr>
<tr><td colspan="3">• Goal: New Knowledge and Understanding
• Focus: Phenomena
• Metric: Knowledge Generation</td><td colspan="3">• Goal: Practical Targets
• Focus: Performance
• Metric: Milestone Achievement</td></tr>
<tr><th colspan="3">Basic Energy Sciences</th><th>ARPA-E</th><th colspan="2">Applied Programs</th></tr>
<tr><td>• Addresses fundamental limitations of current theories and descriptions of matter in the energy range important to most energy technologies.</td><td>• Seeks fundamental new understanding of materials or processes that may revolutionize or transform future energy technologies.</td><td>• Pursues fundamental new understanding, usually focused on scientific showstoppers, to advance energy technologies.</td><td>• Establishes proof of new, higher-risk concepts.
• Prototypes new technology concepts.
• Explores the feasibility of scaling up demonstrated technology concepts in a “quick hit” fashion.</td><td>• Conducts research to meet technical milestones, emphasizing the development, performance, cost reduction, and durability of materials and components or the efficiency of processes.</td><td>• Scales up research.
• Demonstrates small-scale and at-scale technology.
• Reduces costs.
• Involves manufacturing R&D.
• Includes deployment and support activities leading to market adoption.
• Shares cost with industry partners.</td></tr>
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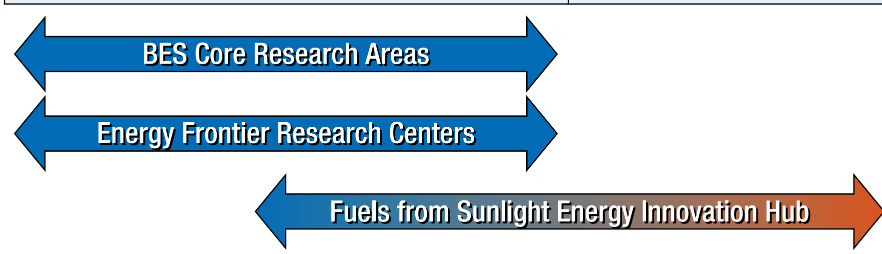


Research, Development, and Deployment Continuum. Each column on the continuum describes a type of R&D, starting with three categories of basic research and moving toward applied research and technology development. The fourth column of bullets indicates the kinds of research conducted by the DOE Advanced Research Projects Agency-Energy (ARPA-E), and the last two columns describe activities within DOE technology offices. Also shown are the goals, foci, and metrics for basic and applied research and technology development.

but also includes a number of group awards. Research conducted at DOE national laboratories primarily consists of large, multi-investigator projects. All BES-funded DOE labs are owned by the federal government and operated by contractors who manage the laboratories and their research activities. BES requires laboratory research to be managed as synergistic, multi-investigator programs rather than collections of projects by individual investigators. This ensures that DOE laboratory projects supported by BES are structured to take unique advantage of national lab capabilities without duplicating BES investments in single-investigator grants in academia. Effective, synergistic team science also is required for the large, core research projects at universities and for all 46 EFRCs. Finally, BES's Fuels from Sunlight Energy Innovation Hub—the Joint Center for Artificial Photosynthesis (JCAP)—is a very large, multidisciplinary R&D center. With approximately 50 senior investigators, JCAP primarily is a partnership between the California Institute of Technology and DOE's Lawrence Berkeley

National Laboratory, with additional university and laboratory participants. JCAP's large scale is required to address the tremendous breadth of scientific and engineering challenges associated with developing a viable artificial photosynthetic system.

The table below compares some essential characteristics of five DOE R&D modalities: (1) core BES research, (2) EFRCs, (3) Energy Innovation Hubs, (4) the DOE Advanced Research Projects Agency-Energy (ARPA-E), and (5) DOE technology offices such as the Office of Energy Efficiency and Renewable Energy. Each modality's characteristics (e.g., investigators and institutions, award period and management, typical award amount, and core motivation and research focus) are well suited to the type of research and objectives the modality pursues along the R&D continuum illustrated on p. 3.

Department of Energy R&D Modalities

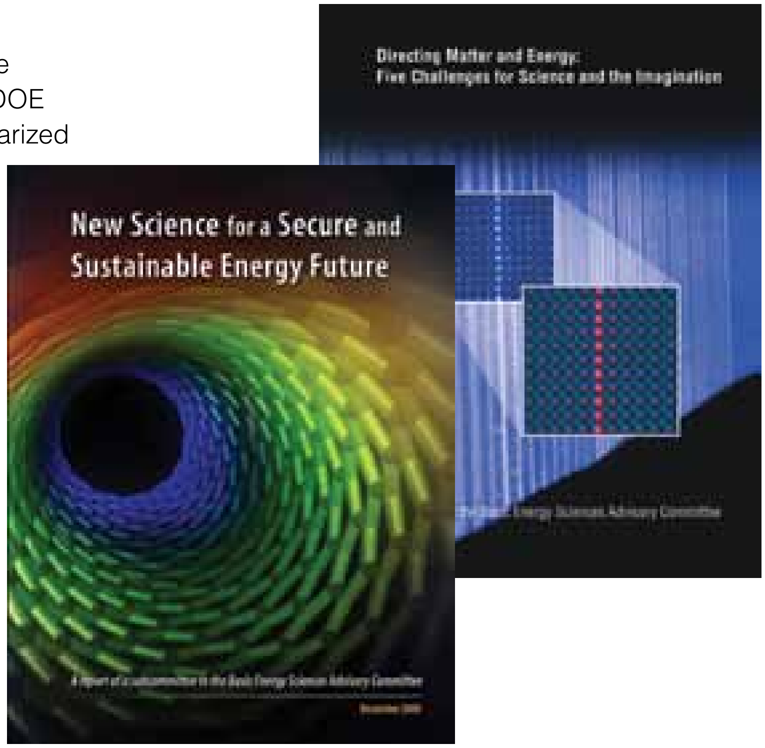
	Investigators and Their Institutions	Period of Award and Management	Typical Annual Award Amount	Core Motivation and Research Focus
Core BES Research	Single investigators, small and large research groups. Led by universities, DOE laboratories, or nonprofits.	Usually 3-year renewable awards managed by BES. Early Career awards are managed separately and are 5-year, nonrenewable awards with set budgets.	\$150K to \$2M	Fundamental research in the grand challenge and use-inspired areas. BES determines the research focus for each core area, with community guidance on new basic research needs.
Energy Frontier Research Centers	Self-assembled groups of about 12 to 20 senior investigators. Led by universities, DOE laboratories, nonprofits, and industry, often with teaming across institutions.	Five years with possible 5-year renewal (pending appropriations). Managed by BES.	\$2M to \$5M	Fundamental research requiring multiple investigators from several disciplines, often with a clear link to new energy technologies. Research focused among a large set of basic research needs developed with community input.
Energy Innovation Hubs	Large group spanning basic and applied R&D. Led by universities, DOE laboratories, industry, or nonprofits, with extensive teaming across institutions.	Five years with possible 5-year renewal. Managed by a single DOE office but with broad coordination across DOE. BES manages the Fuels from Sunlight Energy Innovation Hub.	About \$22M in year one (with up to \$10M for infrastructure but no new construction). Up to \$25M in years two to five.	Purpose-driven research, integrating across basic and applied research toward commercialization. Generally, DOE determines the topical areas addressed by the hubs, and funding opportunity announcements (FOAs) are specific.
ARPA-E	Single investigator to small teams. Led by universities, nonprofits, industry, or consortia of these.	One to 3 years. Managed by ARPA-E, which reports to the Secretary of Energy.	\$500K to \$10M	High-risk research driven by the potential for significant commercial impact. Generally, DOE determines the area of interest, and FOAs are specific.
DOE Technology Offices	R&D teams of varying size. Led by universities, DOE laboratories, industry, or consortia of these.	One to 3 years. Managed by specific DOE technology offices.	Small teams (~\$300K) to large technology demonstrations (>\$1M).	Developmental research and technology demonstration projects with specific deliverables and clear milestones. Generally, DOE determines the area of interest, and FOAs are specific.

Strategic Planning and Research Community Involvement

BES actively engages the research community in strategic planning. The Basic Energy Sciences Advisory Committee (BESAC) is chartered under the Federal Advisory Committee Act to advise BES on its research areas and user facilities (science.energy.gov/bes/besac/). The 2003 BESAC report, *Basic Research Needs to Assure a Secure Energy Future*, set the foundation for the 10 subsequent workshops and reports in the Basic Research Needs series (science.energy.gov/bes/news-and-resources/reports/basic-research-needs/). This series has identified critical basic research required to advance a wide range of energy technologies. BESAC's 2007 report, *Directing Matter and Energy: Five Challenges for Science and the Imagination*, completed this remarkable strategic planning effort by examining the grand challenges confronting science in the realm most significant for much of everyday life.

Together, these workshops attracted more than 1,500 participants from academia, DOE laboratories, and industry. BESAC summarized workshop results and highlighted the role that new science can play in finding transformational energy solutions in a 2008 report, *New Science for a Secure and Sustainable Energy Future*. This set of workshop reports provided the foundation for the solicitation of two significant new research efforts in FY 2009: the EFRCs and a companion program enhancing single-investigator and small-group research (SISGR) across all BES core research programs. BES and BESAC continue to engage the research community in workshops designed to address new scientific opportunities and identify ways that critical needs for advanced energy technologies can inspire new science (science.energy.gov/bes/news-and-resources/reports/workshop-reports/).

Section 2 (p. 6) of this report describes how BES does business (e.g., program management, solicitation and review of BES-funded projects, and external reviews of BES research and user facilities). Descriptions of the BES research and facility portfolio follow, along with representative research accomplishments from 2011 (see Section 3, p. 11). Additional information about BES research projects can be found on the BES website (science.energy.gov/bes/). This site includes summary abstracts of all projects supported by BES core research areas (science.energy.gov/bes/research/) and detailed descriptions of the 46 EFRCs (science.energy.gov/bes/efrc/), the Fuels from Sunlight Energy Innovation Hub (science.energy.gov/bes/research/doe-energy-innovation-hubs/), and BES user facilities (science.energy.gov/bes/suf/).



How Basic Energy Sciences Does Business

Program Management: Organization and Staff

Basic Energy Sciences (BES) is organized into three divisions: Materials Sciences and Engineering (MSE); Chemical Sciences, Geosciences, and Biosciences (CSGB); and Scientific User Facilities (SUF). BES staffing includes about 35 federal program managers who oversee an annual research investment of approximately $700M and manage scientific user facility operations with an annual operating budget of over $760M (see current BES organization chart at science.energy.gov/~/media/bes/pdf/about/BES_Org_Chart.pdf). As Ph.D. scientists, these program managers have research experience well beyond the postdoctoral level in the scientific areas covered by the portfolios they manage. Many come to BES with previous experience in scientific program or facility management at DOE laboratories or other governmental agencies.

The MSE, CSGB, and SUF divisions support about 1,400 research projects organized into 23 core research areas. Each area is overseen by one to two program managers and has a clearly defined scientific emphasis often spanning multiple scientific and engineering disciplines. In addition to the core research areas, 46 Energy Frontier Research Centers (EFRCs) are managed by a committed team of BES program managers, most of whom also have duties in the core programs. Similarly, a team of program managers also oversees the Fuels from Sunlight Energy Innovation Hub.

Solicitation and Review of Funding Applications

BES actively encourages scientists from universities, nonprofit organizations, industry, and DOE laboratories to submit new ideas for research projects. Potential applicants are advised to contact BES program managers and submit preapplications (white papers) describing newly proposed research. Program managers evaluate these preapplications for relevance to BES core research and then encourage or discourage the submission of full applications. New applications in specific research areas also are sought through expressions of interest publicized on the BES website. Major new research initiatives are solicited using special Funding Opportunity Announcements (FOAs). Major examples include FOAs for the EFRCs in FY 2009 and the Fuels from Sunlight Energy Innovation Hub in FY 2010. Another example is the annual FOA for the Early Career Research Program, which is administered across the DOE Office of Science and has special requirements. Although each FOA contains specific eligibility requirements regarding teaming arrangements, FOAs typically are broadly open to universities, nonprofits, industry, DOE laboratories, and other federal laboratories. Renewal applications for eligible ongoing BES research projects are received prior to the end of the grant or project period.

All research proposals submitted to BES are subject to rigorous merit review. The most critical aspect of this process is review by external scientific experts, or peer review. All peer review is conducted according to the criteria codified in 10 Code of Federal Regulations Part 605: (1) scientific and/or technical merit of the

Energy Frontier Research Centers (EFRCs) Summit and Forum. BES invited America's top energy scientists to the May 2011 meeting to promote synergies among the research community and highlight early EFRC successes.

project; (2) appropriateness of the proposed method or approach; (3) personnel competency and adequacy of the proposed resources; and (4) reasonableness and appropriateness of the proposed budget. (For additional details on BES peer review and references to applicable policies and guidance, see science.energy.gov/bes/funding-opportunities/peer-review-policies/.) Special solicitations or FOAs may include additional merit review criteria. Large, multi-investigator grants and national laboratory projects also have additional review criteria that assess synergy within the project.

BES implements peer review in several forms, optimizing this process for the type and number of research proposals under consideration. For single-investigator or small-group research in the core research areas, an individual peer review process is used to evaluate new and renewal applications, which often arrive in small numbers. In such cases, an application is sent to a set of reviewers who return their individual reviews to the appropriate program manager. For multi-investigator activities at DOE laboratories or universities, renewal reviews often are conducted by a panel of reviewers during a site visit to the host institution. These onsite reviews are excellent ways to critically examine group synergy and use of the host institution's unique capabilities. When onsite panel reviews are infeasible or inappropriate, BES may conduct "reverse-site visit" reviews, during which applicants present their research to a review panel at a neutral site. Finally, solicitations or expressions of interest that generate large volumes of applications require the use of review panels to effectively and efficiently complete the peer review process. These panels can be convened in person to evaluate a set of proposals or conducted "virtually" using modern communications tools. Each panel assesses a set of proposals without the applicant present.

Peer review is not the only aspect of a complete merit review process in BES. Another important component is evaluating how well the proposed research fits with a particular BES core research area or responds to the stated objectives of an FOA. These programmatic assessments are made by BES program managers, whose expertise, vision, and judgment are critically important in the development of mission-relevant research programs. Program managers combine these assessments with an analysis of the peer reviews to form a funding recommendation for the application that then is presented to BES management for approval or rejection. BES management may request additional information or justification from the recommending program manager(s) before finalizing the funding decision(s).

Success rates for renewal applications vary, but 10% to 20% of all BES core research projects typically are terminated over the 3-year renewal cycle. Consequently, the BES research portfolio does not remain static. It is constantly renewed so that work that has reached its conclusion, is past its fruition, or has underperformed—as determined by peer review—is terminated, thereby providing funding to initiate more promising research projects.

User facilities also are reviewed using external, independent review committees that operate according to the same basic procedures that BES has established for peer review. A facility review—which is conducted triennially—includes the following important assessments:

- Reliability and availability of the facility to users
- User access policies and procedures
- User satisfaction
- Facility staffing levels
- Research and development activities for facility advancement
- Facility management and long-range goals
- Safety and environmental impact of all activities

The outcomes of these reviews help improve facility operations to better serve the broad scientific user community.

External BES Program Evaluation

Since 2002, the management and oversight of BES research and facility portfolios have been evaluated by an independent, external set of reviewers known as a Committee of Visitors (COV). COVs are convened as subcommittees under the auspices of the Basic Energy Sciences Advisory Committee (BESAC). Each COV is charged with two activities:

1. Assess the efficacy and quality of the processes used to (a) solicit, review, recommend, and document proposal actions and (b) monitor active projects and programs.
2. Within the boundaries defined by DOE missions and available funding, comment on how the award process has affected (a) the breadth and depth of portfolio elements as well as (b) their national and international standing.

