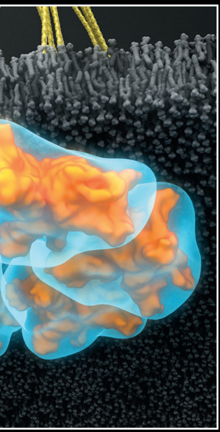
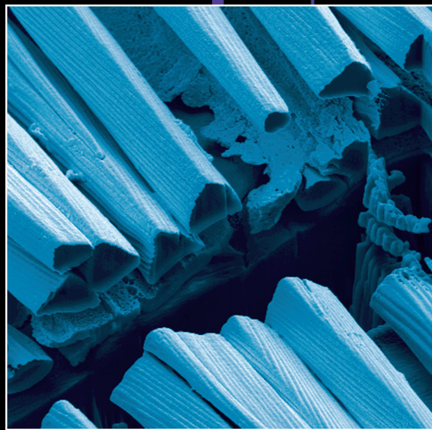
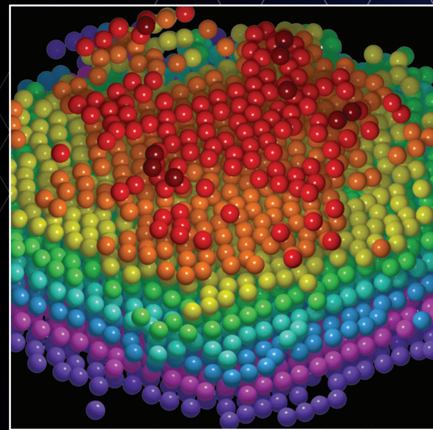
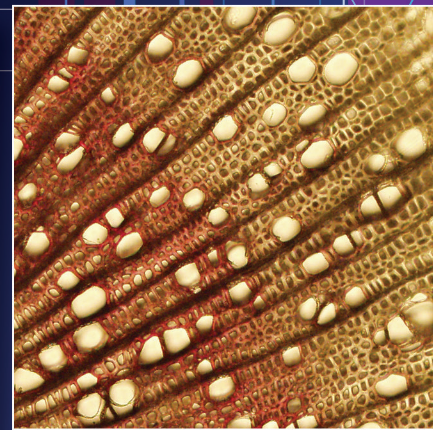

Basic Energy Sciences Summary Report

U.S. DEPARTMENT OF ENERGY | Office of Science

February 2017

Cover Images

Left to right beginning on the back cover: (1) A snapshot from time-lapse oscillatory dynamics of lipid compartments, a simple chemical analogue to a biological cell, responding to a sudden drop in concentration of dissolved sugar in the surrounding water, revealed by fluorescence microscopy. [Courtesy Atul N. Parikh in Oglecka et al. 2014. “Oscillatory phase separation in giant lipid vesicles induced by transmembrane osmotic differentials,” *eLife* **3**, e03695.] **(2)** Cross-section view of the corrugated jaws of the SLAC-RadiaBeam Technology Dechirper illuminated by an alignment laser prior to installation on the Linac Coherent Light Source (LCLS) beam line. When the jaws are closed around the electron beam, it provides a new way to manipulate both the electron energy and the transverse kick given to the head and tail of a single bunch from the accelerator, thereby allowing a whole new class of controlled, multicolor pulses to be produced at LCLS for x-ray chemical analysis with even greater precision. [Courtesy Patrick Krejcik, SLAC National Accelerator Laboratory] **(3)** Scientists track ultrafast creation of a catalyst with x-ray laser. This artistic rendering shows an iron-centered molecule that is severed by laser light (upper left). Within hundreds of femtoseconds (10^{-15} seconds), a molecule of ethanol from a solvent rushes in (bottom right) to bond with the iron-centered molecule. [Courtesy SLAC National Accelerator Laboratory] **(4)** Examining the enzyme complex that makes cellulose microfibrils. See image 7, inside back cover. **(5)** Scanning electron microscopy image of the hair coating of Saharan silver ants, which shows the triangular cross section of the hairs. See image 3, inside back cover. **(6)** The first determination of the exact three-dimensional (3D) coordinates of nine layers of tungsten atoms with a precision of 19 picometers (10^{-12} meters)—about one-third of the radius of a hydrogen atom. This image was created by utilizing the extraordinarily high resolution of the TEAM 1 microscope at Lawrence Berkeley National Laboratory. [Courtesy Mary Scott and Jianwei (John) Miao, University of California, Los Angeles] **(7)** Microscopic stem cross section of transgenic poplar with an engineered enzyme showing a normal developing vasculature but altered cell wall structure. [Courtesy Guichuan Hou, Appalachian State University]

Acronyms

2D, 3D	two, three dimensional
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
EFRC	Energy Frontier Research Center
EPSCoR	Experimental Program to Stimulate Competitive Research
FEL	free-electron laser
FOA	funding opportunity announcement
HFIR	High Flux Isotope Reactor
JCAP	Joint Center for Artificial Photosynthesis
JCESR	Joint Center for Energy Storage Research
LANL	Los Alamos National Laboratory
LBNL	Lawrence Berkeley National Laboratory
LCLS	Linac Coherent Light Source
MSE	Materials Sciences and Engineering
nm	nanometer
NSRC	Nanoscale Science Research Center
ORNL	Oak Ridge National Laboratory
PI	principal investigator
PNNL	Pacific Northwest National Laboratory
R&D	research and development
SLAC	SLAC National Accelerator Laboratory
SNL	Sandia National Laboratories
SNS	Spallation Neutron Source
SUF	Scientific User Facilities

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Acronyms list and cover image information are on inside front cover. Information on banner images for the various BES research and user facility divisions is on inside back cover.