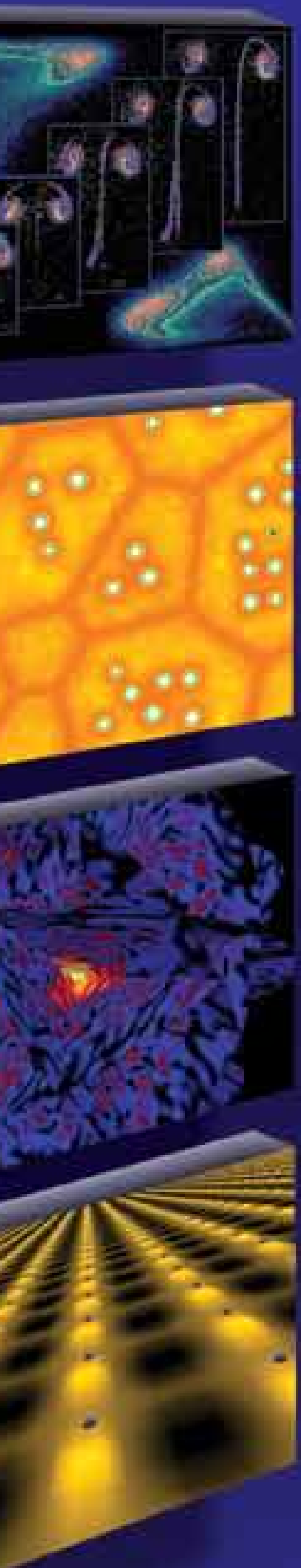
COVs assess each BES division every 3 years. BES responds to COV recommendations, which have resulted in real and measurable changes, particularly in the areas of improved project documentation and information management. COVs also have affirmed the quality of BES scientific programs and the appropriateness of BES merit review procedures and decision-making processes. The COV process helps ensure that BES funding procedures are open and transparent to the research communities that BES serves. All BES COV reports and BES responses are available at science.energy.gov/bes/besac/bes-cov/.

Research Award Oversight

Using several mechanisms, BES program managers actively monitor all research awards during the award period to ensure progress toward the proposed research objectives. Generally, program managers engage in discussions with lead investigators and project directors through regularly scheduled or informal teleconferences and at scientific meetings. University grants typically are funded for their award period in annual budget increments, and formal requests for continued funding must be submitted prior to the next budget period (except for the final budget period when university researchers apply for renewal funding). This formal continuation request includes a detailed progress report on the research and publications generated from BES funding. BES program managers review these requests before approving continued funding.

Under the management and operations contracts between DOE and its laboratories, the contractor manages BES-funded research programs. As with the grant program, national laboratory programs are externally peer reviewed every 3 years. Between these reviews, BES interacts extensively with DOE laboratory management and principal investigators (PIs) during the course of ongoing laboratory research projects to ensure their progress. This interaction includes teleconferences; discussions at scientific meetings; and regular, formal presentations by DOE laboratory managers on research progress and program management.

Finally, BES program managers organize and conduct PI meetings within a particular research or topical area to foster collaboration, cooperation, and the exchange of scientific ideas among researchers and to promote interactions with BES program management. Although PI meetings are not program reviews, they include oral and poster presentations of BES-supported projects and provide excellent opportunities for BES program managers to informally monitor research progress. Perhaps more importantly, PI meetings help investigators understand that BES manages mission-relevant research programs, not just portfolios of disconnected research projects. PI meetings also have been instrumental in developing effective, long-lasting collaborations among investigators. These synergies have significantly strengthened BES research areas by providing interactive mechanisms by which BES fosters a high standard of excellence among its scientists and helps formulate future directions for major research elements of the program. COVs have uniformly supported and enthusiastically endorsed the PI meetings.



Research Portfolio and User Facilities

Basic Energy Sciences (BES) supports a variety of research disciplines—including condensed matter and materials physics, chemistry, geosciences, and aspects of physical biosciences—that seek to discover new materials and design new chemical processes. These disciplines play a role in virtually every aspect of energy resources, production, conversion, transmission, storage, efficiency, and waste mitigation. In addition to this research, BES user facilities provide outstanding capabilities for imaging; characterizing diverse materials ranging from metals, alloys, and ceramics to fragile biological samples; and studying these materials' chemical transformations. This section describes the BES research portfolio and user facilities in detail, along with selected 2011 accomplishments from each.

- Materials Sciences and Engineering Division
- Chemical Sciences, Geosciences, and Biosciences Division
- Scientific User Facilities Division
- Energy Frontier Research Centers and Energy Innovation Hubs

Materials Sciences and Engineering Division

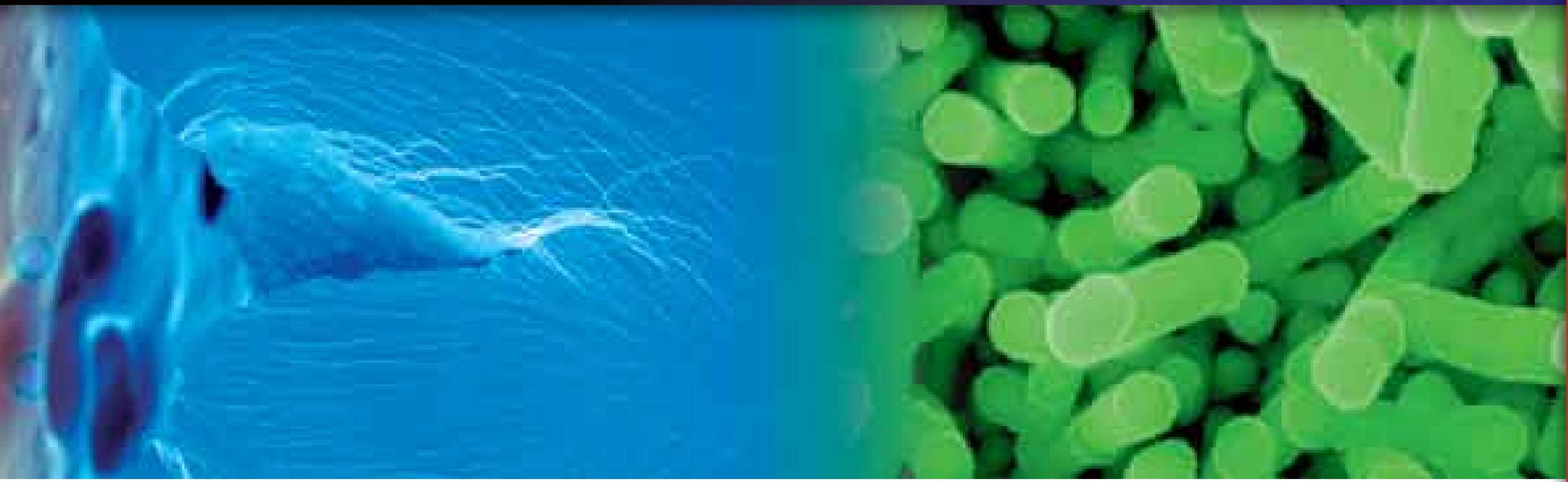
science.energy.gov/bes/mse/

Materials are critical to nearly every aspect of energy generation and use. When they perform inadequately, efforts to improve energy efficiencies, extend infrastructure and device lifetimes, or introduce new energy technologies are impeded. The Materials Sciences and Engineering (MSE) Division within BES supports research to provide fundamental understanding of the synthesis, behavior, and performance of materials. Such knowledge will offer solutions to these wide-ranging challenges and reveal new research directions that cannot be foreseen with current understanding. MSE-sponsored research explores the origin of macroscopic material behaviors and their fundamental connections to a material's atomic, molecular, and electronic structures. At the core of this research is the quest for breakthroughs enabling the deterministic design and discovery of new materials with novel structures, functions, and properties. Such understanding and control are critical to science-guided design of highly efficient energy-related processes, including (1) the conversion of sunlight to electricity; (2) new electromagnetic pathways for enhanced light emission in solid-state lighting; and (3) multifunctional, nanostructured materials for optimum electron and ion transport in batteries and fuel cells.

To accomplish these goals, MSE supports integrated research activities in:

- **Scattering and Instrumentation Sciences** to develop new tools and techniques for characterizing and correlating material performance, structure, and dynamics on multiple time and length scales and in the environments where materials are used.
- **Condensed Matter and Materials Physics** to understand the foundations of material functionality and behavior.
- **Materials Discovery, Design, and Synthesis** to design and precisely assemble structures for controlling material properties and discovering new materials with unprecedented functionalities.

An overarching goal of these activities is understanding how to direct and control energy flow in material systems over multiple time and length scales. This knowledge will enable prediction of material behavior, transformations, and processes in challenging real-world systems (e.g., materials with many atomic constituents, complex structures, and a broad range of defects as well as those exposed to extreme environments). As a leader in materials discovery, MSE research explores new frontiers and unpredicted, emergent behavior in material systems (e.g., magnetism and superconductivity); utilizes nanoscale control; and investigates systems that are metastable or far from equilibrium. MSE also supports research at the



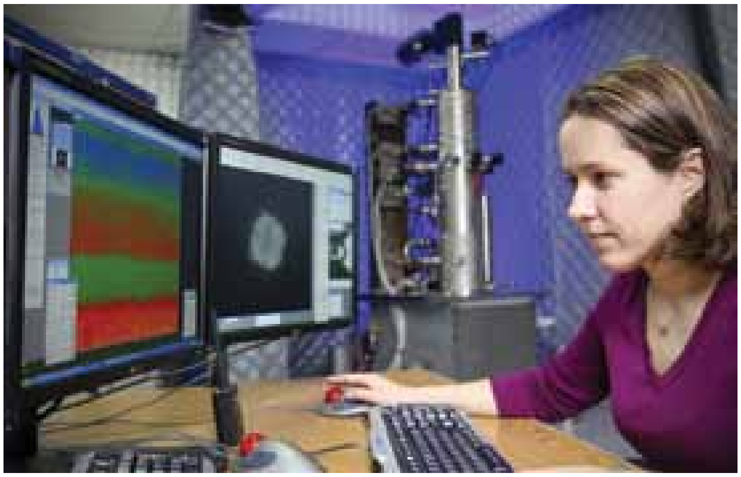
interface between the physical and biological sciences to explore biomimetic processes as new approaches to novel materials design. The MSE Division also is home to DOE's Experimental Program to Stimulate Competitive Research (EPSCoR). EPSCoR supports research activities spanning DOE's diverse science and technology programs in states that historically have received relatively less federal research funding.

MSE Research Activities

Scattering and Instrumentation Sciences

Advanced characterization tools with very high structural and temporal precision are essential for understanding, predicting, and ultimately controlling matter and energy at the level of electrons, atoms, and molecules. Scattering and Instrumentation Sciences supports the development of innovative techniques and instrumentation for scattering, spectroscopy, and imaging using electrons, neutrons, and x-rays. Such tools provide precise information on the atomistic structure and dynamics of materials. Focal points for these research activities are DOE's world-leading electron, neutron, and synchrotron x-ray scattering facilities (see Scientific User Facilities Division, p. 28). Revolutionary advances in these techniques will enable transformational research on advanced materials for DOE missions in energy, environment, and national security.

Understanding complex materials and phenomena requires combinations of tools to determine the roles of individual species and interfaces in multicomponent systems. Because electrons, neutrons, and x-rays interact uniquely with matter, they offer a range of complementary tools with different sensitivities and resolutions for characterizing materials at length and time scales spanning several orders of magnitude.



New Imaging Technique Enables Spin Mapping at the Atomic Scale. Using an electron microscope, Maria Varela views the atomic arrangements of a magnetic oxide interface. Varela and her colleagues are using this advanced instrument to better understand magnetic properties of materials (see Research Accomplishment on p. 18). [Courtesy of Oak Ridge National Laboratory.]

Furthermore, investigations of dynamic phenomena in real time under natural (or operating) conditions provide insights into the real-world functioning of a material. New capabilities for ultrafast science will investigate dynamics related to electronic, catalytic, magnetic, and other transport processes at very fast time scales.

Condensed Matter and Materials Physics

Understanding the scientific basis for controlling and changing the properties of materials is critical to improving their functionality on every level and thus fulfilling DOE's energy mission. Condensed Matter and Materials Physics supports experimental and theoretical research to advance current understanding of phenomena in condensed matter. Specifically, this includes the solids, liquids, and mesoscale materials—whether electronic, magnetic, optical, thermal, or structural—that make up the infrastructure for energy technologies at every level. Research activities encompass four programmatic areas: Experimental Condensed Matter Physics, Theoretical Condensed Matter Physics, Physical Behavior of Materials, and Mechanical Behavior and Radiation Effects.

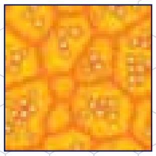
Central goals are characterizing and understanding superconducting, magnetic, and other types of materials whose properties are driven by strong interactions between electrons in their structures. Particularly emphasized are investigations of low-dimensional systems, including nanostructures, and studies of electronic properties under extreme conditions, such as ultralow temperatures and extremely high magnetic fields. Research relevant to energy technologies includes understanding the elementary energy conversion steps in photovoltaics, energetics of hydrogen storage, and electron spin phenomena and basic semiconductor physics related to next-generation information technologies and electronics. Fundamental studies of the interactions of atomic particles and energy (quantum physics) will lead to improved understanding of electrical and thermal conduction in a wide range of material systems. Critically needed is the ability to couple theories describing phenomena at the atomic scale to material properties at the macroscale where the connection between these properties and a material's size, shape, and composition is poorly understood.

Another focus area is learning how materials respond to varying temperature, electromagnetic fields, radiation, and chemical environments. Understanding the influence of material defects and their effects on strength, structure, deformation, and failure over a wide range of length and time scales will enable the design of materials with superior mechanical properties and resistance to damage in different environments.

Materials Discovery, Design, and Synthesis

The discovery and development of new materials have long been recognized as the engines advancing science frontiers and driving technology innovations. Predictive discovery of new types of matter with tailored properties—critical to world leadership scientifically, technologically, and economically—depends on understanding how materials form. Goals of this research area are to grow and maintain U.S. leadership in materials discovery by investing in advanced synthesis capabilities and by coupling synthesis with state-of-the-art user facilities and advanced computational capabilities. A key part of the portfolio is biomimetic materials research, which translates biological processes





Proof-of-Concept Version of Self-Repairing Photoelectrochemical Cell. The cell contains a photoactive solution composed of a mixture of self-assembling molecules in a glass cylinder held in place by a metal clamp. Protruding from the top are two electrodes, one made of platinum (bare wire), the other of silver (in glass tube). For more details, see Research Accomplishment on p. 16. [Courtesy of Massachusetts Institute of Technology.]

into impactful approaches for designing and synthesizing materials with remarkable properties found only in nature (e.g., self-repair and adaptability to changing environments). Research includes activities in Materials Chemistry and Biomolecular Materials and in Synthesis and Processing Science. These activities underpin many energy-related technological areas such as batteries and fuel cells, catalysis, solar energy conversion and storage, friction and lubrication, and membranes for advanced separations.

Materials Chemistry and Biomolecular Materials research emphasizes chemistry- and biology-based approaches to material synthesis and assembly. Major research directions include (1) the controlled synthesis and assembly of functional nanoscale materials with desired properties; (2) mimicking biology's energy-efficient synthesis approaches to generate new, advanced materials for use under harsher, nonbiological conditions; (3) bioinspired materials that assemble autonomously and dynamically; and (4) adaptive and resilient materials that possess self-repairing capabilities.

Synthesis and Processing Science supports fundamental research for developing new processing methods and techniques based on physical concepts (e.g., diffusion, nucleation, and growth) to synthesize materials with desired structures and tailored properties. An important element of this activity is developing real-time monitoring tools, diagnostic techniques, and instrumentation to provide information on the progression of the structure and properties of a material as it forms. Such tools and techniques enable understanding of the underlying physical mechanisms and allow atomic-level control of material synthesis and processing.

Selected 2011 Accomplishments

The following pages describe MSE-supported research on self-repairing solar cells, "smart" microparticles, atomic-scale imaging of magnetic properties, and the behavior of the "pseudogap" phase in superconducting materials. These accomplishments represent only a small portion of the science supported by MSE in 2011.

MSE Research Accomplishment

Nanoscale Solar Cells Capable of Self-Repair

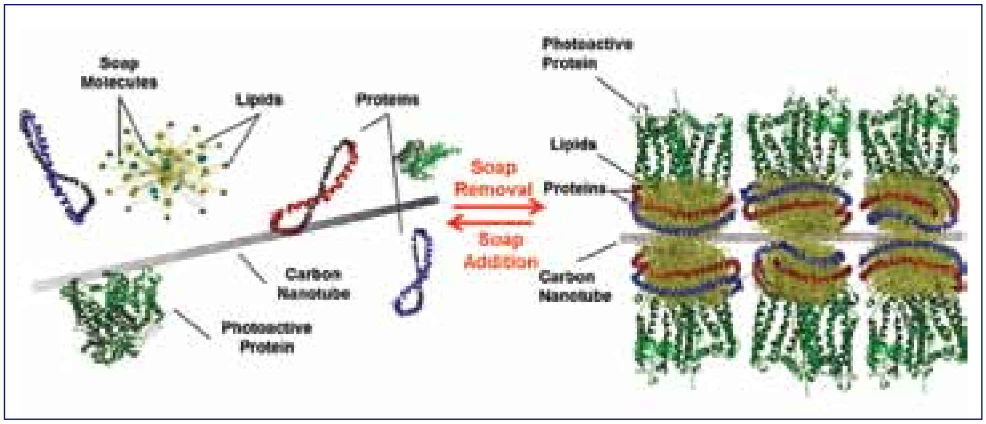
Background: One of the problems with harvesting sunlight for energy is that long-term exposure to the sun's rays can damage many materials, including solar cells, reducing their efficiency. Naturally occurring photosynthetic systems such as plants use elaborate, self-repair pathways to limit the impact of this degradation. They constantly break down their light-capturing modules and then precisely reassemble this machinery from scratch so that the basic structures capturing solar energy are, in effect, always brand new.