Overview of Basic Energy Sciences

science.energy.gov/bes/

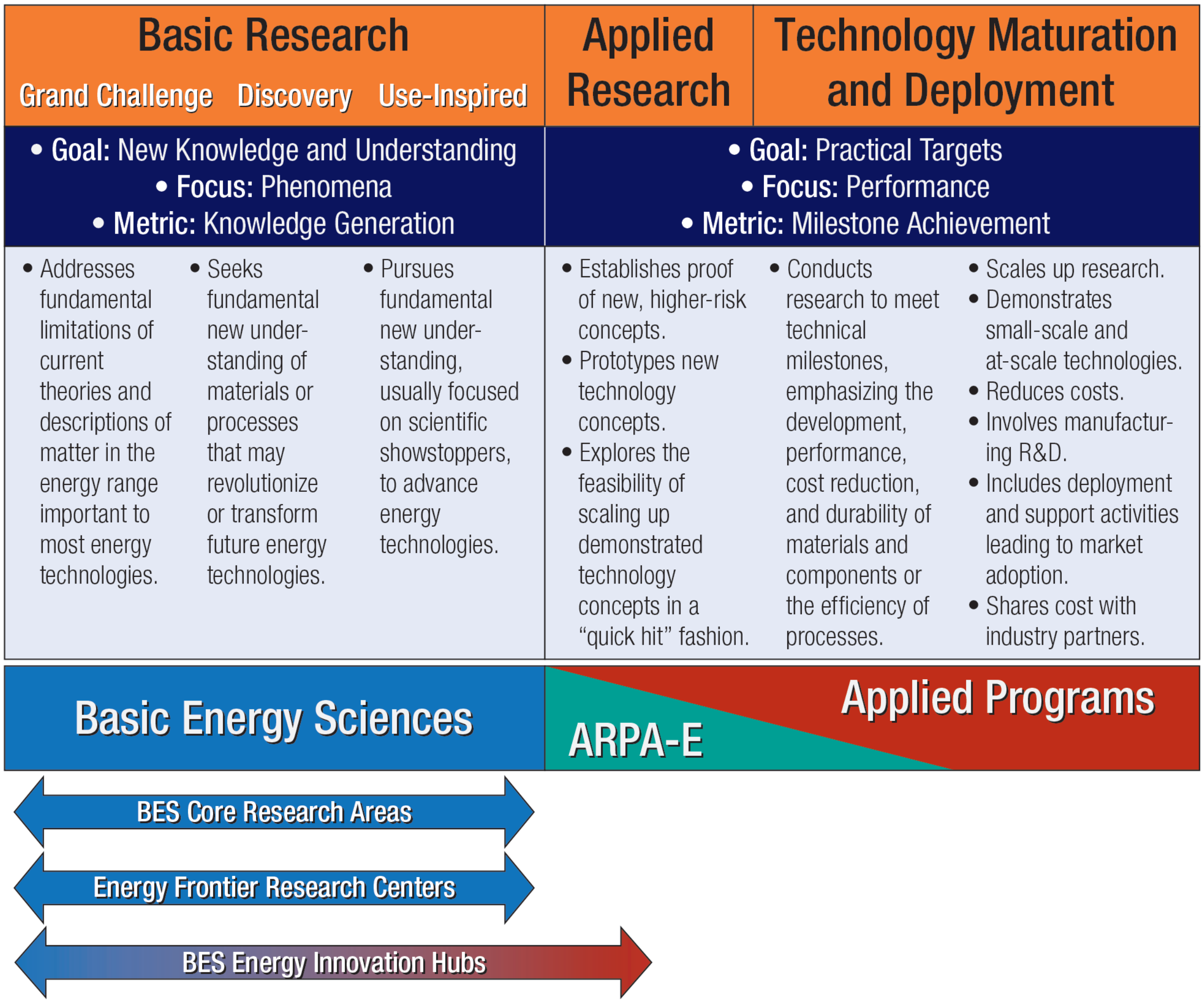
Mission and Research Portfolio

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 2016 invested approximately $717M in research, including over 1,000 core research projects, 36 Energy Frontier Research Centers (EFRCs), and two Energy Innovation Hubs. These investments span diverse sectors across the country, including research at more than 150 academic, nonprofit, and industrial institutions and at 17 DOE laboratories in 47 states and the District of Columbia. BES also supports world-class, open-access, and complementary scientific user facilities such as intense x-ray sources, neutron scattering facilities, and research centers for nanoscale science. The total annual operating budget of these facilities is about $897M.

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 scientific 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 to build basic understanding of physical and chemical phenomena. Discovery research seeks new understanding of materials or chemical processes related more directly to transformative energy technologies. Use-inspired research, while still addressing fundamental issues, is focused on 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, p. 3) must have practical, achievable targets with specific milestones and deliverables. Failure to meet an applied research goal does not present new opportunities; instead, alternative approaches must be adopted to achieve the milestone and deliver the product. Although they primarily explore basic research activities, the two Energy Innovation Hubs are unique in the BES portfolio because they intentionally integrate basic and early-stage applied research.

From single-investigator studies to large multidisciplinary research centers, BES uses several modalities to address the needs spanning its basic research activities. The university portfolio in the BES core research areas is dominated by single-investigator grants but also includes a number of group awards. Research conducted



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 bulleted column 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.

at DOE national laboratories primarily consists of large, multi-investigator projects. 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 laboratory 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 of the EFRCs. Finally, BES's Energy Innovation Hubs—the Joint Center for Artificial Photosynthesis (JCAP) and the Joint Center for Energy Storage Research (JCESR)—are very large, multidisciplinary R&D centers. Led by the California Institute of Technology in primary partnership with Lawrence Berkeley National Laboratory, JCAP brings together leading researchers in catalysis and photocatalysis to build foundational scientific approaches for converting water, carbon dioxide, and sunlight to fuels. Headquartered at Argonne National Laboratory, JCESR leverages the expertise of world-class battery researchers to overcome fundamental challenges in improving energy storage systems. The large scale of the Hubs is required to address the tremendous breadth of their scientific and engineering challenges.

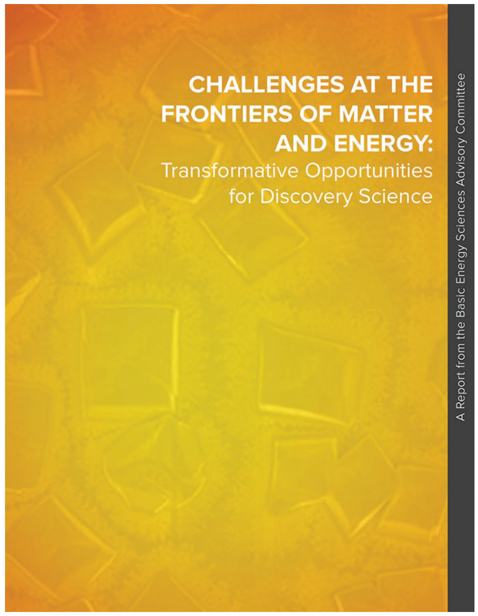
Strategic Planning and Research Community Involvement

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 Workshop Reports

For more information: science.energy.gov/bes/community-resources/reports/

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 subsequent workshops and reports in the Basic Research Needs series (see BES Workshop Reports, p. 4; science.energy.gov/bes/community-resources/reports/). This series has identified critical basic research required to advance a wide range of energy technologies. Together, these workshops attracted more than 2,000 participants from academia, DOE laboratories, and industry.



In 2007, BESAC capped the remarkable strategic planning effort represented by the initial Basic Research Needs workshops with the report, *Directing Matter and Energy: Five Challenges for Science and the Imagination*. With a focus on directing and controlling matter down to the molecular, atomic, and electronic levels, this report defined grand challenges for the research community. Most recently, BESAC completed a follow-on report, *Challenges at the Frontiers of Matter and Energy: Transformative Opportunities for Discovery Science*. This report highlights how recent discoveries made in pursuit of the original grand challenges have inspired compelling new research directions that could potentially transform the methods, reach, and impact of basic energy science.

BES and BESAC continue to engage the research community in workshops designed to address new scientific opportunities and identify critical needs for advanced energy technologies to inspire new science. BES is updating the Basic Research Needs series of reports, giving highest priority to areas with major scientific and technological advances in the last decade. New and emergent topics will also be considered for subsequent workshops.

The next section 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 portfolios follow (see p. 11). For additional information about BES research projects, see 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 EFRCs (science.energy.gov/bes/efrc/), Energy Innovation Hubs (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