Research: An artificial solar cell that mimics this self-repair process recently was demonstrated for the first time. A novel, dynamic system consisting of carbon nanotubes, protein lipids, and bacterial photosynthetic reaction centers can be made to spontaneously assemble and disassemble itself through the removal or addition of soap, or surfactant, molecules. When a surfactant is added, the system's components come apart and form a soupy solution. When the surfactant is removed, the compounds automatically reassemble into a perfectly formed, rejuvenated photocell. The photoconversion efficiency of this artificial solar cell increased by more than 300% through self-repair over 168 hours of operation.

Impact: This regeneration process provides a bioinspired route for designing more robust, fault-tolerant solar energy conversion schemes, potentially extending their lifespans indefinitely.

Reference

Ham, M.-H., et al. 2010. "Photoelectrochemical Complexes for Solar Energy Conversion that Chemically and Autonomously Regenerate," *Nature Chemistry* **2**, 929–36.



Self-Repair of an Artificial Solar Cell. The photosynthetic complex can assemble and disassemble itself in a reversible process enabling replacement of damaged components. [Image reprinted by permission from Macmillan Publishers Ltd: From Ham et al. 2010.]

MSE Research Accomplishment

Smart Microparticles Perform Robotic Functions

Background: Self-assembly enables synthesis of materials that have far more functional diversity than traditional metals, ceramics, and polymers. However, complex and dynamic structural characteristics of the ensuing materials, whose organization often occurs across many coexisting length and time scales, can make these new materials difficult to control and manipulate.

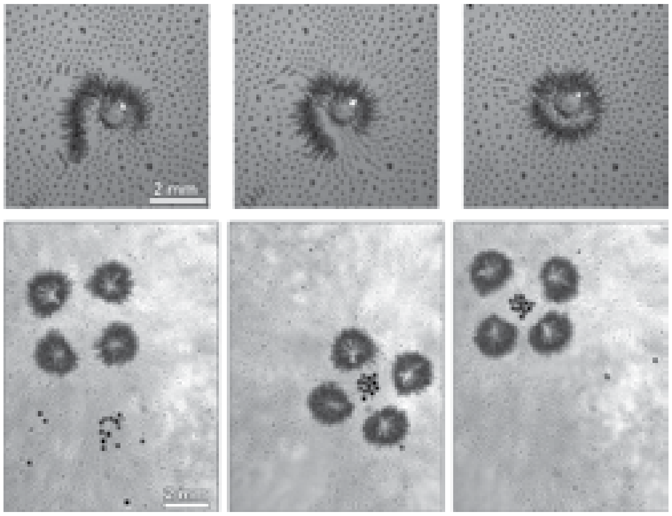
Research: Teams of tiny microrobots, each a mere half millimeter wide, can now be directed and manipulated to perform elaborate mechanical functions such as grasping, transporting, and releasing cargo. These new structures are made of remarkably simple, inexpensive constituents: magnetic microparticles confined between two nonmixing liquids. When subjected to a magnetic field, the particles self-assemble into miniature star-like structures, or asters. By manipulating the magnetic field, individual asters and aster arrays can be directed to open and close around a target particle, swim, and then release the captured particle at a desired location. These structures can even self-repair, so if particles are lost, the aster simply reshuffles itself.

Impact: This discovery demonstrates control of functionality and provides new insights into the design and fabrication of "smart" synthetic materials with self-repairing, multitasking, and reconfiguring capabilities. Intriguing applications include self-assembled grippers or tweezers for manipulating microparticles on the surface of liquids.

Reference

Snezhko, A., and I. S. Aranson. 2011. "Magnetic Manipulation of Self-Assembled Colloidal Asters," *Nature Materials* **10**, 698–703.

Magnetic Manipulation of Microrobots. Energized and directed by a magnetic field, microparticles assembled into a star-like structure, or aster, capture a targeted particle (top), and an aster array captures and relocates multiple targeted particles (bottom). [Image reprinted by permission from Macmillan Publishers Ltd: From Snezhko and Aranson 2011.]



MSE Research Accomplishment

Seeing Magnetism at the Atomic Scale

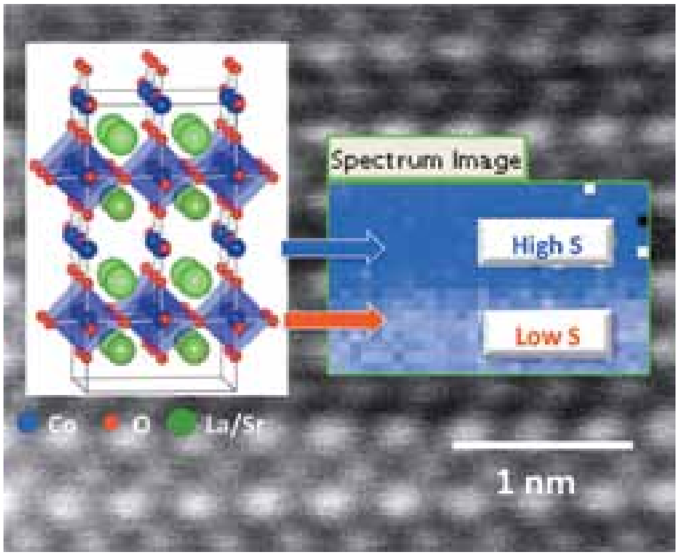
Background: Magnetic properties are critical for a vast array of material applications including computer hard drives, motors, generators, and permanent magnets used in many technologies. Developing the next generation of magnetic materials requires understanding these properties at the atomic scale, where their thin-film architecture or small defects dominate behavior. Current measurement techniques often are limited in that they provide “bulk measurements” of a sample, without spatial resolution. Z-contrast electron microscopy has demonstrated its ability to probe structural, chemical, and electronic properties with atomic-scale resolution and now also has provided magnetic information at this length scale in exquisite detail.

Research: For the first time, the “spin” of individual atomic planes—the atomic behavior that controls magnetic properties—has been imaged in an electron microscope. Being able to map spin at an atomic scale will provide the understanding necessary to resolve many of the mysteries of magnetism. These experiments took advantage of the most advanced electron microscopes and focused on cobalt, a technologically important element found in batteries, magnets, and structural materials. In this investigation, the spin of cobalt atoms in thin films showed unexpected ordering not observed in bulk materials. Theoretical calculations indicate that the mechanism responsible may be associated with the strain in the thin film.

Impact: This new imaging technique, coupled with predictive modeling, offers the potential to design and control spin structure, enabling the fine-tuning of material properties.

Reference

Gazquez, J., et al. 2011. “Atomic-Resolution Imaging of Spin-State Superlattices in Nanopockets within Cobaltite Thin Films,” *Nanoletters* **11**, 973–76.



Real-Space, Atomic-Resolution Mapping of a Spin-State Superlattice in a Cobalt Oxide. The background is a microscopy image of a cobaltite thin film ($La_{0.5}Sr_{0.5}CoO_{3-\delta}$), where each “dot” corresponds to a row of atoms. On a matching scale, the left inset is a schematic of the crystal structure; the right is an image reconstructed from an analysis of the energy loss. The brightness of each data point (pixel) corresponds to the spin state at that place in this compound. [Image reprinted with permission from Gazquez et al. 2011. Copyright American Chemical Society.]

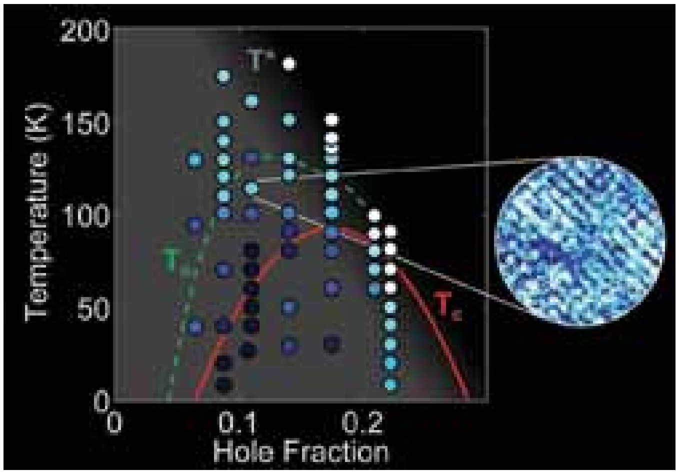
MSE Research Accomplishment

Unraveling Superconductivity's Pseudogap

Background: Superconductors are materials that conduct electricity with 100% efficiency, losing zero energy to resistance from the conducting material itself. All known superconducting materials, even the so-called "high-temperature" superconductors, exhibit superconductivity only at temperatures close to absolute zero, which requires expensive cooling systems. Dramatically increasing this working temperature, thereby making superconductors easier and cheaper to use, is a key research and technological goal. Achieving this objective has been hampered by a long-standing, unanswered question that centers on the origin and electronic behavior of the so-called "pseudogap" phase, a nonsuperconducting state observed in many superconductors' electronic spectrum at temperatures above the superconducting state. Pseudogap refers to an energy range with very few electronic states, whereas a "gap" is an energy range containing no states. Research has yet to reveal clearly whether the pseudogap phase is a static state with a stable electronic structure or a dynamic state whose electronic structure fluctuates in time. Also unclear is how the pseudogap phase relates to the superconducting phase.

Research: New understanding of these mechanisms is emerging from observations obtained through a combination of unique techniques exploring the structure at temperatures above the superconducting phase. One set of measurements indicates that electrons do not form pairs but exhibit a new, distinctive ordering. This new phase persists when the material becomes superconducting. Other measurements reveal stripe-like fluctuations of charge and spin that normally are seen only in the superconducting phase but were predicted for a broader range of conditions. Each of these new findings is an important step toward a full understanding of the mechanism behind high-temperature superconductivity.

Impact: This new knowledge may help enable the discovery and rational design of new high-temperature superconductors, possibly even ones that operate at room temperature. Such an advance would revolutionize energy generation, storage, and transmission technologies.



Strength of Fluctuating Stripes at the Onset of the Pseudogap in a Copper Oxide Superconductor. The right inset of this phase diagram shows the approximately four atomic-length patterns in the spatial structure of electronic wave functions as a result of the stripe formation. Shown are the superconducting transition temperature (T_c), the upper bound for the onset of superconducting fluctuations (T_o), and the pseudogap temperature (T^*). The fluctuating stripes are seen throughout the pseudogap phase but are strongest near a hole concentration of one-eighth (the darker the symbols, the stronger the fluctuations). [Image reprinted by permission from Macmillan Publishers Ltd: From Parker et al. 2010.]

References

Parker, C. V., et al. 2010. "Fluctuating Stripes at the Onset of the Pseudogap in the High-T_c Superconductor $Bi_2Sr_2CaCu_2O_{8+x}$," *Nature* **468**, 677–80.

He, R.-H., et al. 2011. "From a Single-Band Metal to a High-Temperature Superconductor via Two Thermal Phase Transitions," *Science* **331**, 1579–83.

Chemical Sciences, Geosciences, and Biosciences Division

science.energy.gov/bes/csgb/

The transformation of energy between types (e.g., optical, electrical, chemical, and thermal) and the rearrangement of matter at the atomic, molecular, and nano scales are critically important in every energy technology. The Chemical Sciences, Geosciences, and Biosciences (CSGB) Division within BES supports research exploring fundamental aspects of chemical reactivity and energy transduction to develop a broad spectrum of new chemical processes, such as catalysis, that can contribute significantly to new energy technologies.

CSGB research focuses on understanding physical and chemical phenomena over a tremendous range of spatial and temporal scales and at multiple levels of complexity. Spatial scales span the subnanometer, for studying the structure of atoms and molecules, to kilometers, for examining the behavior of subsurface geological structures. Time scales range from attoseconds (10^{-18} seconds), for investigating electron motions in atoms, to millennia, for understanding geological change. Central to all CSGB research is the quest to understand and control atomic- and molecular-level chemical change and its concomitant transformation of energy.

Knowledge of the quantum mechanical behavior of electrons, atoms, and molecules is being translated into the ability to control and direct chemical behavior to achieve a desired result. Such results include, for example, optimal conversion of solar energy into excited electronic states and then into separation of electrical charge in macromolecular assemblies. This unprecedented degree of control represents a new era for chemical science, which CSGB research seeks to expand further by enabling the tailoring of chemical transformations with atomic and molecular precision. The challenge is to predictively assemble and manipulate large, complex chemical, geochemical, and biochemical systems at the same level of detail now possible for simple molecular systems.

To address these challenges, CSGB's portfolio is organized into three coordinated activities:

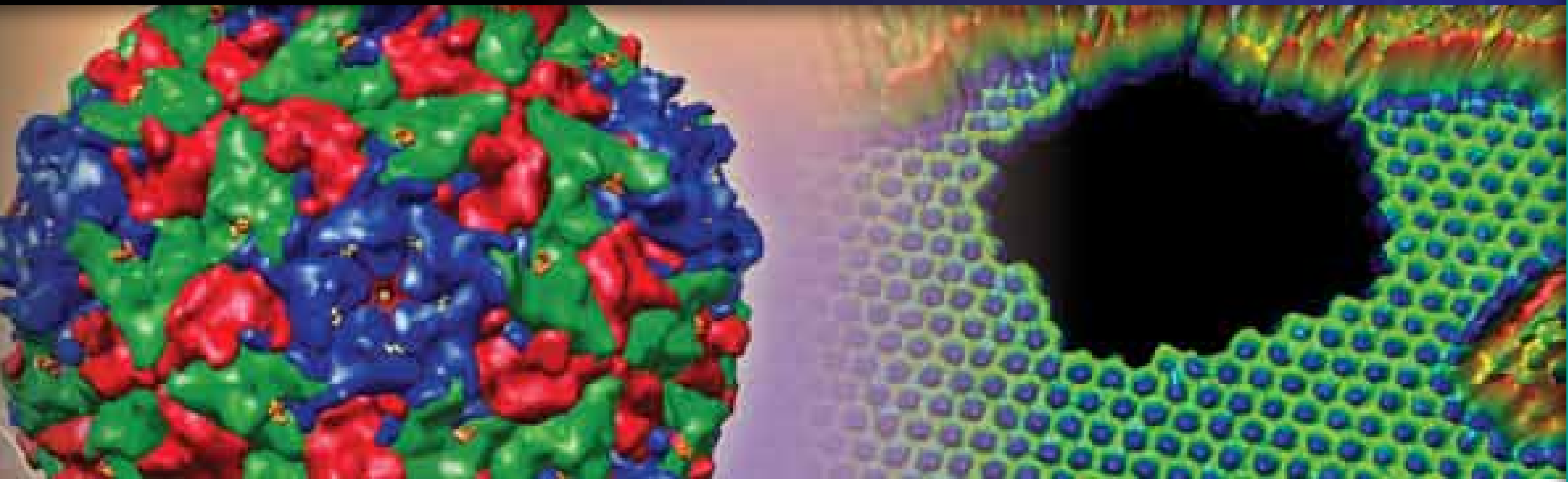
- **Fundamental Interactions**
- **Chemical Transformations**
- **Photochemistry and Biochemistry**

The division encourages interdisciplinary science bridging the above areas, and its activities all exhibit strong synergy among experiment, theory, and computational modeling and simulation.

CSGB Research Activities

Fundamental Interactions

This activity builds the fundamental science basis essential for technological advances in a diverse range of energy processes. Research emphasizes structural and dynamical studies of atoms, molecules, and nanostructures to provide complete knowledge and rigorous

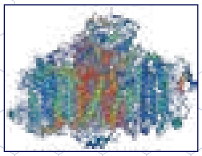


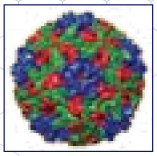
understanding of reactive chemistry in gas and condensed phases. These studies also investigate the chemistry occurring at phase interfaces (e.g., gas-liquid, gas-solid, liquid-solid) because of its critical importance in energy technologies—from catalysis to electrical energy storage. The Fundamental Interactions portfolio includes significant efforts to develop new sources of photons, electrons, and ions for characterizing and controlling atomic, molecular, and nanoscale matter. Computational and theoretical efforts focus on novel algorithms with increased accuracy and efficiency that aim to provide a predictive modeling and simulation capability for scientific discovery across multiple time and length scales. Research is conducted to understand molecular-scale chemical and physical properties as well as interactions governing chemical reactivity, solute and solvent structure, and transport.