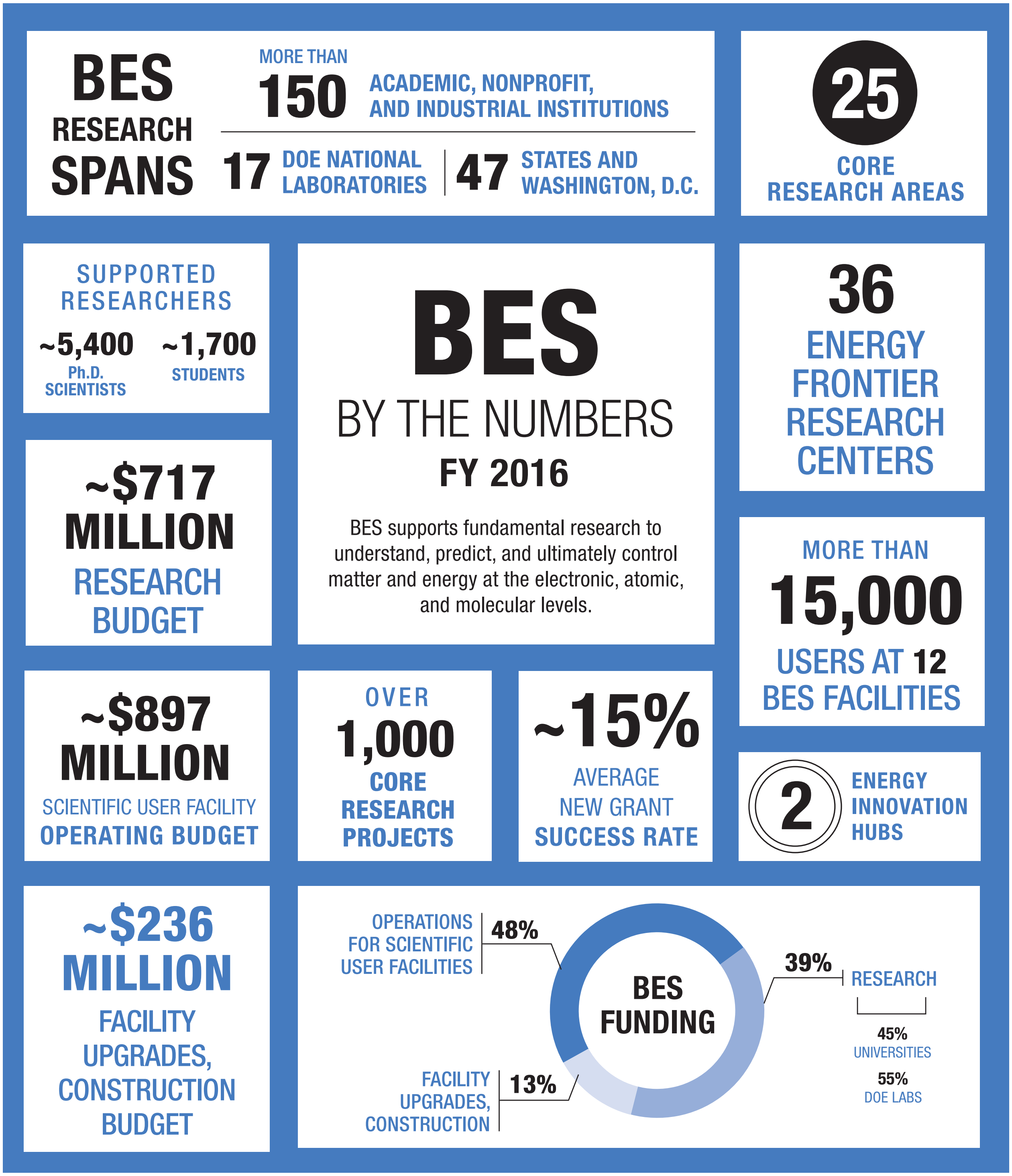
Basic Energy Sciences (BES) is organized into three divisions: Materials Sciences and Engineering (MSE); Chemical Sciences, Geosciences, and Biosciences (CSGB); and Scientific User Facilities (SUF). BES staffing includes about 35 federal program managers who oversee an annual research investment of approximately $717M and manage scientific user facility operations with an annual operating budget of about $897M (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 over 1,000 research projects organized into 25 core research areas. Each area is overseen by one or two program managers and has a clearly defined portfolio often spanning multiple scientific and engineering disciplines. In addition to the core research areas, the Energy Frontier Research Centers (EFRCs) are managed by a senior technical advisor and a committed team of BES program managers, who also have duties in the core programs. Similarly, a team of program managers oversees the Energy Innovation Hubs.

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. Major new research initiatives are solicited using special funding opportunity announcements (FOAs). For example, BES issued FOAs for EFRCs in FY 2014 and FY 2016, Ultrafast Materials and Chemical Sciences in FY 2014, and Computational Materials Sciences in FY 2015 and FY 2016. Other examples include FOAs with special requirements for both the Early Career Research Program administered annually across the DOE Office of Science and for the Experimental Program to Stimulate Competitive Research (EPSCoR) issued about once a year. Although each FOA contains specific eligibility requirements regarding teaming arrangements, FOAs (with the exception of EPSCoR) typically are broadly open to universities, nonprofits, industry, DOE laboratories, and other federal laboratories. Renewal applications for eligible BES research projects are received before the end of the grant or project period.

Prior to funding, research proposals submitted to BES are subject to rigorous merit review. The most critical aspect of this process is review by external scientific experts. This 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 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 arrive throughout the year. In such cases, an application is sent to a set of reviewers who return their individual reviews to the appropriate program manager. For large, multi-investigator activities at DOE laboratories or universities, renewal reviews may include 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. In all cases, panel reviews in BES result in individual peer review reports from each panel member; there are no "consensus" review reports.

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).

The average success rate for new applications is about 15 percent. Success rates for renewal applications vary, but 10 percent to 20 percent of all BES core research projects are typically terminated when they come up for renewal. 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 are also 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:

- Quality and quantity of research performed at the facility and impact of that research
- 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. For large awards, program managers engage in discussions with lead investigators and project directors through regularly scheduled teleconferences. Site visits are scheduled as appropriate and formal mid-term reviews are standard for awards with initial award periods over 3 years. For single-investigator awards, oversight involves email exchanges, informal teleconferences, and discussions at scientific meetings. University grants are typically funded 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 operating 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) to ensure their progress. This interaction includes teleconferences; discussions at scientific meetings; periodic (often annual) progress reports as required by the program; 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 formal 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.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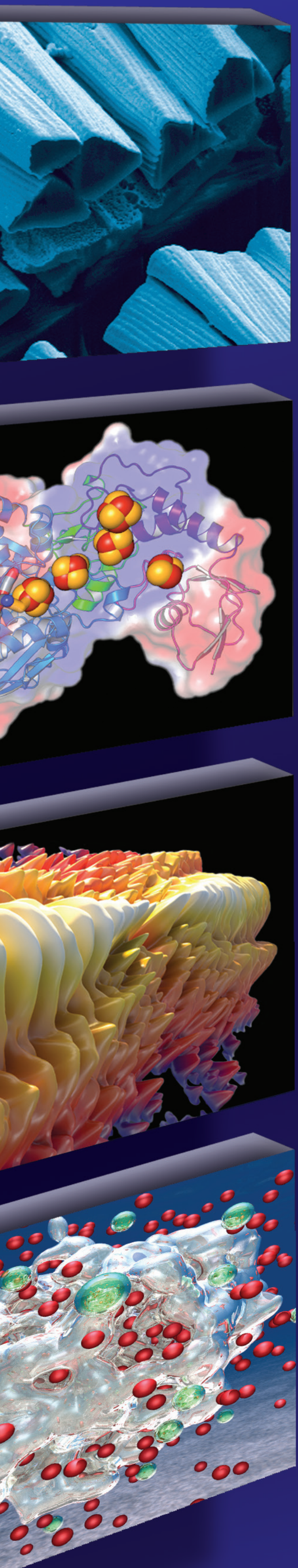
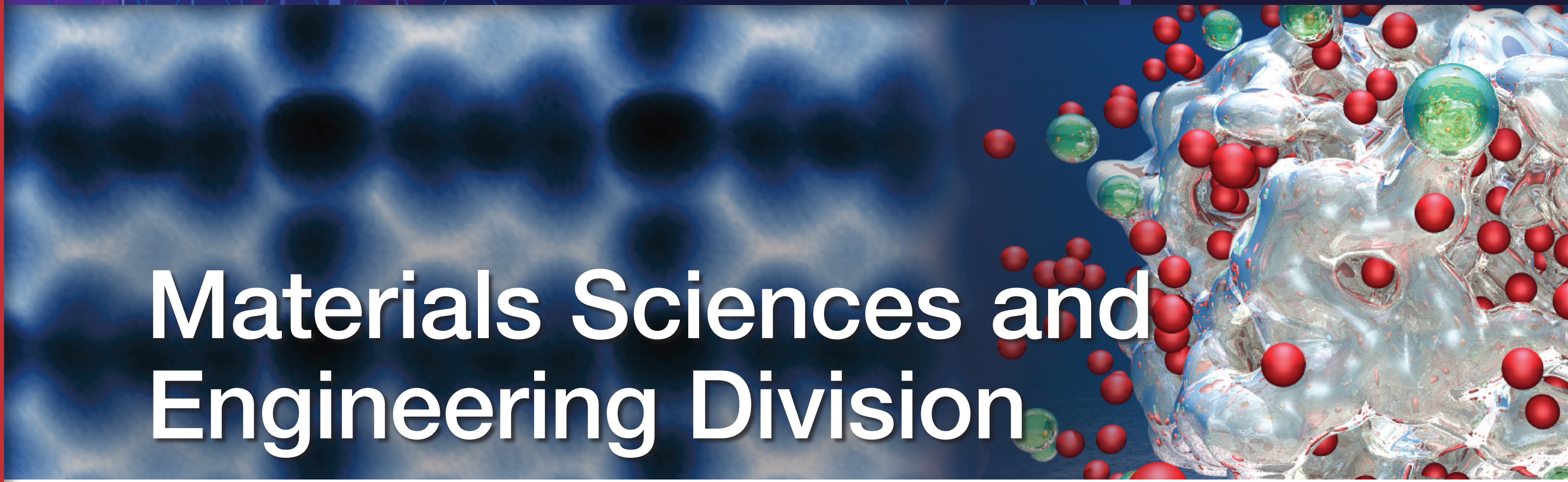