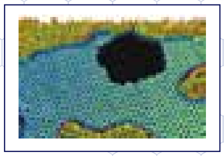
Strong emphasis is placed on ultrafast optical and x-ray techniques to explore and direct molecular dynamics and chemical reactions. These tools enable studies of energy transfer within isolated molecules, illuminating the making and breaking of chemical bonds. They also allow direct observation of the formation and evolution of excited states, a capability central to understanding elementary energy conversion processes. The Fundamental Interactions activity exploits the nation's most advanced x-ray light sources, particularly the Linac Coherent Light Source (LCLS) at the SLAC National Accelerator Laboratory, where researchers use the world's fastest and most intense x-ray pulses to explore new frontiers in x-ray interactions with matter.

Catalysis Science Researcher Jose Rodriguez.
[Courtesy of Brookhaven National Laboratory.]

Another unique feature of this activity is its world-leading fundamental research into the clean and efficient combustion of 21st century transportation fuels. The ultimate objective is to provide science-based combustion simulations enabling the design of new devices, such as internal combustion engines. Studies focus on the dynamics and rates of gas-phase chemical reactions at energies characteristic of combustion, identifying key combustion intermediates, and understanding their chemical and physical properties. This knowledge is integrated into combustion models that may involve hundreds, or even thousands, of reactions necessary to describe a combustion process. These models also incorporate the complex turbulent flow and energy transport characteristics of real combustion processes.



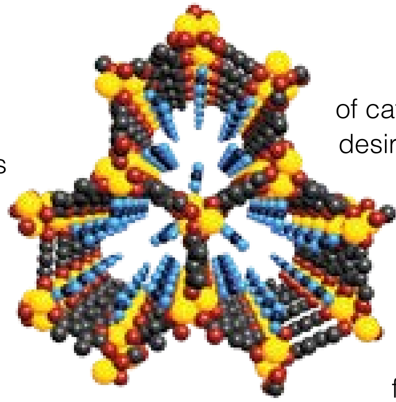




Chemical Sciences, Geosciences, and Biosciences

Chemical Transformations

Research in this activity emphasizes the design, synthesis, characterization, and optimization of chemical processes underpinning current and emerging energy strategies. Encompassing the areas of catalysis, separations and analysis, heavy-element chemistry, and geosciences, this effort seeks to inform advanced technical solutions in fuel production, nuclear energy, and disposal options for byproducts of energy technologies (e.g., deep underground sequestration of carbon dioxide). Activities span a wide breadth of novel chemistry—including nanostructured surfaces; electrochemistry; nanoscale membranes; bioinspired chemistry; inorganic, organic, and hybrid molecular complexes; and analytical and physical geochemistry. This activity also develops unique tools needed for chemical analysis and molecular detection, emphasizing the imaging of chemically distinct species.



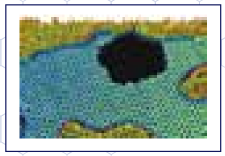
Schematic of a Molecular Framework Molecule Capable of Capturing Carbon Dioxide. [Courtesy of University of California–Los Angeles.]

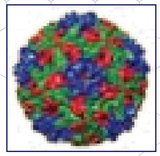
The Chemical Transformations research portfolio includes the nation's largest federal effort in applying basic science to unravel the principles that define how catalysts accelerate and direct chemistry. Such knowledge enables the rational synthesis of new nanoscale catalysts that will lead to increased energy efficiency and chemical selectivity. Because so many fuel and chemical production processes rely on catalysts, improving catalytic efficiency and selectivity has enormous economic and energy consequences. The grand challenge is to use fundamental understanding of catalytic chemistry for the rational design and synthesis of catalysts that perform precisely as desired. To address this challenge, this activity promotes synergy among several scientific and engineering disciplines; integrates heterogeneous, homogeneous, and bioinspired catalysis studies; and encourages the use of BES user facilities to significantly advance catalysis research.

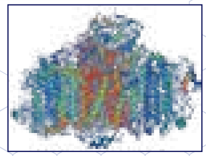
Exploring the fundamental chemistry of heavy elements—the actinides and transactinides—is another unique focus of this portfolio. Knowledge about the chemical characteristics of actinide and fission-product materials under realistic conditions provides a basis for the fission fuel cycles envisioned for advanced nuclear energy systems. Combined experimental and theoretical research is supported to develop a predictive understanding of the chemical and physical properties of these elements, including their solution, interfacial and solid-state bonding, and reactivity. Related studies explore the science by which heavy-element compounds can be more effectively separated, research important for both nuclear fuels and waste remediation. More recently, this effort was expanded to consider carbon dioxide removal from postcombustion streams, an area of research essential to making carbon capture an economic reality.

Photochemistry and Biochemistry

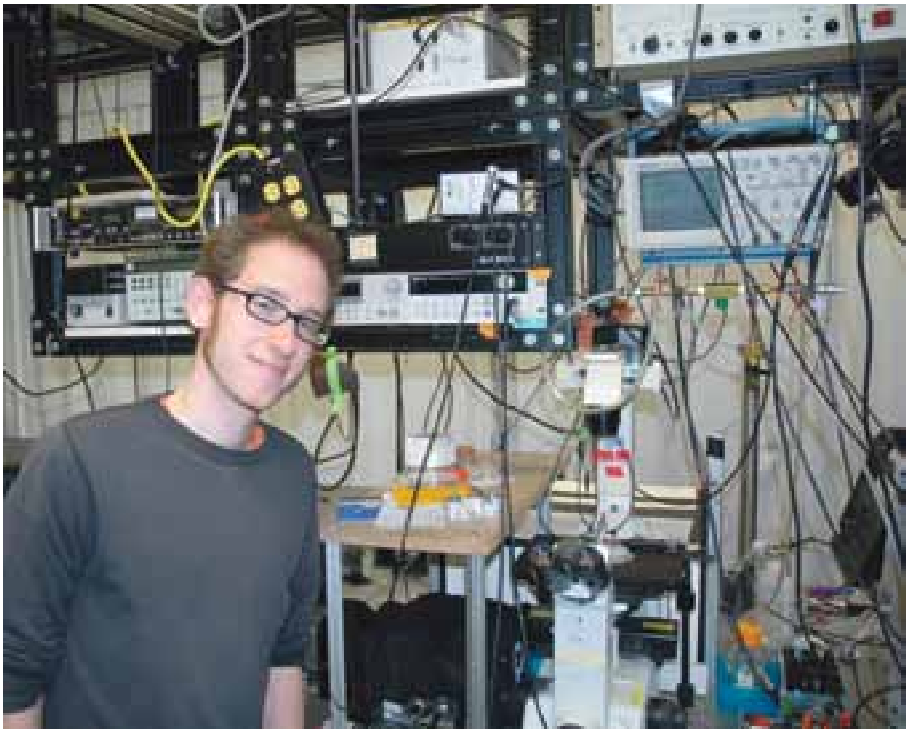
Research in the Photochemistry and Biochemistry activity focuses on molecular mechanisms that capture light energy and convert it into chemical and electrical energy in both natural and manmade systems. This effort is critical





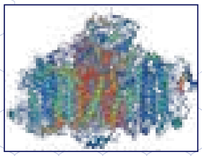
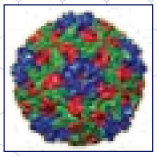
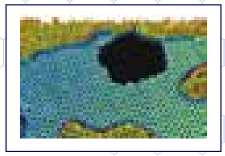


for effectively using our most abundant energy source—the sun, whose light strikes Earth with enough energy each hour to fuel a year's worth of human activity. To tap into this potential, natural photosynthesis is studied to provide roadmaps for creating robust artificial and biohybrid designs. Tools developed elsewhere in BES for the physical sciences are used extensively to understand the mechanisms of biological energy transduction, including processes beyond primary photosynthesis (e.g., carbon reduction and deposition of reduced carbon into energy-dense carbohydrates and lipids). Complementary research in synthetic systems encompasses organic and inorganic photochemistry for energy capture and conversion in artificial photosynthetic assemblies.



Trapping Single Biomolecules in Solution. In groundbreaking research, Randall Goldsmith (pictured here) and W. E. Moerner developed and applied a technique for confining and studying an individual protein without having to pin it down and potentially alter its fundamental behavior (see Research Accomplishment, p. 27). [Courtesy of Stanford University.]

Research in natural photosynthesis emphasizes intersections between the biological sciences and energy-relevant chemical sciences and physics. Such studies explore self-assembly of photosynthetic components, natural mechanisms of photon capture and charge separation, and self-regulating and -repairing properties of the photosynthetic apparatus. This work provides vital scientific knowledge underlying artificial photosynthetic fuel production and more efficient generation of biomass as a renewable energy source. Downstream from primary photosynthesis, physical biosciences research combines experimental and computational tools from the physical sciences with biochemistry and molecular biology to develop fundamental insights into the complex processes transforming energy in living systems. Because nature's largest repository of solar energy resides in plant cell walls, research seeks a greater understanding of cell-wall architecture at the molecular level, knowledge required for catalytic conversion of biomass into chemical fuels.

Chemical Sciences, Geosciences, and Biosciences

Solar photochemistry research uses insights from nature to develop efficient artificial photosynthetic systems, emphasizing a molecular-level understanding of solar energy capture and conversion in the condensed phase and at interfaces. The ultimate goal is to harvest this energy as fuel or electricity. Investigations include the elementary steps involved in light absorption and energy transfer, charge separation, and charge transport within a number of chemical systems. This research advances the use of solar electrochemistry as an alternative to photovoltaics for renewable electricity generation. By contrast, solar photocatalysis—achieved by coupling artificial photosynthetic systems for light harvesting and charge transport with the appropriate electrochemistry—provides a direct route for generating fuels such as hydrogen, methane, and complex hydrocarbons.

Selected 2011 Accomplishments

The following pages describe CSGB-supported research that has led to a new technique for determining protein structures, a more energy-efficient method for synthesizing nitrogen compounds, and a new technology enabling the visualization of molecules in solution. These studies are only a fraction of the many research projects supported by CSGB in 2011.

CSGB Research Accomplishment

New X-Ray Sources Provide Unprecedented Probes of Matter

Background: X-rays are ideal probes of the structure of matter, pinpointing the locations of atoms in a sample. New x-ray sources, including the world's first x-ray free electron laser—the Linac Coherent Light Source (LCLS)—provide capabilities that are revolutionizing our ability to image matter at the atomic scale. The intensity and ultrashort duration of LCLS x-ray pulses can produce snapshots of atomic motion to be sequenced into movies that demystify intimate details about the inner workings of materials and chemical processes.

Research: Researchers have used LCLS to take single-shot, x-ray images of intact viruses, paving the way for capturing live microbes and other organisms in action. In separate studies, researchers used LCLS capabilities to develop a new approach for determining the three-dimensional structures of proteins. The laser's brilliant pulses of x-ray light pull structural data from tiny protein nanocrystals, avoiding the need to use large protein crystals that can be difficult or impossible to prepare.

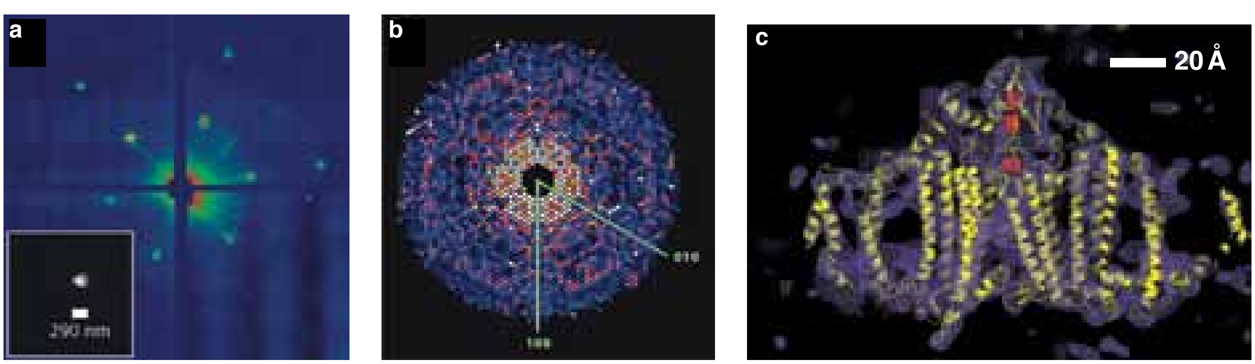
Impact: This technique will take years off the time required for structural analysis of some proteins and allow scientists to decipher tens of thousands of other macromolecules out of reach today, including many involved in energy technologies and biopharmaceutical applications. Moreover, it opens the door to whole new realms of scientific possibilities, including the ability to observe atoms moving and chemical bonds forming and breaking in real time.

References

Chapman, H. N., et al. 2011. "Femtosecond X-Ray Protein Nanocrystallography," *Nature* **470**, 73–77.

Seibert, M. M., et al. 2011. "Single Mimivirus Particles Intercepted and Imaged with an X-Ray Laser," *Nature* **470**, 78–81.

Femtosecond X-Ray Protein Nanocrystallography. The Photosystem I protein plays a key role in photosynthesis. Crystallizing this protein, although difficult, is a prerequisite to using standard x-ray crystallography to obtain its structure. In a new approach enabled by the ultrafast, ultraintense x-ray pulses at the Linac Coherent Light Source, a single x-ray pulse yields a diffraction pattern used to image the shape of a single nanocrystal **(a)**. An accumulation of such diffraction patterns from nanocrystals (>15,000 in this example) is used to build the full three-dimensional diffraction pattern **(b)**, which is then analyzed to give the molecular structure **(c)**. [Images reprinted by permission from Macmillan Publishers Ltd: From Chapman et al. 2011.]



CSGB Research Accomplishment

Breaking Nature's Strongest Chemical Bonds

Background: Nitrogen (N_2) is converted to ammonia (NH_3) using catalysis through the Haber-Bosch process, arguably one of the most important chemical processes that society has ever devised. Approximately 50% of the world's population relies on fertilizer derived from this process to grow food. However, the extreme temperature and pressure required for the reaction also make this one of the most energy-intensive, carbon dioxide–producing processes used by the chemical industry. Although finding more efficient methods for breaking the N_2 triple bond is paramount to worldwide energy and economic interests, this technology has remained largely unchanged since it was invented more than a century ago. Fundamental research is essential for discovering new and more energy-efficient methods to synthesize NH_3 and other N-containing chemicals.

Research: New synthetic methods now promote these challenging chemical transformations under much milder conditions. For example, a recently discovered hafnium metal complex uses carbon monoxide (CO) to break the N_2 bond, while making new carbon-carbon and carbon-nitrogen bonds. Adding some hydrogen creates oxamide, an important agrochemical currently made from fossil fuels. Remarkably, the whole process operates at ambient temperature, rupturing two of the strongest chemical bonds found in nature, those in N_2 and CO. This core molecule can be elaborated further with CO_2.

Impact: This research begins to establish low-energy pathways to a broad variety of everyday products such as fertilizers, pesticides and herbicides, polymers and polymer fibers, and pharmaceuticals.

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Semproni, S. P., E. Lobkovsky, and P. J. Chirik. 2011. "Dinitrogen Silylation and Cleavage with a Hafnocene Complex," *Journal of the American Chemical Society* **133**, 10406–09.

Energy-Efficient Process Breaks Nature's Strongest Chemical Bonds. Nitrogen and carbon monoxide are strongly bound molecules, so breaking their bonds to take advantage of these abundant feedstocks can expend a great deal of energy. In a newly discovered process, an organometallic hafnium compound efficiently breaks these bonds while simultaneously forming new carbon-carbon and carbon-nitrogen bonds. [Courtesy of Princeton University.]

CSGB Research Accomplishment

Molecular Movies Illuminate Dynamics of Light-Harvesting Proteins in Solution

Background: Light-capturing, biological molecules exploit various structural and electronic changes to harvest sunlight. This behavior is a critical part of the natural process by which the sun's energy is converted into chemical energy. However, studying these fleeting changes in fine detail poses a formidable experimental challenge for molecules in solution, where diffusion randomly moves molecules in and out of the sample volume. Until now, spectroscopic studies have been forced to rely on the analysis of many molecules over time, resulting in an averaged depiction that lacks molecular detail. This averaging obscures important rare or unsynchronized events experienced by only a few molecules at a time. Examples include fluctuations in a molecule's solvent environment and structural changes occurring during the course of a reaction. Physically immobilizing molecules under study on a surface is self-defeating because this approach can completely alter the molecules' behavior.