Research Portfolio and User Facilities

Basic Energy Sciences (BES) supports a variety of research disciplines including condensed matter and materials physics, chemistry, geosciences, and aspects of biosciences that seek to understand, predict, and ultimately control matter and energy at the electronic, atomic, and molecular levels. 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 a unique suite of analytical tools for studying the atomic structure and functions of complex materials and chemical transformations. This section describes the BES research portfolio and user facilities in detail.

- 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

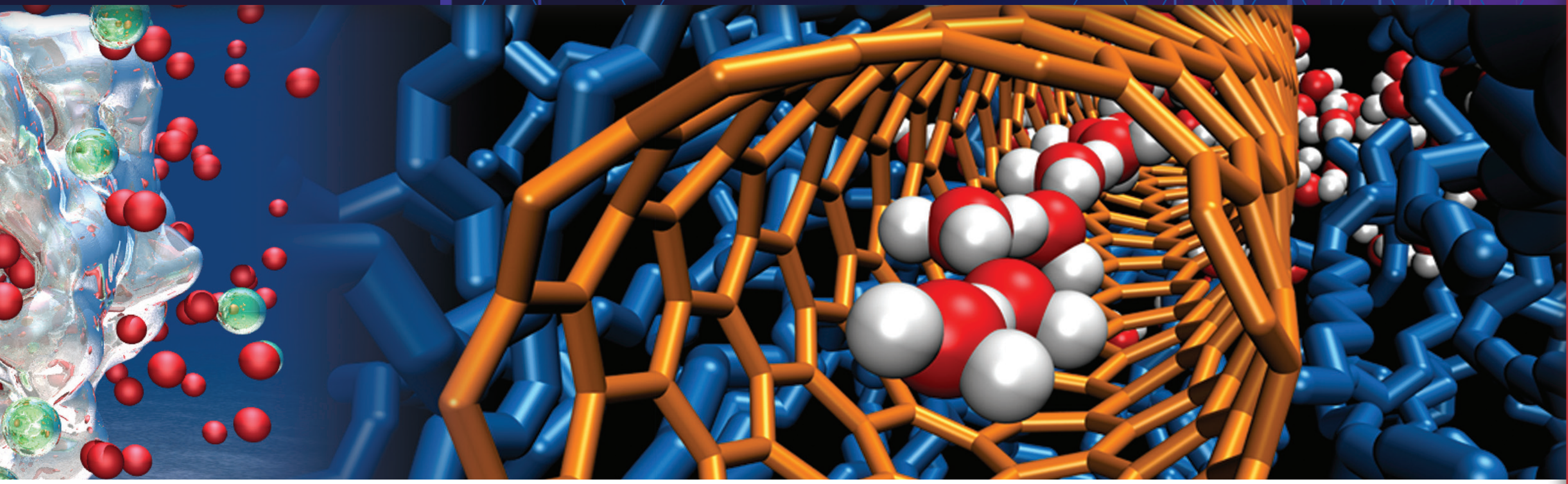
science.energy.gov/bes/mse/

Materials are critical to nearly every aspect of energy generation and use. Improving material performance is vitally important to enhancing energy efficiencies, extending infrastructure and device lifetimes, or introducing new energy technologies. The Materials Sciences and Engineering (MSE) Division within BES supports research to provide fundamental understanding of the synthesis, structure, behavior, and performance of materials. Such knowledge will offer solutions to wide-ranging energy challenges and reveal new research directions that cannot be foreseen with current materials and 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 scientific 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 next-generation batteries and fuel cells.

To accomplish these goals, MSE supports the following basic research activities:

- **Materials Discovery, Design, and Synthesis** to design and precisely assemble structures for controlling material properties and discovering new material phenomena and unprecedented functionalities.
- **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 discover new phenomena and understand the foundations of material functionality and behavior.

An overarching goal of these activities is understanding how to direct and control energy flow in material systems over different time and length scales. This knowledge will enable prediction of a material's 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 of structure and properties; 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 and bioinspired processes as new approaches to novel materials design and synthesis. The MSE Division



is also home to DOE's Experimental Program to Stimulate Competitive Research (EPSCoR). DOE EPSCoR supports research activities spanning diverse science and technology programs across all DOE offices in states that historically have received relatively less federal research funding.

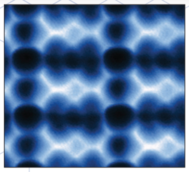
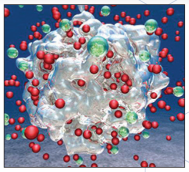
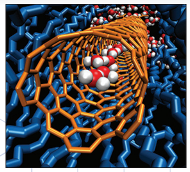
MSE Research Activities

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 our understanding of how materials form. The Materials Discovery, Design, and Synthesis activity aims to nurture 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 principles and processes 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, 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, membranes for advanced separations (of gases, ions, hazardous contaminants), and carbon capture and storage.

Synthesizing New Materials at High Pressure. Staff scientist Hong Zheng prepares to grow crystals in the extreme conditions of Argonne National Laboratory's (ANL) high-pressure floating zone furnace. The high temperatures and pressures produced by the furnace enable the discovery of new quantum materials that cannot be grown under ambient conditions. [Courtesy ANL]

Materials Chemistry and Biomolecular Materials research emphasizes chemistry- and biology-based approaches to materials synthesis and assembly. Major research directions include: (1) the controlled synthesis and assembly of functional nanoscale and mesoscale materials with desired properties; (2) control of surface and interfacial chemistry and morphology; (3) mimicry of biology's energy-efficient synthesis

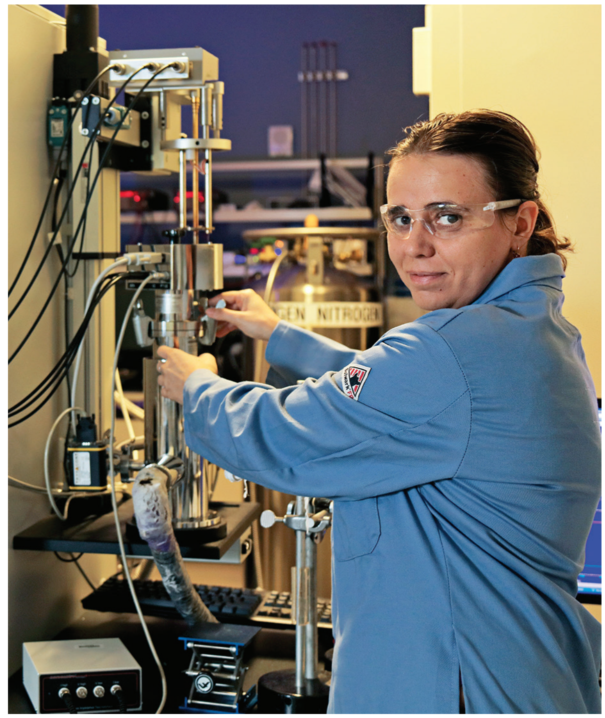




approaches to generate new, advanced materials for use under harsher, non-biological conditions; (4) development of bioinspired materials that assemble autonomously and dynamically and are adaptive, resilient, and self-repairing.

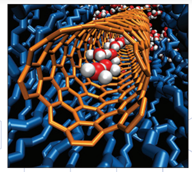
Synthesis and Processing Science supports fundamental research for developing new processing methods and techniques based on physical concepts (e.g., diffusion, nucleation, and growth) to synthesize materials with desired structures and tailored properties. An important element of this activity is the development of real-time monitoring tools, *in situ* 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 atomic-level control to advance understanding of the underlying physical mechanisms of material synthesis and processing.

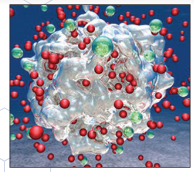
Scattering and Instrumentation Sciences

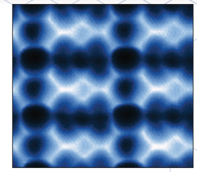
Advanced characterization tools with very high structural and temporal precision are essential for understanding, predicting, and ultimately controlling matter and energy at the level of electrons, atoms, and molecules. The Scattering and Instrumentation Sciences activity supports the science that utilizes and advances techniques and instrumentation for scattering, spectroscopy, and imaging using electrons, neutrons, and x-rays. Such tools provide detailed 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. 20). 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. 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,

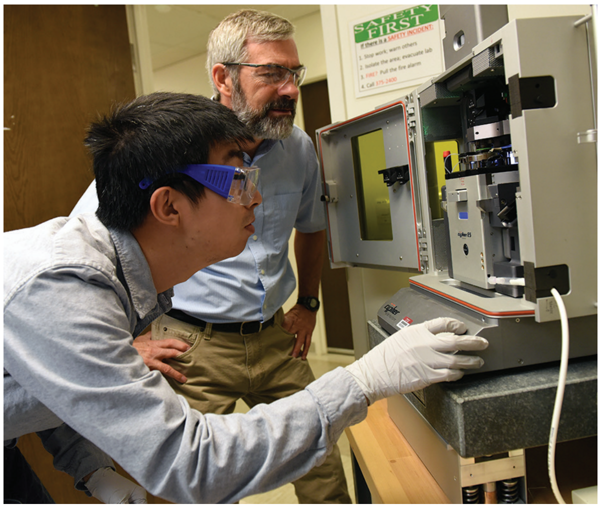


Developing Complex Materials with Enhanced Properties. Vera Bocharova, of Oak Ridge National Laboratory (ORNL), performs broadband dielectric spectroscopy, a technique capable of capturing a variety of material synthesis mechanisms and phenomena by probing temperature-dependent dynamics on time scales from 10^{-8} to 100 seconds. [Courtesy ORNL]









Understanding and Controlling Formation of Hierarchical Materials. Jim De Yoreo, Director of the Materials Synthesis and Simulations Across Scales Initiative at Pacific Northwest National Laboratory (PNNL), shown here in front of an atomic force microscope with Shuai Zhang, leads an effort to understand and control formation of hierarchical materials by combining synthesis, computer simulations, and *in situ* imaging of assembly processes in both inorganic and biomimetic systems. [Courtesy PNNL]

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. The Condensed Matter and Materials Physics activity supports experimental and theoretical research to advance current understanding of phenomena in condensed matter and to discover new phenomena. Specifically, this activity includes research on the behavior and properties of bulk, nanoscale, and mesoscale materials—whether electronic, magnetic, optical, thermal, or structural—that underpin 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 include 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 interfacial phenomena, and studies of electronic properties of materials under extreme conditions, such as ultralow temperatures and very high magnetic fields. Research relevant to energy technologies includes understanding the elementary energy conversion steps in photovoltaics and electron spin phenomena and basic semiconductor physics related to next-generation information technologies and electronics. Fundamental studies of the interactions of electrons 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 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 harsh environments.

Chemical Sciences, Geosciences, and Biosciences Division

science.energy.gov/bes/csgb/

The transformation of energy among types (e.g., optical, solar, electrical, chemical, and thermal) and the rearrangement of matter at the atomic, molecular, and nanoscales 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 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 changes and their 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:

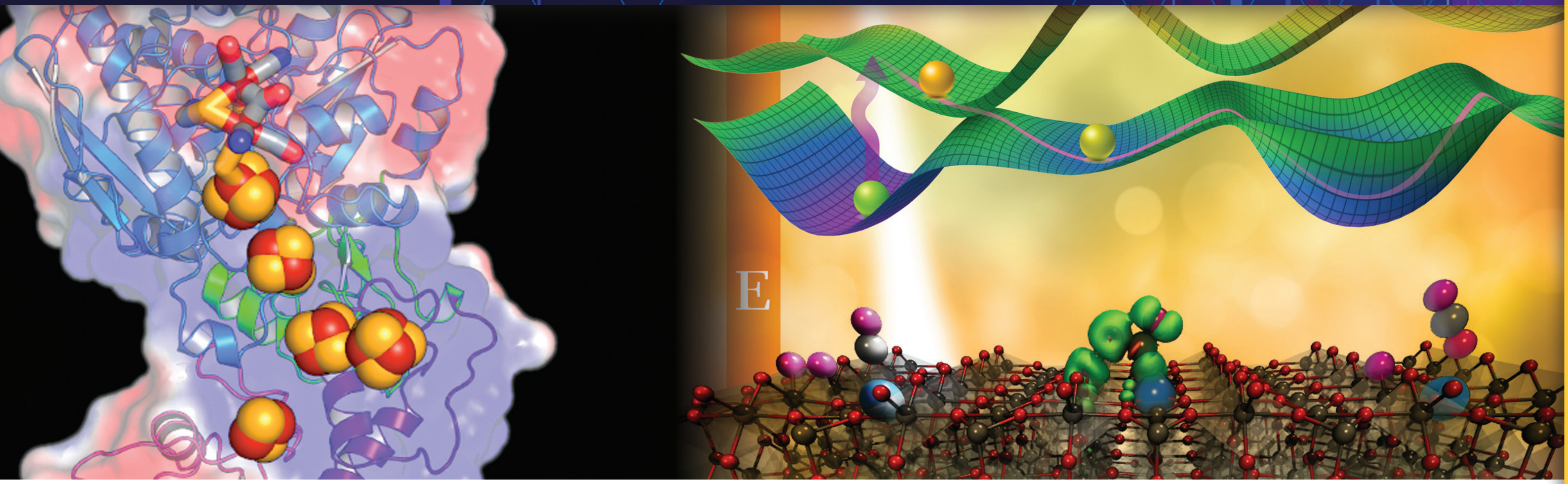
- **Fundamental Interactions**
- **Chemical Transformations**
- **Photochemistry and Biochemistry**

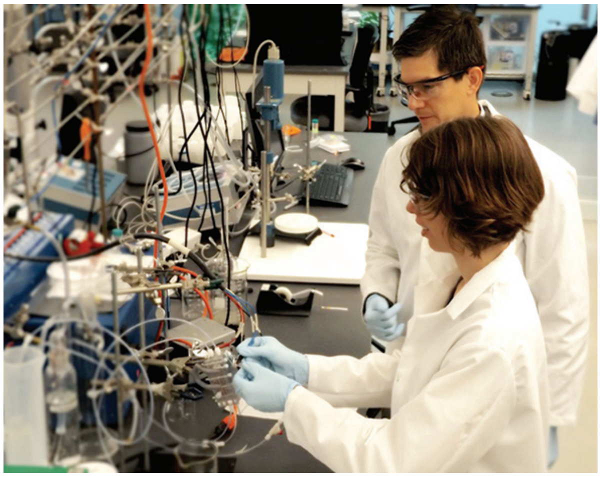
The division encourages interdisciplinary science bridging these three areas, and its activities all exhibit strong synergy among experiment, theory, and computational modeling and simulation.