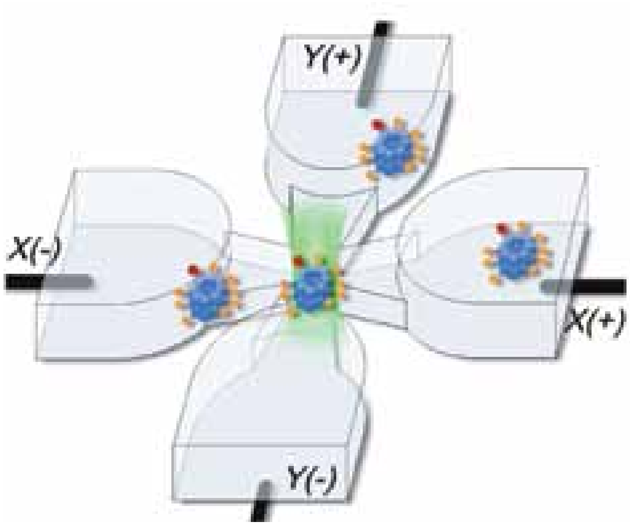
Research: Researchers recently overcame this vexing problem by developing the ABEL (Anti-Brownian Electrokinetic) trap. The ABEL trap maintains the position of a single fluorescent protein molecule at the center of a microfluidic cavity, where it can be probed for prolonged periods (often >1 second) without surface immobilization. The trap uses electric fields to induce motions that cancel the random movement of the single protein, known as Brownian motion. In other words, the trap figuratively freezes a single biomolecule of interest in a solution of many solvent molecules, allowing spectroscopic analyses of just that molecule. In this case, the target was allophycocyanin, an important photosynthetic antenna protein. Experiments revealed unexpected electronic and structural changes that occur when this protein harvests sunlight. Moreover, the timeframe during which these changes occurred was determined, resulting in a movie of the molecule undergoing its transformation.

Impact: This new, structural-dynamic view of how allophycocyanin responds to light expands our understanding of natural light-harvesting systems, which can help further the design of synthetic systems for solar energy conversion.

References

Goldsmith, R. H., and W. E. Moerner. 2010. "Watching Conformational- and Photodynamics of Single Fluorescent Proteins in Solution," *Nature Chemistry* **2**, 179–86.

Wang, Q., and W. E. Moerner. 2011. "An Adaptive Anti-Brownian Electrokinetic Trap with Real-Time Information on Single-Molecule Diffusivity and Mobility," *ACS Nano* **5**, 5792–99.



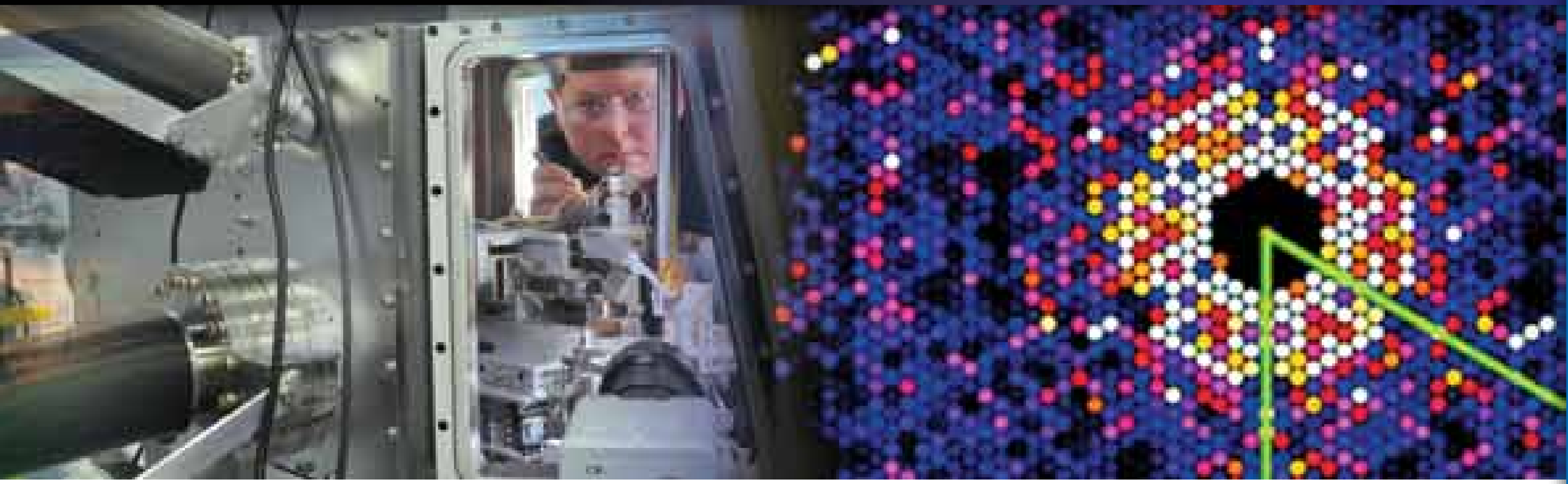
Investigating the Dynamics of a Single Biomolecule. Electrokinetic forces compensate for diffusion to trap single molecules of a photosynthetic antenna protein in solution for more than 1 second. [Courtesy of Stanford University.]

Scientific User Facilities Division

science.energy.gov/bes/suf/

BES operates a suite of scientific user facilities through its Scientific User Facilities (SUF) Division. These facilities provide unique technical tools—including x-ray light sources, neutron scattering facilities, Nanoscale Science Research Centers (NSRCs), and Electron-Beam Microcharacterization Centers (EBMCs)—for advancing science in basic and applied energy-related disciplines. Research conducted at the facilities involves characterizing materials at the

BES Scientific User Facilities



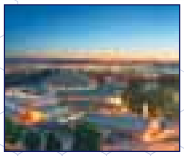
highest level of spatial, spectral, and temporal resolution. The breadth of instrumentation available across the facilities enables complementary evaluations of material structure, composition, and function and the evolution of such properties over time in a variety of operating conditions. In addition, the NSRCs (located near one or more x-ray, neutron, or electron scattering facilities) have capabilities for synthesizing, fabricating, and exploring matter at the nanoscale.

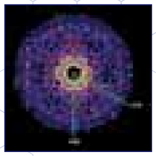
These premier scientific facilities are open access, based on acceptance of user proposals through a competitive merit review process, allowing scientists from academia, federal laboratories, and industry to use the facilities' unique capabilities and sophisticated instrumentation. In FY 2011, the facilities supported more than 14,000 users from many science and technology disciplines, including chemistry, physics, geology, materials science, environmental science, biology, and a wide range of engineering fields (see table at right). The facilities make possible experimental studies that cannot be conducted in ordinary laboratories, enabling leading-edge research that benefits from a merging of ideas and techniques from different disciplines.

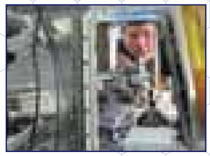
Breakdown of Scientific Users in FY 2011

Facility	Users
X-Ray Light Sources	**10,261**
Advanced Light Source	1,931
Advanced Photon Source	3,986
National Synchrotron Light Source	2,313
Stanford Synchrotron Radiation Lightsource	1,515
Linac Coherent Light Source	516
Neutron Scattering Facilities	**1,675**
High Flux Isotope Reactor	477
Lujan Neutron Scattering Center	308
Spallation Neutron Source	890
Nanoscale Science Research Centers	**1,780**
Center for Nanoscale Materials	368
Center for Functional Nanomaterials	363
Molecular Foundry	327
Center for Nanophase Materials Sciences	374
Center for Integrated Nanotechnologies	348
Electron-Beam Microcharacterization Centers	**618**
National Center for Electron Microscopy	188
Electron Microscopy Center for Materials Research	220
Shared Research Equipment User Facility	210
Total Users in FY 2011	**14,334**

Continuous development and upgrades of scientific capabilities and advanced instrumentation are important components of the performance of a facility. Consequently, the SUF research portfolio includes accelerator and detector research to explore technology options for next-generation x-ray and neutron sources. In addition, construction activities support new and upgraded facilities and beamlines. A 2011 highlight was the ongoing construction of the National Synchrotron Light Source-II at Brookhaven National Laboratory.







Scientific User Facilities

X-Ray Research

Since their discovery in 1895, x-rays have tantalized scientists and engineers with their ability to reveal the interior structures of solid objects. They also have been the principal way of determining the atomic structure of materials for nearly a century. Today's most advanced synchrotron radiation light sources can produce x-rays billions of times brighter than the x-ray technology used in laboratories and hospitals. These highly focused, intense x-rays enable the study of materials ranging from metals and semiconductors to proteins and pharmaceutical drugs. The tiny wavelengths of x-rays can resolve structural details at the molecular to atomic level, providing information for understanding and controlling material functionality. This understanding then can be used to synthesize materials with desired behaviors to advance technological growth.

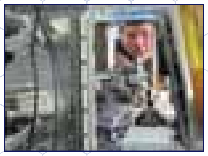
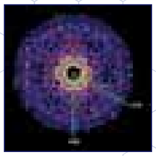
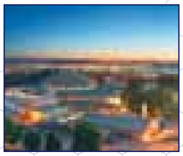
Synchrotron radiation has vastly enhanced the utility of x-ray techniques including diffraction, spectroscopy, and imaging. Moreover, the broad energy range of x-rays allows researchers to tailor characterization techniques to the individual materials and functions to be analyzed. Finally, the ability to control x-ray beam properties—such as polarization (both linear and circular), coherence, beam size, and time scale—has opened many new research avenues. The most recent advance in x-ray technologies is the advent of ultrafast x-ray pulse time structures using free electron lasers (FELs) to generate the x-ray beams.

BES supports and operates five synchrotron radiation light sources. Four of these are storage ring–based sources: the Advanced Light Source at Lawrence Berkeley National Laboratory (LBNL), Advanced Photon Source at Argonne National Laboratory (ANL), National Synchrotron Light Source at Brookhaven National Laboratory (BNL), and Stanford Synchrotron Radiation Lightsource at SLAC National Accelerator Laboratory. The newly constructed fifth light source, the Linac Coherent Light Source (LCLS) at SLAC, is a free electron laser. More than 10,000 scientists conduct research at these five facilities annually, making discoveries and advancing science and technology. They come from a wide range of fields including materials science, physical and chemical sciences, metrology, geosciences, environmental sciences, biosciences, medical sciences, and pharmaceutical sciences. Many unexpected scientific communities, such as forensic science and archaeology, also are exploring opportunities to use synchrotron radiation for their research.

Neutron Scattering

A goal of BES science is to understand the factors that determine the properties of matter on the atomic scale and then use this knowledge to optimize those properties or develop new materials and functionality. With expanding applications in geology, biology, and physics, neutron scattering is among the most powerful tools for characterizing matter to understand and develop new materials and chemistries.

Neutrons have several unique advantages among the different probes used to investigate atomic-scale structure and dynamics. For studying structure with atomic resolution, neutrons have a wavelength similar to the spacing between atoms, and for investigating dynamics, they have energies similar to those

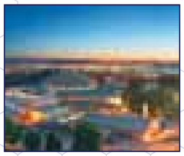
Advanced Instrumentation for New Materials. Kathleen Gregar checks an instrument used to grow pure complex oxide films at the Center for Nanoscale Materials, which supports basic research and instrument development for creating innovative materials with unique functionality. [Courtesy of Argonne National Laboratory.]

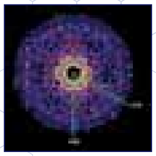
of atoms in materials. Neutrons have no charge, allowing them to penetrate deep into a bulk material. They are scattered similarly by both light and heavy atoms but differently by different isotopes of the same element. Substitution of isotopes for atoms in structures thus allows characterization of specific chemical sites in, for example, organic and biological materials. Neutrons also have a suitable magnetic moment for probing magnetism in condensed matter. Finally, neutron scattering cross-sections are precisely measurable on an absolute scale, facilitating straightforward comparison with theory and computer modeling.

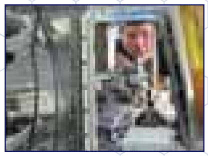
Neutrons can be generated via fission in a research reactor, such as the High Flux Isotope Reactor (HFIR) at Oak Ridge National Laboratory (ORNL). In addition to supporting neutron scattering experiments, HFIR also provides other capabilities including radiation damage studies required to develop fusion and advanced fission reactors, as well as isotope production for a wide range of research, technological, and medical applications. Another approach for producing neutrons is to use an accelerator to generate protons that strike a heavy-metal target. The impact produces neutrons in a process known as spallation. Since accelerators are naturally pulsed, the resulting neutron source also is pulsed, enabling highly efficient use of the neutrons produced in time-of-flight experiments. The Lujan Neutron Scattering Center (Lujan Center) at Los Alamos National Laboratory (LANL) and the new Spallation Neutron Source (SNS) at ORNL are pulsed spallation neutron sources. Each year more than 1,600 scientists, engineers, and industrial researchers from across the United States conduct their research at HFIR, Lujan Center, and SNS.

Nanoscale Science and Electron Microscopy

Nanoscience is the study of materials and their behaviors at the nanometer (nm) scale, a length equivalent to tens of atoms. New scientific understanding and technologies are emerging through the probing and manipulation of single atoms and molecules, discrete clusters of atoms and molecules, and systems with nanoscale components. The scientific quest of this research is to design, observe, measure, and understand how these systems function and how they interact with the environment. Scientific discoveries at the nanoscale have the potential to contribute significantly to the understanding of energy and matter and advance innovations and technologies for national, economic, and energy security.





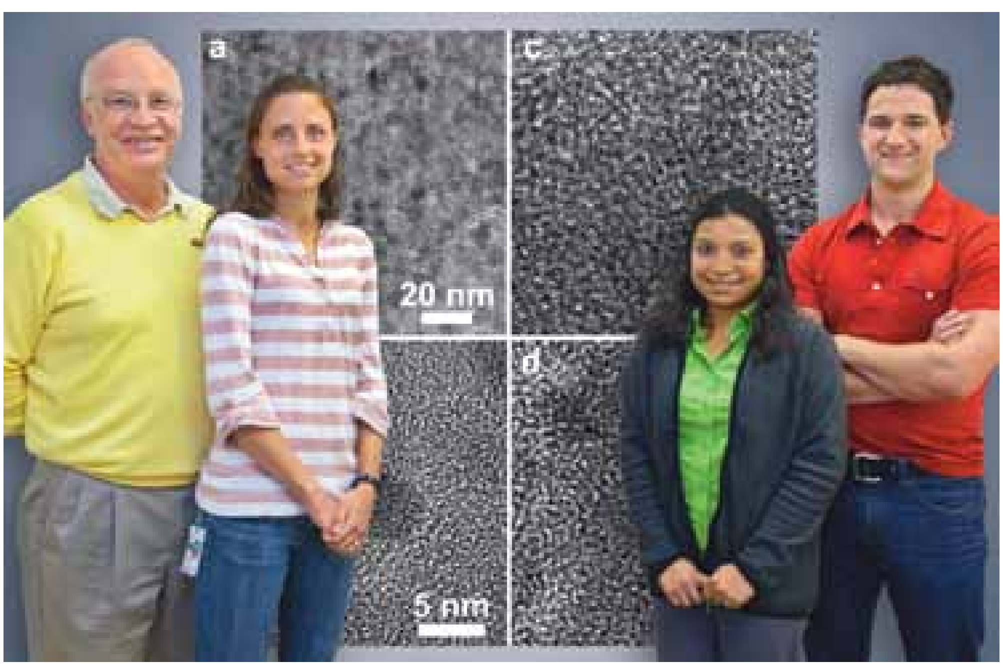


Scientific User Facilities

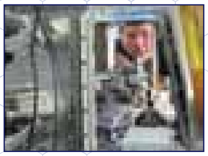
As DOE's premier user facilities for interdisciplinary nanoscale research, the Nanoscale Science Research Centers (NSRCs) serve as the basis for a nationwide program encompassing new science, tools, and computing capabilities. The five NSRCs are the Center for Nanoscale Materials at ANL, the Center for Functional Nanomaterials at BNL, the Molecular Foundry at LBNL, the Center for Nanophase Materials Sciences at ORNL, and the Center for Integrated Nanotechnologies at Sandia National Laboratories and LANL. Each center has particular expertise and capabilities in selected theme areas such as nanomaterial synthesis and characterization; catalysis; theory, modeling, and simulation; electronic materials; nanoscale photonics; soft and biological materials; imaging and spectroscopy; and nanoscale integration.

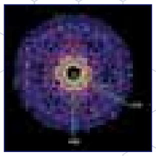
A key aspect of nanoscale science and the broader field of characterization is electron-beam microcharacterization, including microscopy and diffraction. Since first being used to investigate materials in the 1930s, electron microscopes have evolved into a forefront technique for characterizing the atomic structure of materials. The technique is used commercially across a range of industries, in medical diagnostics as well as in physical and life science research. Electron beams offer unique characterization capabilities and provide both structural and chemical information over critical length scales complementary to those probed by neutrons and photons.

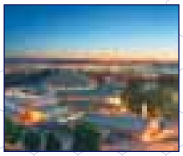
As important components of the user facility portfolio, BES's three Electron-Beam Microcharacterization Centers (EBMCs) seek to develop next-generation electron-beam instrumentation and conduct corresponding



Developing a Breakthrough Nanocomposite for High-Capacity Hydrogen Storage. The scientific team that designed the new nanomaterial included, from left, Christian Kisielowski, Anne Ruminski, Rizia Bardhan, and Jeff Urban. Their research is described on p. 36. [Courtesy of Lawrence Berkeley National Laboratory.]







research. The net results are unsurpassed spatial resolution with a world-record 50 picometers (0.05 nm) and the ability to simultaneously obtain structural, chemical, and other types of information from subnanometer regions. Such capabilities allow study of the fundamental mechanisms of catalysis, energy conversion, corrosion, charge transfer, magnetic behavior, and many other processes. Moreover, they are critical for understanding and improving materials for energy applications and the associated physical characteristics and changes governing material performance. These centers are the National Center for Electron Microscopy at LBNL, the Electron Microscopy Center for Materials Research at ANL, and the Shared Research Equipment User Facility at ORNL.

The NSRCs and EBMCs are co-located with one or more major BES user facilities for x-ray and neutron scattering, which complement and leverage the centers' capabilities.

Accelerator and Detector Research

Accelerator research is the cornerstone for developing new technologies that will improve the performance of light sources and neutron spallation facilities. The research explores new areas of science and technologies that will facilitate construction of next-generation, accelerator-based user facilities. A major emphasis is on assessing new capabilities for developing novel accelerator components such as high-repetition-rate electron beam injectors and improved cathode materials to enhance lifetime and performance. Research also includes beam physics studies to produce ultrahigh-brightness beams from origin to x-ray production and ultrafast beam control via the design and characterization of subfemtosecond (hundreds of attoseconds) FEL pulses. Such capabilities are opening new avenues for understanding chemical, material, and biological behaviors and phenomena.

This research activity was a major supporter of the theoretical and experimental studies leading to rapid development of LCLS, the world's brightest light source. These studies addressed many of the fundamental physics questions concerning FELs and high-brightness beams, resulting in remarkably successful experiments and demonstrating that high peak beam brightness is possible with a very low average current, as realized at LCLS. This activity also is investing in research to develop a new and more efficient generation of photon and neutron detectors, crucial for optimizing beam use. The detector studies include developing new designs and materials, as well as "smart" three-dimensional detectors that adapt to beam quality and perform initial analysis of data as it is received at the detector.

Selected 2011 Accomplishments

The following pages describe examples of how DOE scientific user facilities have been used to improve industrial battery technology, identify nanoscale phenomena that control thermal conductivity in thermoelectric materials, synthesize new high-capacity hydrogen storage materials, and develop a novel scheme for enhancing x-ray measurements of processes lasting just trillionths of a second. These accomplishments highlight only a few of the scientific advances enabled by BES user facilities in 2011.

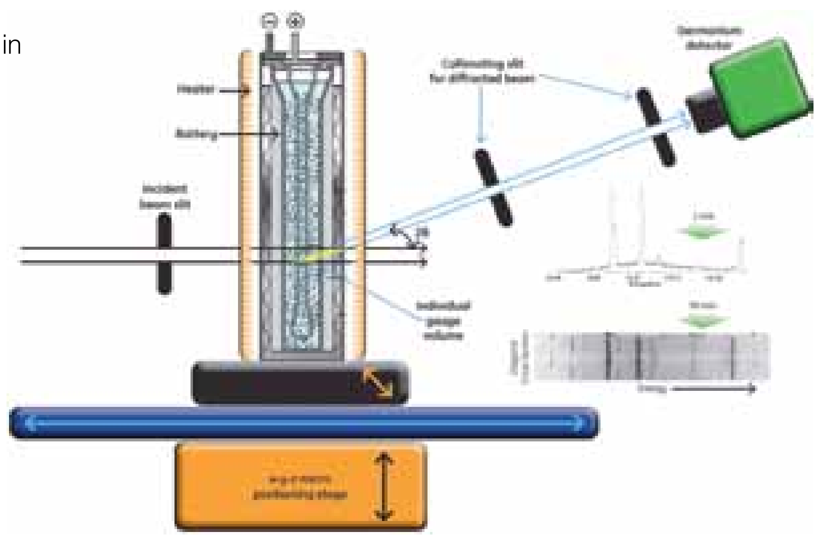
SUF Research Accomplishment

Revolutionary Industrial Battery Technology Developed Using Light Source Facilities

Background: Maximizing battery performance and reliability requires an in-depth fundamental understanding of the complex chemical processes, microstructural changes, and degradation that occur in real time as a battery is charged and discharged. To peer into the inner workings of a battery, researchers have traditionally used battery designs with windows in external layers that let x-rays through. However, these batteries specifically designed for experimental work often had structures considerably different from those of commercial batteries and were limited in the cycling conditions that could be investigated.

Research: One type of high–energy density battery with internal chemistry that previously had been inaccessible to x-ray analysis is the sodium-metal-halide cell, which is more than 3 cm thick and operates at 300°C. Using high-energy x-ray beams capable of penetrating through dense materials, a General Electric (GE)–led research team was able to obtain a detailed view of the chemical fluctuations deep within this full-size commercial battery in real time. These beams—generated by the National Synchrotron Light Source at Brookhaven National Laboratory and the Advanced Photon Source at Argonne National Laboratory—were used to produce x-ray diffraction patterns that researchers analyzed to track where and when chemical reactions occurred while the battery was charged and discharged. Additional studies of battery cross-sections helped the engineers further understand the evolution of chemical processes at the interfaces within the system. Aided by the results of this research, GE refined the chemistry and components of the sodium-metal-halide cell to create new batteries that boast three times the energy density and charging power of lead-acid batteries currently used for industrial transportation and stationary power applications. These new batteries also have expected lifetimes of up to 20 years and can operate in a wide range of temperature environments.

Impact: Enabled by breakthroughs in understanding the chemistry driving the sodium-metal-halide technology, GE is launching a new line of heavy-duty batteries known as Durathon™ that will be manufactured in a facility now under construction in Schenectady, New York. Production of these advanced batteries, which will be used for transportation and by telecoms, utilities, and data centers, will create more than 300 jobs.



Experimental Setup on X-Ray Beamline X17B1 at the National Synchrotron Light Source. The powerful x-ray beam penetrates deep into a full-size sodium-metal-halide battery during charging and discharging. Using a detector to measure the energy and intensity of the diffracted x-ray beam, researchers can track chemical fluctuations inside the battery. [Courtesy of General Electric.]

Reference

Rijssenbeek, J., et al. 2011. “In Situ X-Ray Diffraction of Prototype Sodium Metal Halide Cells: Time and Space Electrochemical Profiling,” *Journal of Power Sources* **196**(4), 2332–39.

SUF Research Accomplishment

Neutrons Point to New Routes for Designing High Thermoelectric Efficiency Materials

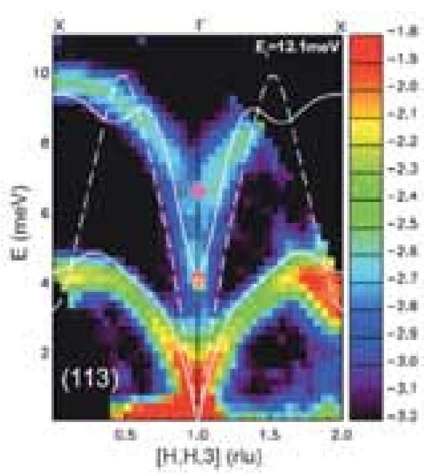
Background: Understanding and controlling how heat moves through solid materials are increasingly important to improving how thermoelectric materials can be used to transform heat into electricity. To maintain the large temperature differences needed to generate electricity, good thermoelectric materials should readily conduct electrons but block the flow of heat. At the nanoscale level, heat is essentially the motion or vibration of atoms. In a solid crystal, the atoms are arranged in a three-dimensional lattice. Phonons—units of vibrational energy—carry heat throughout a crystal by traveling with wave-like motion along the atoms. Studying the different kinds of phonons and their seemingly chaotic movement within a crystal lattice is key to determining the origins of a material's ability to conduct heat.

Research: The powerful neutron scattering instruments at the Spallation Neutron Source (SNS) at Oak Ridge National Laboratory (ORNL) provide researchers with a unique opportunity to investigate all the different types of atomic vibrations within a sample in a single experiment. The SNS Cold Neutron Chopper Spectrometer uses neutrons with wavelengths and low energy levels ideal for probing the vibrations of atoms in a crystal lattice. Researchers analyzed the energy and direction of neutrons scattered by phonons in lead telluride, a thermoelectric material particularly resistant to conducting heat. Once multiple neutron scattering datasets were acquired for different orientations of the crystal, researchers used the HB-3 Triple-Axis Spectrometer at ORNL's High Flux Isotope Reactor to pinpoint anomalous phonon behavior detected in particular regions of the crystal. Results of this research revealed an unusual, strong interaction between different phonon modes that disrupt the transport of thermal energy in lead telluride.

Impact: By uncovering nanoscale processes that control thermal conductivity, this research is helping to build the foundational knowledge needed to design new materials with tailored nanostructural features that obstruct heat flow but preserve electrical conductivity. These results point toward a new direction for obtaining very high thermodynamic efficiencies in materials that concentrate solar energy for electricity generation, recover waste heat to power industrial and transportation processes, and support many other application areas.

Reference

Delaire, O., et al. 2011. "Giant Anharmonic Phonon Scattering in PbTe," *Nature Materials* **10**, 614–19.



Neutron Scattering Data from the Cold Neutron Chopper Spectrometer at the Spallation Neutron Source. By analyzing the intensities of neutrons scattered from a single crystal of lead telluride, researchers discover an anomalous interaction between phonons moving in different directions, disrupting the flow of heat within the crystal. [Image reprinted by permission from Macmillan Publishers Ltd: From Delaire et al. 2011.]

SUF Research Accomplishment

Breakthrough Nanocomposite Material for High-Capacity Hydrogen Storage

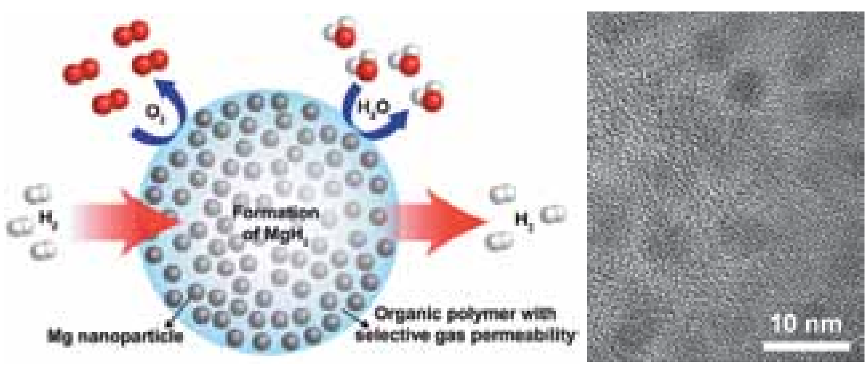
Background: With high energy density, hydrogen (H_2) is a promising alternative energy carrier that can be derived from many sources such as water, biomass, and organic materials. A key challenge to advancing H_2 as an energy carrier is finding effective ways to store more H_2 gas in less space and to easily access the stored H_2 when needed. One approach involves reacting H_2 with light metals such as lithium, sodium, or magnesium to form metal hydrides, but many of these compounds absorb and release H_2 too slowly and require excessive heating to unlock their stored H_2. Preventing these metals from interacting with oxygen or water in unwanted oxidation reactions is another obstacle. Advances in nanoscience are helping to overcome these limitations.

Research: Using the Molecular Foundry and the National Center for Electron Microscopy at Lawrence Berkeley National Laboratory, researchers have designed and synthesized a new nanostructured composite material that can efficiently store and release H_2 on demand under relatively moderate conditions. Nanosized crystals of magnesium (about 5 nanometers in diameter), which have much more surface area for interacting with H_2 than bulk magnesium, enable faster H_2 uptake and release at lower temperatures (200°C). By embedding magnesium nanoparticles within a flexible polymer matrix that is permeable only to H_2, the magnesium was protected from oxidative degradation by oxygen and water. In addition to accelerating reaction rates without requiring expensive metal catalysts, the resulting nanocomposite can store more H_2 per unit volume than a tank of the compressed gas.

Impact: This research represents a major breakthrough in the design of low-cost, hydrogen-storing materials for fuel cells and other power generation technologies. Besides providing a promising proof-of-principle for advancing hydrogen storage, this study shows how researchers can leverage the unique properties of nanostructures encased in gas-selective polymers to overcome thermodynamic and kinetic barriers underlying related problems in other areas of energy research.

Reference

Jeon, K.-J., et al. 2011. "Air-Stable Magnesium Nanocomposites Provide Rapid and High-Capacity Hydrogen Storage Without Using Heavy-Metal Catalysts," *Nature Materials* **10**, 286–90.



Hydrogen-Storing Magnesium Nanoparticles Embedded in Polymer. Illustration (left) and transmission electron microscope (TEM) image (right) show magnesium nanoparticles embedded within an organic polymer that is permeable to H_2 but blocks oxygen and water. The TEM image clearly shows the uniform distribution of the nanoparticles throughout the polymer. [Image reprinted by permission from Macmillan Publishers Ltd: From Jeon et al. 2011.]

SUF Research Accomplishment

Optimizing Electron Beams to Produce Ultrashort X-Ray Pulses

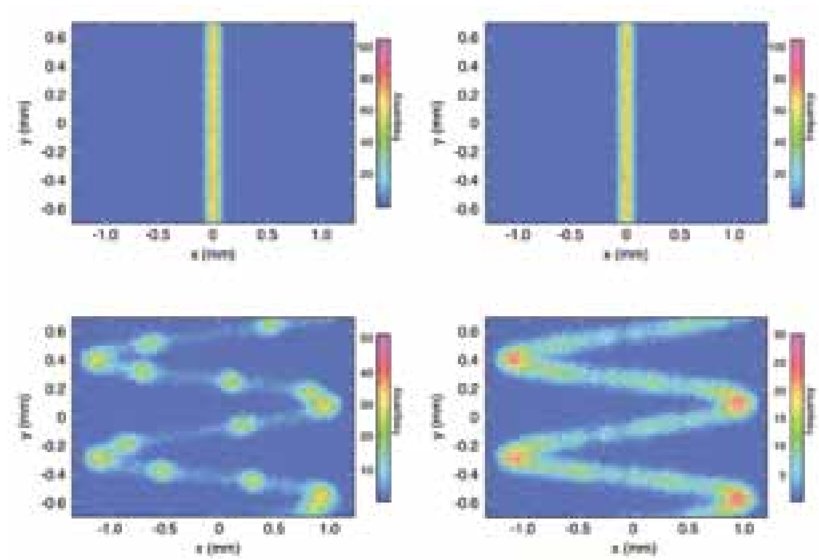
Background: The joining and splitting of molecular bonds in chemical reactions are incredibly quick—lasting less than a picosecond (a trillionth of a second). To precisely image details at near atomic scales and at the time scale of chemical reactions, measurements need to be taken very quickly and over short enough time periods to understand how the process evolves. These experiments require high-quality, well-defined electron beams to generate these ultrashort x-ray pulses.

Research: To tackle this challenge, a novel scheme capable of measuring subpicosecond "bunches" of electrons with exceptional time resolution has been developed. The scheme involves modulation of the beam in perpendicular directions to maximize the measurable information from the beam including insights on beam instability, enabling the creation of x-ray beams that are both spatially and temporally coherent.

Impact: This scheme is proposed to be used to examine the fine longitudinal structure of the electron beam at the Next Linear Collider Test Accelerator at SLAC National Accelerator Laboratory. It can be incorporated easily into any advanced accelerator facility as a diagnostic tool for optimizing beam performance.

Reference

Andonian, G., et al. 2011. "Longitudinal Profile Diagnostic Scheme with Subfemtosecond Resolution for High-Brightness Electron Beams," *Physical Review Special Topics – Accelerators and Beams* **14**, 072802.



Novel Scheme Can Measure Ultrashort Electron Bunches (Subpicoseconds) with Exceptional Temporal Resolution (Hundreds of Attoseconds) and Dynamic Range. The top figures show the transverse beam profile resulting from the radiofrequency streak-camera when the beam density modulation is generated by only one laser (left) and the profile when the density modulation is generated by the interplay of two lasers in an echo-FEL scheme (right). The bottom figures show the enhanced resolution produced by adding the laser-based horizontally streaking module. [From Andonian et al. 2011.]