CSGB Research Activities

Fundamental Interactions

This activity builds the fundamental science 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,



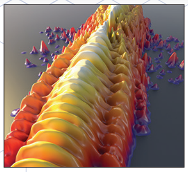
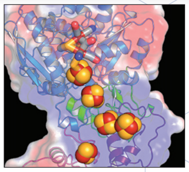
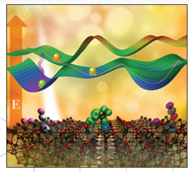


Converting Carbon Dioxide to Fuels and Chemicals. Stephanie Nitopi, a Stanford University graduate student, and Professor Thomas Jaramillo set up a carbon dioxide reduction experiment in the Jaramillo group's custom electrochemical cell. [Courtesy SLAC National Accelerator Laboratory]

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 enable chemistry by design using predictive modeling and simulation capabilities that facilitate 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.

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 exploring 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 Transformations

Research in this activity emphasizes the design, synthesis, characterization, and optimization of chemical processes underpinning current and emerging technologies that support DOE missions in energy, environment, and national security. 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 energy-production byproduct disposal.

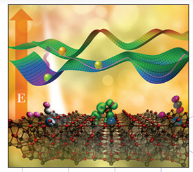
Catalysis science research in this portfolio comprises basic studies to unravel mechanisms by which catalysts accelerate and direct chemical conversions. Since many fuel and chemical production processes rely on catalysts, improving catalytic efficiency and selectivity by developing novel pathways and novel catalysts has enormous economic and energy consequences. The grand challenge is to rationally design and synthesize durable catalysts that perform as predicted from first principles, particularly for converting uncommon feedstocks into commodity and specialty chemicals and materials. To address this challenge, this activity supports efforts that integrate the most current scientific and instrumentation advances to discover how the atomistic structure of matter relates to reactivity and to control reaction products under conditions relevant to energy-related chemical processes.

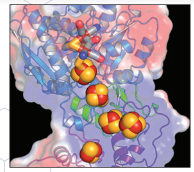
A unique focus of this portfolio is the exploration of fundamental chemistry at the extreme end of the periodic table, primarily the energy-significant actinides. Knowledge about the chemical characteristics of actinide and

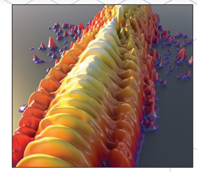
Exploring the Physical Properties of Ionic Liquids. Under the direction of chemist James Wishart (left), Brookhaven National Laboratory (BNL) summer research students prepare to measure the viscosity of an ionic liquid. Nicole Zmich (right, undergraduate), Adafih Blackburn (center, high school student), and Damian Ewko (rear, undergraduate) prepare the experiment. Ionic liquids have a number of potential uses as powerful solvents in electric battery applications and in improved processes to separate and safely dispose of nuclear waste. [Courtesy BNL]

environmentally persistent fission products under realistic conditions is essential for the development of advanced energy systems and nuclear security. Combined experimental and theoretical research is pursued on the chemical and physical properties of these elements, focusing on their solution chemistry, interfacial and solid-state bonding, and chemical reactivity.

Research in this portfolio also seeks to predictively understand the basic chemical and physical principles involved in separations systems at molecular and nanoscale dimensions. These research activities examine, for example, removal of combustion byproducts from flue stacks, separation of hydrocarbon mixtures into their







components, and extraction of heavy elements from nuclear fission products. Activities also focus on developing chemical analysis tools for the discovery and advancement of innovative solutions to DOE mission-related problems.

Geosciences research includes basic experimental and theoretical research in geochemistry and geophysics. Geochemical research emphasizes fundamental understanding of geochemical processes and reaction rates, focusing on aqueous solution chemistry, mineral-fluid interactions, and isotopic distributions and migration in natural systems. Geophysical research explores new approaches to understanding the subsurface physical properties of fluids, rocks, and minerals and develops techniques for determining such properties at a distance.

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 artificial systems. This effort is critical for effectively using our most abundant energy source—the sun. The light from the sun 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 understand how plants, algae, and photosynthetic bacteria capture sunlight and convert it into other forms of energy. Understanding this process in natural systems can provide roadmaps for creating robust artificial and biohybrid designs. Tools for the physical sciences developed elsewhere in BES are used extensively to understand different mechanisms of biological energy capture and conversion, including processes beyond primary photosynthesis (e.g., reduction of carbon and its deposition into energy-dense carbohydrates and lipids). Complementary research in organic and inorganic photochemical systems is providing important insights into energy capture and conversion in artificial photosynthetic assemblies.

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 self-repairing properties of the photosynthetic apparatus. This work provides vital scientific knowledge that forms a foundation for photosynthetic fuel production in artificial systems 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 understand the complex processes transforming energy in living systems. These studies examine a variety of energy-relevant biochemical and biophysical phenomena, including cellular regulatory processes, biopolymer structures, plant cell wall architectures, and protein active site chemistry.

Solar photochemistry research focuses on developing efficient artificial photosynthetic systems and emphasizes 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 conventional photovoltaics for renewable electricity generation. 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.

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, and Nanoscale Science Research Centers (NSRCs)—for advancing science in basic and applied energy-related disciplines. Research conducted at the facilities involves characterizing materials at the 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 have capabilities for synthesizing, fabricating, and exploring matter at the nano- to microscale.

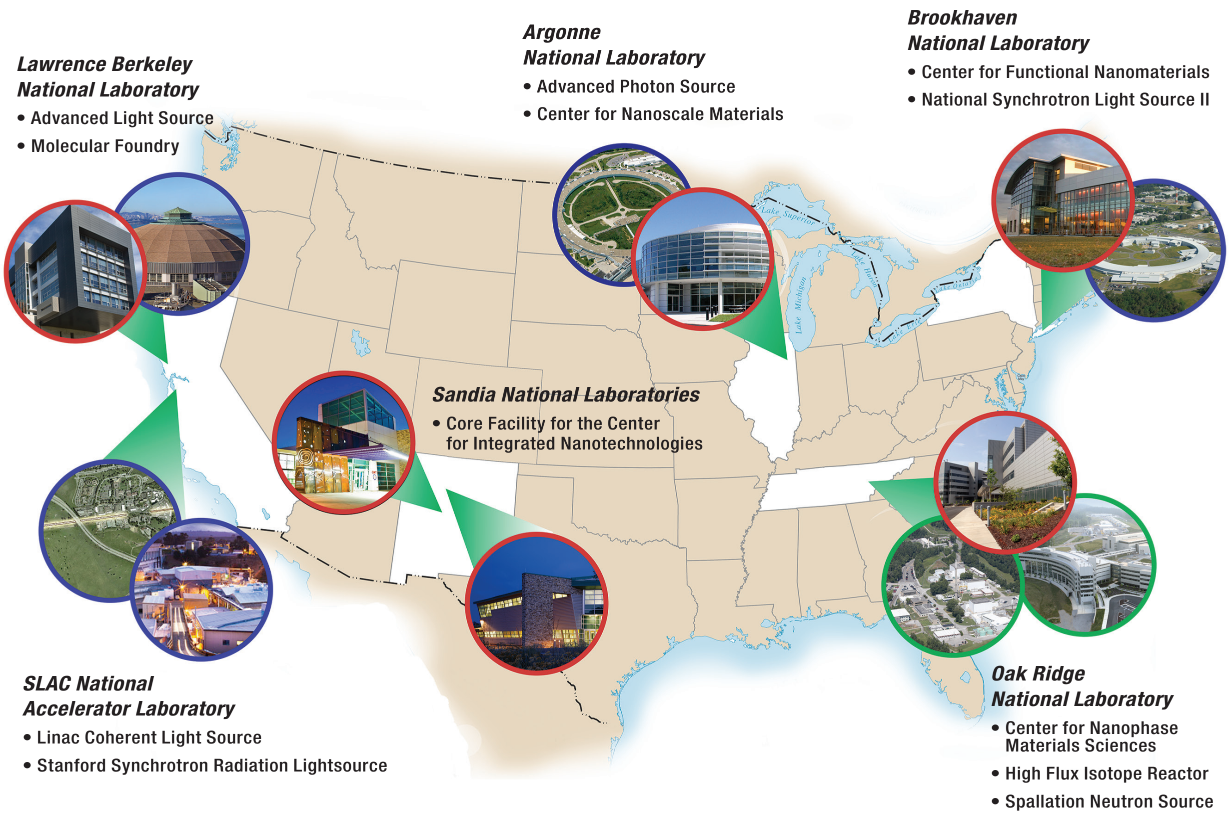
These premier scientific facilities are open access, based on acceptance of user proposals through a competitive merit review process, allowing scientists from academia, federal laboratories, and industry to use the unique capabilities and sophisticated instrumentation of the facilities. In FY 2016, the facilities supported more than 15,000 users (see table at right) from many science and technology disciplines, including chemistry, physics, geology, materials science, environmental science, biology, and a wide range of engineering fields. 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 2016