Energy Frontier Research Centers and Energy Innovation Hubs

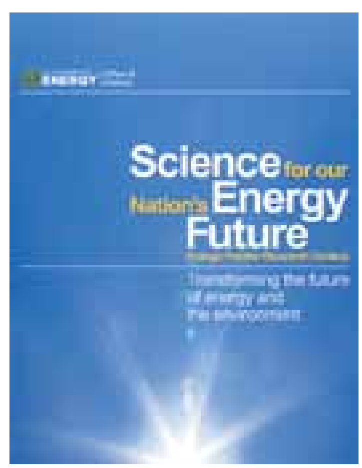
science.energy.gov/bes/efrc/
energy.gov/hubs/

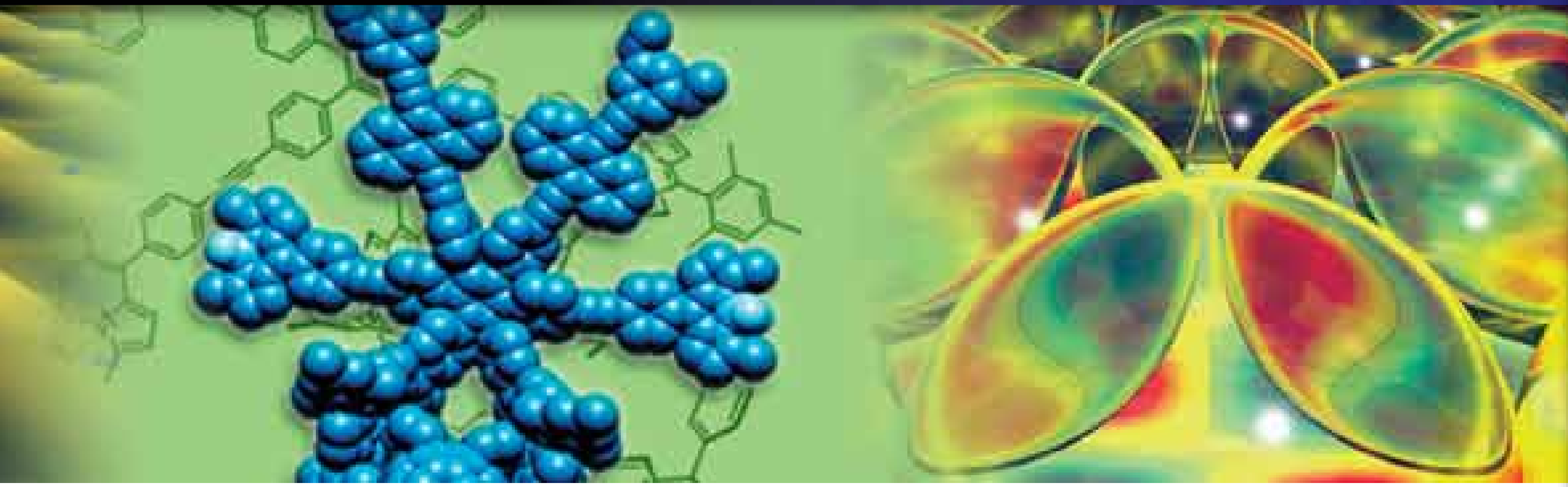
Energy Frontier Research Centers

BES established the Energy Frontier Research Centers (EFRCs) in 2009 in response to community recommendations to create science and engineering "dream teams" focused on addressing basic research challenges identified during community-based strategic planning (see Section 2, p. 5). The EFRCs support energy-relevant, basic research with a scope and complexity beyond that found in standard, single-investigator or small-group awards. The research from these multi-investigator, multidisciplinary centers will lay the groundwork for transformative energy technologies of the future. In all, there are 46 EFRC awards, 16 with full support from the American Recovery and Reinvestment Act of 2009. The remaining 30 are funded annually through BES. The EFRC program includes some 860 senior investigators, with an additional 2,000 postdoctoral associates, students, and technical staff participating on a full- or part-time basis at more than 115 institutions in 35 states and the District of Columbia.

BES provides effective EFRC oversight and management through regular and frequent interactions with the Centers, including tele-conferences, site visits, and meetings with the EFRCs as a group. To facilitate communication of research advances and technology needs and ensure that research activities are not duplicated, the EFRC management team (science.energy.gov/bes/efrc/contacts/) coordinates EFRC research within BES and with the DOE technology offices.

During the first year of operation, each EFRC was subject to an early operations and management review by an external panel. These reviews ensured that the Centers were appropriately managed and structured to achieve their research objectives. A reverse-site visit allowed EFRC investigators to present their research vision, organizational structure, and management strategies to an external review panel at a neutral site. The peer review panel consisted of reviewers with technical and managerial expertise who critically examined the vision, structure, strategy, and synergy of the EFRC, as well as utilization of the host institution's unique capabilities. Also evaluated was the ability of each EFRC to become "more than the sum of its constituent parts." BES provided formal guidance to each center both on areas of exemplary performance and on those requiring



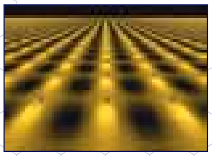
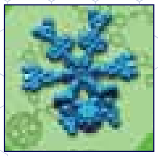
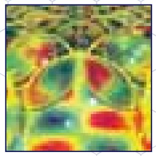


Plenary Session at the Energy Frontier Research Centers Summit and Forum. Energy Secretary Steven Chu highlighted the need to "unleash America's science and research community" to achieve energy breakthroughs in his presentation, "Energy Frontier Research Centers: Helping Win the Energy Innovation Race."

improvement. From these management reviews, a "Best Practices" Management Reference Document was prepared and distributed to all EFRCs to promote better understanding of this collaborative modality and the impact it has on scientific performance.

In May 2011, BES hosted a major scientific meeting to highlight early successes of the EFRCs and strengthen connections with the broader technical community. Titled "Science for Our Nation's Energy Future: Energy Frontier Research Centers Summit and Forum," this three-day meeting welcomed more than 1,000 of America's top energy researchers and policymakers to Washington, D.C., for a showcase of early EFRC science (see figure at left). The summit included plenary presentations by senior policymakers, and panel discussions focused on international and industrial perspectives as well as challenges for science and the imagination. All 46 EFRCs contributed a combination of technical oral and poster presentations to the forum, and the popular Life at the Frontiers of Energy Research Video Contest (www.energyfrontier.us/video-contest) was hugely successful. As a result of this meeting, the mission and early achievements of each EFRC were summarized in a publicly available, nontechnical brochure (science.energy.gov/~/media/bes/efrc/pdf/EFRC_Brochure_05132011.pdf). EFRC technical summaries also are available (science.energy.gov/~/media/bes/efrc/pdf/efrc/ALL_EFRC_technical_summaries_2011.pdf).

The EFRCs have established effective collaborations among themselves and with the larger scientific community. Activities among the centers include the EFRC Community Website (www.energyfrontier.us/), which facilitates the sharing of research highlights and meeting

information and also serves as a repository for BES communications with the centers. A grassroots effort by early career scientists working within the EFRCs has resulted in the Frontiers in Energy Research newsletter (www.energyfrontier.us/newsletter/201105/intro). This themed electronic publication contains research highlights contributed and edited quarterly by a board of early career scientists invested in the public communication of science. Communication efforts outside the EFRCs include numerous outreach and education activities geared toward the public. EFRC scientists also have organized several well-attended symposia on energy-relevant basic science at major meetings of various professional societies, including the American Chemical Society, Materials Research Society, and American Vacuum Society.

Synthetic Catalyst Outperforms Nature. Scientists at the Center for Molecular Electrocatalysis—including Morris Bullock (foreground)—have designed a hydrogen-producing catalyst that works 10 times faster than the naturally occurring enzyme that inspired its design (see Research Accomplishment on p. 42). Pictured with Bullock are researchers Jenny Yang and Kevin Welch. [Courtesy of Pacific Northwest National Laboratory.]

Selected 2011 Accomplishments

The following pages describe EFRC science that has led to synthetic catalysts that produce hydrogen much faster than natural enzymes and a new device that improves the efficiency of harvesting electricity from the sun's thermal energy. These highlights represent a small fraction of the total research output of the 46 EFRCs. Updated highlights of EFRC research can be found at science.energy.gov/bes/efrc/highlights/.

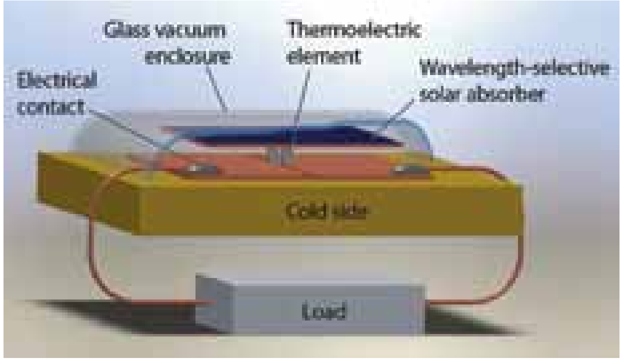
EFRC Research Accomplishment

Harvesting Electricity from the Sun's Thermal Energy

Background: When most people think of solar cells, they think of the flat, electricity-generating panels installed on the roofs of residential and commercial buildings or other surfaces. These conventional solar devices directly convert sunlight into electricity via the photovoltaic effect—a process in which photons of light strike a specially treated semiconductor material like silicon, releasing electrons that form an electrical current. A less common approach for capturing the sun's energy is solar thermal electricity generation (STEG), which converts sunlight into heat that then is used to make electricity. A key challenge for STEG has been maintaining the large temperature difference needed to drive electron flow between the hot and cold sides of a device without attaching expensive sun-tracking systems for concentrating incoming solar radiation.

Research: Researchers at the Solid-State Solar-Thermal Energy Conversion Center, an EFRC at the Massachusetts Institute of Technology, have built a new prototype that can achieve sunlight-to-electricity conversion efficiencies of about 5%—roughly eight times more efficient than previous flat-panel STEG devices. Several factors contribute to the improvements. Foremost is a better fundamental understanding of how to design thermoelectric material at the nanoscale, resulting in a semiconductor material that conducts electricity but not heat. Engineering of the prototype also is important. At the top sun-facing side of the device is a copper plate coated in a wavelength-selective, solar-absorbing material that captures almost all the sunlight striking it. As the absorbed solar radiation is converted to heat and concentrated, the top side warms to 200°C. Electrons migrate from the hot side to the cold side (20°C) below via thermoelectric elements made of the new semiconductor material, thereby producing electricity. Sealing the hot part of the device in a glass vacuum enclosure nearly eliminates heat loss because contact with air molecules is cut off. The thermoelectric material does not conduct heat well, so the temperature difference between the hot and cold sides is maintained, allowing continued operation of the device.

Impact: Although efficiency levels still need to be increased for commercial purposes, the leap in performance is a critical advance toward viable thermoelectric systems as potential complements to traditional solar cells that together can maximize the transformation of sunlight into useful energy. This research also holds promise for developing applications that capture and reuse heat lost from vehicle exhaust systems or power plants.



Key Components of a New Solar Thermoelectric Generator for Capturing the Sun's Energy. Encased in a glass vacuum tube to minimize heat loss, the solar absorber soaks up sunlight, which is converted into heat. An electrical current is produced as electrons flow from the hot solar absorber panel to the lower cold side of the device. [Image reprinted by permission from Macmillan Publishers Ltd: From Kraemer et al. 2011.]

Reference

Kraemer, D., et al. 2011. "High-Performance Flat-Panel Solar Thermoelectric Generators with High Thermal Concentration," *Nature Materials* **10**, 532–38.

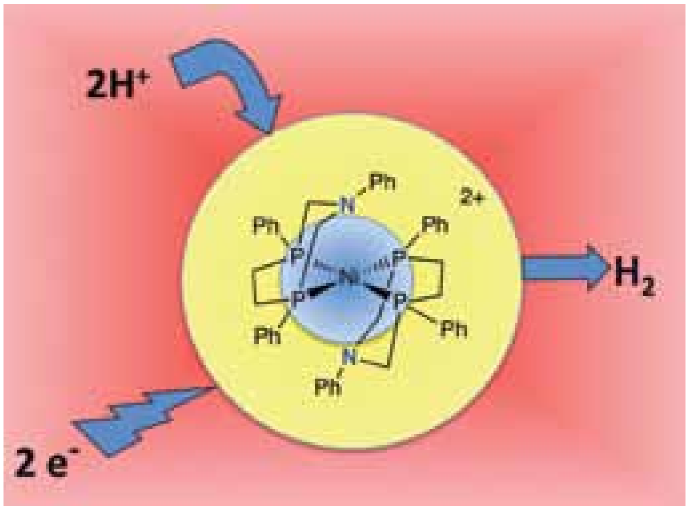
EFRC Research Accomplishment

Hydrogen-Producing Catalyst Mimics and Beats Nature

Background: The intermittent nature of sustainable energy sources, such as the sun and wind, require reliable systems for storing and delivering the electrical energy these sources generate. A tremendous amount of energy can be stored in the chemical bonds of molecules such as hydrogen (H_2). Catalysts are needed to convert electrical energy into the chemical energy of hydrogen bonds, reverse this process, and then release electricity as needed. Platinum is an excellent catalyst of these reactions, but this metal is too scarce and expensive for large-scale use. Microbes naturally produce enzymes that catalyze these reactions using Earth-abundant metals such as nickel or iron, but these enzymes often are difficult to produce in large quantities and unstable outside their native environment.

Research: Researchers at the Center for Molecular Electrocatalysis, an EFRC at Pacific Northwest National Laboratory, have used a naturally occurring enzyme to guide the design of a remarkable new catalyst for storing electrical energy by producing H_2 gas. Generating more than 100,000 hydrogen molecules per second, the synthetic catalyst works a record-breaking 10 times faster than the original enzyme. Preparing these catalysts for commercial applications will require additional research to minimize the amount of electrical energy input lost as heat during this conversion.

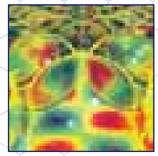
Impact: These results demonstrate how researchers can identify the most important features enhancing natural enzyme efficiency and then combine them in synthetic streamlined structures readily produced in bulk and able to withstand industrial conditions. This important breakthrough in electrocatalyst design could enable the effective interconversion of electrical and chemical energy. New low-cost electrocatalysts that are faster and more stable than natural enzymes are key to improving systems for storing, delivering, and using electricity generated from numerous sources.

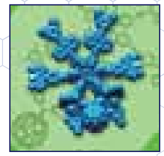


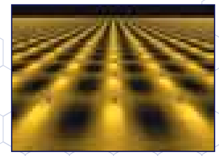
New Synthetic Catalyst for Converting Electrical Energy into Chemical Energy Stored in H_2 Molecules. The new complex uses nickel (Ni) instead of more expensive metals like platinum to set record-breaking conversion speeds that outperform natural enzymes. [Courtesy of Pacific Northwest National Laboratory.]

Reference

Helm, M. L., et al. 2011. “A Synthetic Nickel Electrocatalyst with a Turnover Frequency above 100,000 s^{-1} for H_2 Production,” *Science* **333**, 863–66.







Energy Innovation Hubs

DOE's Energy Innovation Hubs are multi-disciplinary, multi-investigator efforts aimed at overcoming critical scientific and engineering barriers to disruptive advances in energy technology. Highly integrated teams of leading scientists conduct high-risk, high-reward research in priority areas selected by DOE. BES provides the lead program management for two hubs: the existing Fuels from Sunlight and the proposed Batteries and Energy Storage hubs.

Fuels from Sunlight Hub

solarfuelshub.org

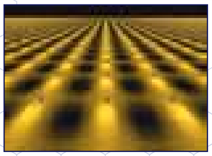
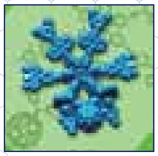
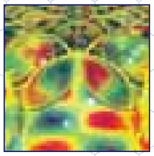
The sun is one of our most remarkable and durable energy resources. Although enough sunlight strikes Earth each hour to power human energy needs for an entire year, only a tiny fraction of this enormous energy potential is being tapped. Scientists have long sought to emulate photosynthesis, nature's system for capturing sunlight and converting it into useful chemical energy. Natural photosynthesis is an amazingly complex process requiring an intricate collection of parts working in concert to collect sunlight, turn it into electrical energy, and then use catalytic electrochemistry to convert water and carbon dioxide into complex chemicals (i.e., biomass). Decades of research have gone into understanding each part of the natural photosynthesis puzzle, and complementary studies have revealed how to build nonbiological mimics of the parts of the photosynthetic apparatus (see figure, p. 44). Researchers may now have the knowledge and ability to create a scalable, manufacturable solar-fuels generator that uses Earth-abundant elements to robustly produce fuel from sun, water, and carbon dioxide more efficiently than current crops. No direct solar-to-fuels industry exists, so the development of a viable solar-fuels generator has the potential for profound environmental and economic impacts. This development would establish U.S. global leadership in renewable energy, reduce dependence on imported oil, decrease greenhouse gas emissions, and provide new jobs in an emerging high-tech field.

In September 2010, BES initiated the Fuels from Sunlight Energy Innovation Hub as one of DOE's first three hubs. This hub, the Joint Center for Artificial Photosynthesis (JCAP), is led by the California Institute of Technology with partners at LBNL, SLAC, and the Universities of California at Irvine and San Diego.