Facility	Users
X-Ray Light Sources	**11,018**
Advanced Light Source	2,317
Advanced Photon Source	5,521
Linac Coherent Light Source	1,062
National Synchrotron Light Source II	477
Stanford Synchrotron Radiation Lightsource	1,641
Neutron Scattering Facilities	**1,343**
High Flux Isotope Reactor	450
Spallation Neutron Source	893
Nanoscale Science Research Centers	**3,020**
Center for Functional Nanomaterials	505
Center for Integrated Nanotechnologies	574
Center for Nanophase Materials Sciences	601
Center for Nanoscale Materials	566
Molecular Foundry	774
Total Users in FY 2016	**15,381**

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.

BES Scientific User Facilities



Nanoscale Science Research Centers

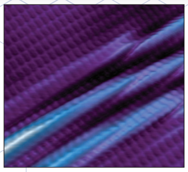
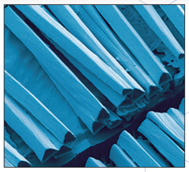
- Center for Functional Nanomaterials (BNL)
- Center for Integrated Nanotechnologies (SNL and LANL)
- Center for Nanophase Materials Sciences (ORNL)
- Center for Nanoscale Materials (ANL)
- Molecular Foundry (LBNL)

X-ray Light Sources

- Advanced Light Source (LBNL)
- Advanced Photo Source (ANL)
- Linac Coherent Light Source (SLAC)
- National Synchrotron Light Source II (BNL)
- Stanford Synchrotron Radiation Lightsource (SLAC)

Neutron Scattering Facilities

- High Flux Isotope Reactor (ORNL)
- Spallation Neutron Source (ORNL)


Scientific User Facilities

X-Ray Research

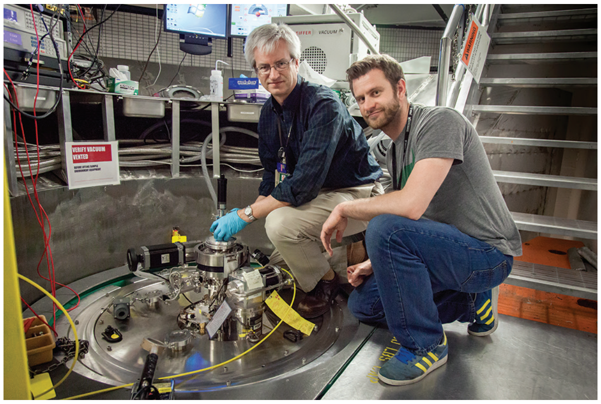
Since their discovery in 1895, x-rays have tantalized scientists and engineers with their ability to reveal the interior structures of solid objects. They also have been the principal way of determining the atomic structure of materials for nearly a century. Today's most advanced synchrotron radiation 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 from molecular to atomic levels, 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.

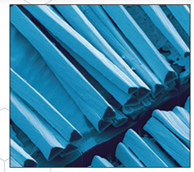
BES supports and operates five synchrotron radiation light sources. Four of these are storage ring–based sources: the Advanced Light Source at Lawrence Berkeley National Laboratory (LBNL), Advanced Photon Source at Argonne National Laboratory (ANL), National Synchrotron Light Source II at Brookhaven National Laboratory (BNL), and Stanford Synchrotron Radiation Lightsource at SLAC National Accelerator Laboratory (SLAC). The fifth light source, the Linac Coherent Light Source (LCLS) at SLAC, is an FEL. More than 11,000 scientists conduct research at these five facilities annually, making discoveries and advancing science and technology. They come from a wide range of research 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.

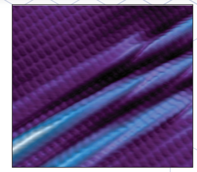
Neutron Scattering

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



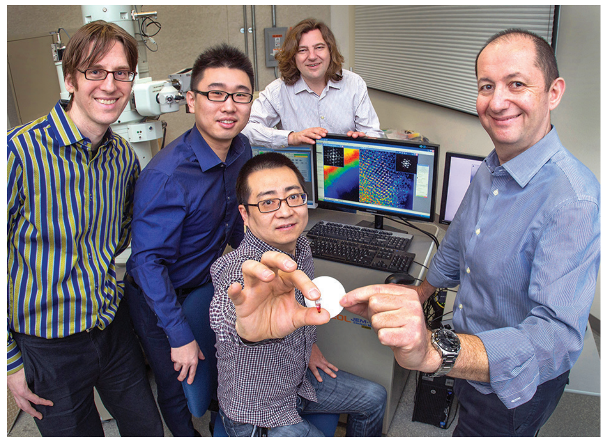
Discovering "Missing" Magnetism in Plutonium. Marc Janoschek (right) from Los Alamos National Laboratory and Doug Abernathy, instrument scientist, prepare for an experiment on plutonium using the Wide Angular-Range Chopper Spectrometer at the Spallation Neutron Source. They discovered that plutonium is magnetic but on a rapidly fluctuating time scale, resolving a decades-long controversy about this element. [Courtesy Oak Ridge National Laboratory]





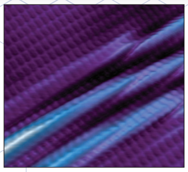
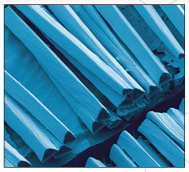
materials and functionality. With expanding applications in materials science, geology, biology, and condensed matter physics, neutron scattering is among the most powerful tools for characterizing matter to understand and develop new materials and chemistries.

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; for investigating dynamics, they have energies similar to those of atomic vibrations and magnetic excitations in materials. Neutrons have no charge, allowing them to penetrate deep into a bulk material. They are scattered equally well by both light and heavy atoms but differently by isotopes of the same element. Judicious substitution of atomic isotopes in structures thus enables characterization of specific chemical sites in, for example, organic and biological materials that would not be possible by other techniques. Neutrons also have a magnetic moment and are additionally scattered by magnetic spins on atoms in condensed matter systems, allowing a direct probe of the magnetic structure. Finally, neutron scattering cross-sections are precisely measurable on an absolute scale, facilitating straightforward comparison with theory and computational modeling.