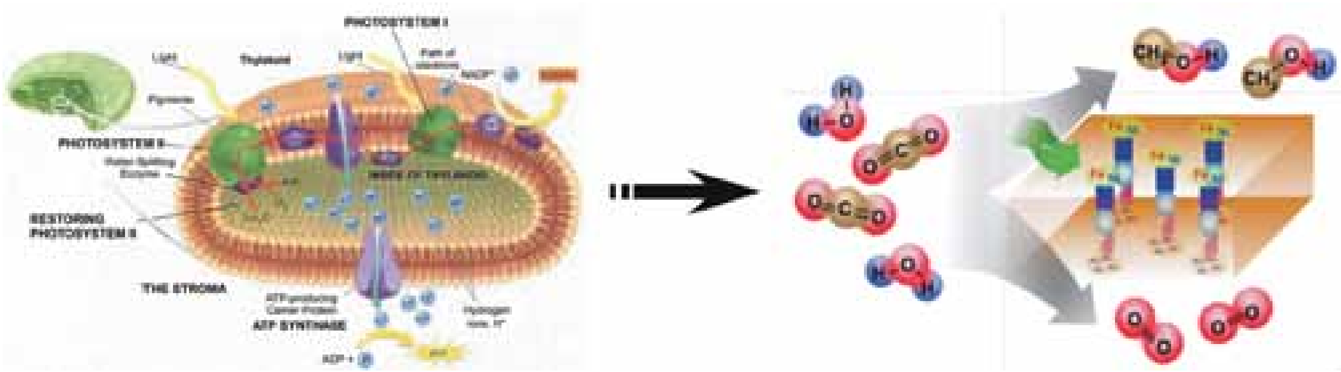
JCAP focuses specifically on the design and development of artificial photosynthetic prototypes for the commercial marketplace and is organized into two research divisions:

- **Accelerated Discovery**
- **Science-Based Scaleup**

Accelerated Discovery seeks to dramatically expand the range of available light absorbers, catalysts, membranes, and system components for creating a fully nonbiological photosynthetic system. New high-throughput systems enable millions of catalyst formulations to be investigated

Energy Frontier Research Centers and Energy Innovation Hubs

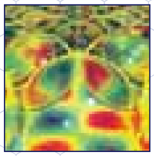
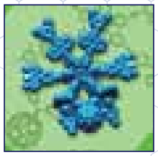
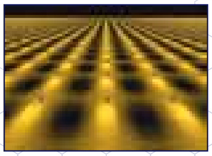


Photosynthesis   Artificial Photosynthesis

Process of Photosynthesis. Researchers from across disciplines are working together to create energy and fuels directly from sunlight by mimicking the natural process of photosynthesis in an economically viable way.

daily. Science-Based Scaleup will develop the scientific understanding and capabilities for linking together nanoscale objects to form fully functional artificial photosynthetic units and then assemble these units into systems that function on increasingly larger scales. JCAP also will (1) create enabling technologies to benchmark component combinations and optimize prototype performance; (2) develop theoretical tools for guiding pre-experiment discovery and modeling; and (3) produce public databases for mining JCAP-generated results, thereby accelerating research efforts through greater participation.

In its first full year of operation (corresponding roughly to FY 2011), JCAP was in the startup phase, establishing and equipping research facilities, hiring personnel, setting up collaborative agreements, and instituting an overall business model. Nearly 60 graduate students, postdoctoral researchers, technical and administrative staff, and principal investigators were hired in the first year. JCAP staffing will reach 150 to 180 scientists and engineers, with an additional 30 to 50 visitors from the EFRCs, other DOE programs, and foreign countries. Video and telecommunications networks now link every laboratory within the hub so that ideas and data can be freely exchanged. JCAP's management model generally follows that of a startup company, so the hub has worked diligently to establish formal mechanisms to protect intellectual property, license materials and devices, and secure confidential advice from collaborators and two external advisory boards. BES oversight of JCAP has included monthly teleconferences between JCAP management and BES staff, quarterly and annual written reports, and informal site visits. In April 2011, BES conducted a reverse-site review to assess JCAP's management and early operations. Notably, the external review panel unanimously commented on the imperative need for a Fuels from Sunlight Hub to integrate the efforts of the solar-fuels community and endorsed JCAP's bold vision and aggressive strategy to achieve its very challenging goal.

Initial research conducted by JCAP in 2011 has produced several scientific publications and invention disclosures. These include:

- Synthesis and characterization of Earth-abundant semiconductor materials with suitable band gaps for water splitting and carbon dioxide activation. Current materials use expensive or rare metals unsustainable for large-scale or long-term use.
- Design of a new high-throughput screening system for preparing and testing up to one million semiconductor formulations daily.
- Establishment of catalyst benchmarking parameters for water splitting and carbon dioxide activation studies. As evidenced by formal letters of collaboration with 20 EFRCs, the solar-fuels community recognizes JCAP for its leadership role in integrating and benchmarking discoveries made throughout the entire solar-fuels community. In September 2011, JCAP hosted the first Artificial Photosynthesis Futures Meeting to discuss opportunities for collaborative efforts, exchange of students and postdoctoral fellows, and intellectual property rights.

Batteries and Energy Storage Hub

The expanded use of renewable but intermittent energy sources (e.g., sun, wind, and tide), coupled with increasing demand for electric transportation vehicles, has greatly enhanced the need for advanced energy storage solutions. BES's proposed Batteries and Energy Storage Energy Innovation Hub would focus on understanding and overcoming critical performance limitations of electrochemical energy storage while enabling the next generation of technologies. This proposed hub would address fundamental barriers to large-scale energy storage as identified in the BES workshop report, *Basic Research Needs for Electrical Energy Storage* (science.energy.gov/~/media/bes/pdf/reports/files/ees_rpt.pdf). In 2011, primary planning activities for the Batteries and Energy Storage Hub included cross-DOE coordination efforts and discussions as well as a public information meeting. A team of program staff from BES, Energy Efficiency and Renewable Energy (EERE), and Advanced Research Projects Agency-Energy (ARPA-E) was responsible for this activity and for coordinating DOE's R&D efforts on batteries and energy storage to optimize their impact.

Selected 2011 Accomplishment

The following page highlights DOE hub research on a new approach that enhances light absorption and efficiency of solar-driven, water-splitting reactions by eliminating bubble formation.

Hub Research Accomplishment

Splitting Water Without the Bubbles

Background: A key reaction in the pursuit of an artificial photosynthetic system is photoelectrolysis, or the splitting of water by sunlight. This process usually occurs in liquid water and starts with a light absorber that captures energy from sunlight and uses a catalyst to drive the water-splitting reaction. In a liquid environment, the hydrogen and oxygen gases produced by this reaction form bubbles that refract or scatter incoming light and slow the transfer of water molecules to the catalyst. As a result, less sunlight reaches the absorber, reducing the conversion efficiency of this solar-driven process.

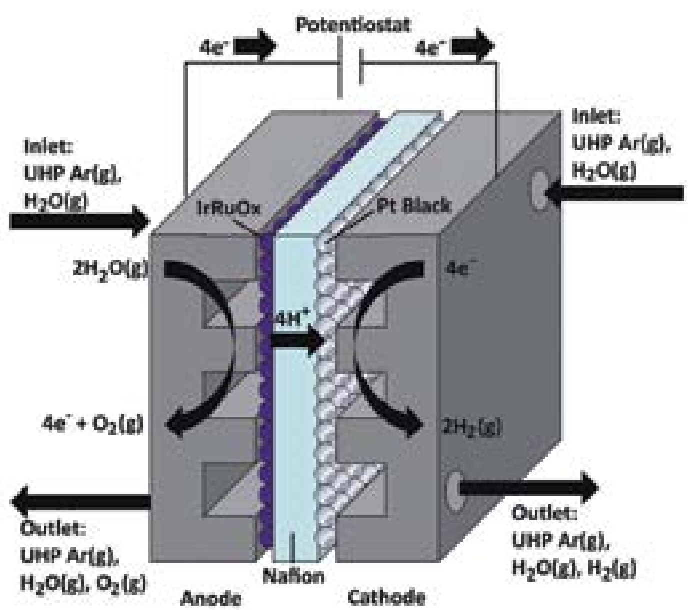
Research: To eliminate the inefficiencies due to bubble formation, researchers at the Joint Center for Artificial Photosynthesis (JCAP) have created a proton exchange membrane (PEM) electrolyzer that generates hydrogen and oxygen from water vapor instead of liquid water. Since both the reactants (water molecules) and the products are gases, no bubbles emerge to interfere with light absorption and catalyst activity. Remarkably, the new approach displays electrolysis rates higher than those of current systems using liquid water under these conditions. The results of this work provide proof-of-concept that a solar-powered PEM electrolyzer can operate with only water vapor as input, even at ambient temperatures in the absence of active heating.

Impact: Producing hydrogen by splitting water is one option for converting intermittent solar energy into chemical energy that can be stored and used as needed. By learning how to harness the sun's energy to make less complex fuel products such as hydrogen, researchers are building the body of knowledge needed to synthesize more chemically complicated solar fuels, such as natural gas or possibly even gasoline, from carbon dioxide. The fundamental insights gained from this discovery may lead to an entirely new approach to photoelectrolysis that, in turn, could alter the strategy for building a commercially viable solar-fuels generation system.

Reference

Spurgeon, J. M., and N. S. Lewis. 2011. "Proton Exchange Membrane Electrolysis Sustained by Water Vapor," *Energy & Environmental Science* **4**, 2993–98.

Caltech Invention Disclosure, "Use of Water Vapor as a Feedstock in Solar-Driven Water Splitting," J. M. Spurgeon, P. Marcus, and N. S. Lewis, filed March 2011.



Schematic Cross-Section of the Proton Exchange Membrane Electrolyzer. This new approach uses water vapor instead of liquid water as a feedstock for generating hydrogen and oxygen. [From Spurgeon and Lewis 2011.]

Acronyms

ABEL Anti-Brownian Electrokinetic

ANL Argonne National Laboratory

ARPA-E Advanced Research Projects Agency-Energy

BES Basic Energy Sciences

BESAC Basic Energy Sciences Advisory Committee

BNL Brookhaven National Laboratory

COV Committee of Visitors

CSGB Chemical Sciences, Geosciences, and Biosciences

DOE Department of Energy

EBMC Electron-Beam Microcharacterization Center

EERE Energy Efficiency and Renewable Energy

EFRC Energy Frontier Research Center

EPSCoR Experimental Program to Stimulate Competitive Research

FEL free electron laser

FOA funding opportunity announcement

GE General Electric

HFIR High Flux Isotope Reactor

JCAP Joint Center for Artificial Photosynthesis

LANL Los Alamos National Laboratory

LBNL Lawrence Berkeley National Laboratory

LCLS Linac Coherent Light Source

MSE Materials Sciences and Engineering

NSRC Nanoscale Science Research Center

ORNL Oak Ridge National Laboratory

PEM proton exchange membrane

PI principal investigator

R&D research and development

SISGR single-investigator and small-group research

SNL Sandia National Laboratories

SNS Spallation Neutron Source

STEG solar thermal electricity generation

SUF Scientific User Facilities

TEM transmission electron microscope

Images

Research Portfolio and User Facilities

P. 10–11, Row one, from left: **(1)** Molecular-beam sampling of a model flame (blue) conducted to better understand combustion chemistry [Sandia National Laboratories (SNL)]. **(2)** Schematic of an artificial photosynthetic device [Lawrence Berkeley National Laboratory (LBNL)]. **(3)** The synthesis and confinement of gas-phase nanoparticles imaged using laser ablation [Oak Ridge National Laboratory (ORNL)].

Row two, from left: **(4)** The Advanced Light Source at Lawrence Berkeley National Laboratory overlooking San Francisco Bay [LBNL]. **(5)** Schematic of a molecular framework molecule capable of capturing carbon dioxide. [University of California–Los Angeles]. **(6)** Computer model showing how nanometer-sized, atom-free regions called voids (white circles) form under irradiation and affect heat flow in nuclear fuels [Center for Materials Science of Nuclear Fuel, an Energy Frontier Research Center (EFRC)].

Row three, from left: **(7)** Three-dimensional rendering of an electron microscope image showing atoms repositioning themselves along the edge of a hole blown through a sheet of graphene, a one-atom-thick layer of carbon atoms. Raised features are adsorbed molecules [LBNL]. **(8)** Computer simulation of the spin dynamics of magnetic-moment relaxation in an iron-platinum (FePt) nanoparticle composed of 14,400 atoms embedded in an FePt random alloy matrix [ORNL]. **(9)** Simulated pattern of the diffraction of an x-ray pulse at the Linac Coherent Light Source (LCLS) from a single molecule [LCLS at SLAC National Accelerator Laboratory].

Row four, from left: **(10)** Detector array for the TOPAZ Single-Crystal Diffractometer instrument at the Spallation Neutron Source [ORNL]. **(11)** Computer simulation of diesel combustion [University of California–Davis and SNL]. **(12)** Pattern showing the tunneling potential of electrons in a network of copper oxide units (yellow) of a superconductor in the pseudogap phase [Brookhaven National Laboratory].

Materials Sciences and Engineering

P. 12–13, from left: **(13)** See image 6. **(14)** Fine white shear lines forming to prevent crack extension in a new damage-tolerant metallic glass stronger and tougher than any other known material [LBNL]. **(15)** Silicon-coated nanowires assembled using viruses [Nanostructures for Electrical Energy Storage EFRC].

Chemical Sciences, Geosciences, and Biosciences

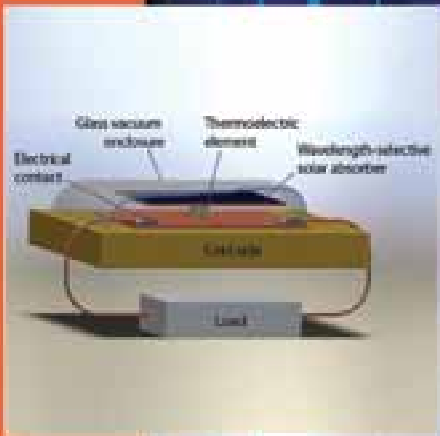
P. 20–21, from left: **(16)** Structure of Photosystem I, a complex membrane-bound molecular machine in plant cells that converts sunlight to energy during photosynthesis [Protein Data Bank (www.rcsb.org) PDB ID 3PCQ visualized using iMol]. **(17)** Three-dimensional structure of Seneca Valley Virus-001, a virus that attacks certain cancer cells without harming normal human cells [Advanced Photon Source, Argonne National Laboratory (ANL)]. **(18)** See image 7.

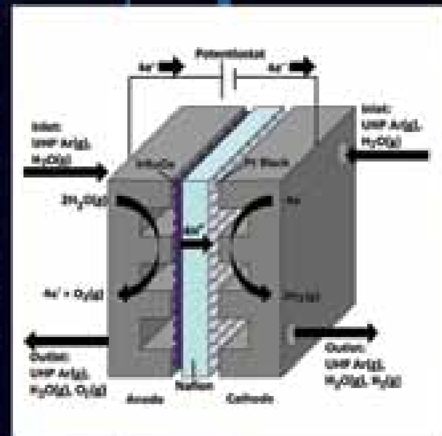
Scientific User Facilities

P. 28–29, from left: **(19)** See image 4. **(20)** Beamline scientist Robert Winarski peering at a sample inside the Hard X-Ray Nanoprobe at ANL's Center for Nanoscale Materials [ANL]. **(21)** Diffraction patterns from more than 15,000 protein nanocrystals obtained using the ultrafast, ultraintense x-rays at LCLS. [Reprinted by permission from Macmillan Publishers Ltd.: From Chapman et al. 2011.]

Energy Frontier Research Centers and Energy Innovation Hubs

P. 38–39, from left: **(22)** See image 12. **(23)** Artificial photosynthetic structure capable of enhanced light absorption [Center for Bio-Inspired Solar Fuel Production EFRC]. **(24)** Light-concentrating nanospheres that coat thin-film solar cells to boost light-harvesting efficiency [Light-Material Interactions in Energy Conversion EFRC].


Glass vacuum enclosure
Thermoelectric element
Electrical contact
Wavelength-selective solar absorber
Cold side
Load


Potentiostat
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Inlet: UHP Ar(g), $H_2O(g)$
Pt Black
Outlet: UHP Ar(g), $H_2O(g)$, $O_2(g)$
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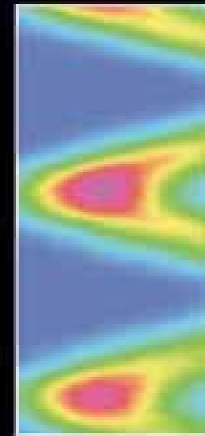
Nafion
Anode
Cathode



2011