Guiding Gold Nanoparticles to Form "Diamond" Superlattices. Using bundled strands of DNA to build tetrahedral cages, scientists at Brookhaven National Laboratory (BNL) have devised a way to trap and arrange nanoparticles in a way that mimics the crystalline structure of diamonds. The ability to build this complex yet elegant arrangement may open a path to new materials that take advantage of the optical and mechanical properties of this crystalline structure for applications such as optical transistors, color-changing materials, and lightweight yet tough materials. [Courtesy BNL]

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 isotope production for a wide range of research, technological, and medical applications and radiation damage studies important for developing materials for fusion and advanced fission reactors. Neutrons also can be generated by a proton beam from a high-power accelerator that strikes a heavy metal target. The impact of the protons on the atoms of the target produces neutrons in a process known as spallation. Utilizing an accelerator in pulse mode, the resulting neutron beam also is pulsed, enabling highly efficient time-of-flight neutron scattering techniques to study material systems. The Spallation Neutron Source (SNS) at ORNL is the world's highest-power pulsed spallation neutron source. Each year more than 1,300 scientists, engineers, and industrial researchers from around the world conduct their research at HFIR and SNS.

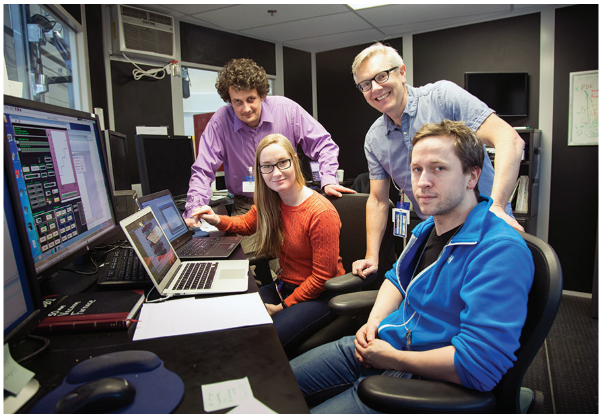




Nanoscale Science

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.

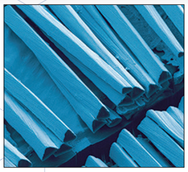
As DOE's premier user facilities for interdisciplinary nanoscale research, the NSRCs serve as the basis for a nationwide program encompassing new science, tools, and computing capabilities. The five NSRCs are the Center for Nanoscale Materials at ANL, the Center for Functional Nanomaterials at BNL, the Molecular Foundry at LBNL, the Center for Nanophase Materials Sciences at ORNL, and the Center for Integrated Nanotechnologies at Sandia National Laboratories and Los Alamos National Laboratory. Each NSRC has particular expertise and capabilities in selected scientific 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 has commercial uses across a range of industries, such as medical diagnostics and 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.



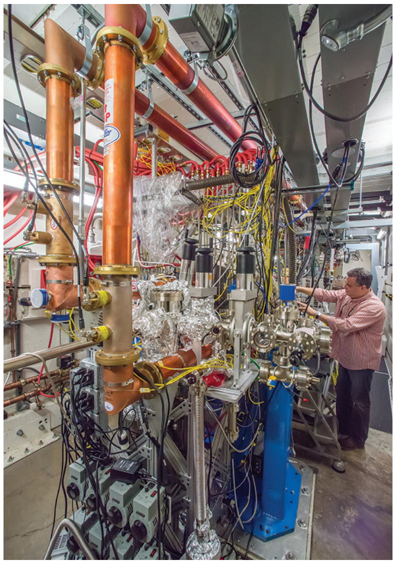
Linking Atomic Structure to Material Phase Transitions. Emil Bozin (left) from Brookhaven National Laboratory, Simon Billinge (standing right) from Columbia University, and Sandra Skaervø and Sverre Magnus Selback (seated, both from the Norwegian University of Science and Technology) examine data generated by the Nanoscale-Ordered Materials Diffractometer at the Spallation Neutron Source. The team used neutron diffraction to examine the structure of a multiferroic material as it passed through a series of structural and magnetic phase transitions. Understanding structure-transition relationships is foundational to potential applications such as memory storage devices. [Courtesy Oak Ridge National Laboratory]

As important components of the user facility portfolio, the NSRCs seek to develop next-generation electron-beam instrumentation and conduct corresponding research. The net results are an unsurpassed atomic 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.

The NSRCs are co-located with major BES user facilities for x-ray scattering, neutron scattering, and high-performance computing. These facilities complement and leverage the centers' capabilities to provide a collaborative multidisciplinary research environment for users.



Laying the Groundwork for Superior Beams. The Advanced Photo-Injector Experiment Accelerator at Lawrence Berkeley National Laboratory (LBNL) is dedicated to demonstrating the capability of an electron injector based on a novel electron gun that aims to deliver the beam quality required by next-generation free-electron laser facilities. [Courtesy LBNL]

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. This 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 cathode 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 innovative optics instrumentation and new and more efficient 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 being generated.

Energy Frontier Research Centers and Energy Innovation Hubs

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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" that address the grand challenges identified in the Basic Research Needs workshop reports (science.energy.gov/bes/community-resources/reports/, see p. 5). These workshops solicited community input to define the basic research necessary for advancing clean energy technologies including solar energy utilization, clean and efficient combustion, electrical energy storage, carbon capture and sequestration, advanced nuclear systems, catalysis, materials in extreme environments, hydrogen science, solid-state lighting, superconductivity, and environmental management.

As part of this effort, the EFRCs support energy-relevant, basic research that will lay the groundwork for the transformative energy technologies of the future. To date, BES has funded 60 EFRCs, 36 of which are currently active. The EFRC program currently supports nearly 600 senior investigators and an additional 1,635 full- or part-time postdoctoral associates, students, and technical staff at more than 110 institutions in 34 states and the District of Columbia.

The EFRCs leverage the skills and talents of multiple investigators to enable fundamental research of a scope and complexity not possible with smaller projects. As such, the EFRCs strengthen and complement the portfolio of single-investigator and small-group research projects supported within BES core research areas, as well as larger-scale research and development (R&D) activities supported by DOE's Energy Innovation Hubs including the Joint Center for Artificial Photosynthesis (JCAP) and Joint Center for Energy Storage Research (JCESR). The EFRCs bring together world-class scientists from different disciplines to tackle challenging problems in new ways; provide an environment that encourages high-risk, high-reward research; integrate synthesis, characterization, theory, and computation to accelerate the rate of scientific progress; develop innovative experimental and theoretical tools that illuminate fundamental processes in unprecedented detail; and create an enthusiastic, interdisciplinary community of energy-focused scientists.

BES provides effective oversight and management through frequent interactions with the EFRCs, including annual progress reports, monthly phone calls, site visits, and EFRC meetings. 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/contact/) coordinates EFRC research within BES and with the DOE technology offices. A 2016 Committee of Visitors Report concluded that:

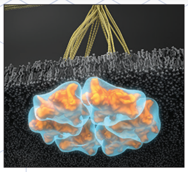
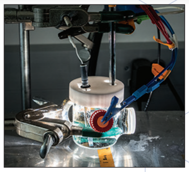
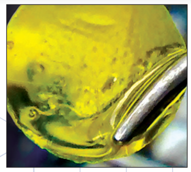
> "… the EFRC procurement processes resulted in the funding of research centers of extraordinary quality, led by internationally recognized and highly accomplished scientists, and that possess high potential for substantive scientific impact in areas relevant to the BES-DOE mission. The high quality and productivity of the centers selected for funding are clearly evident in the documentation of the initial review process and, more importantly, in the mid-term reviews of centers selected for support." (science.energy.gov/bes/besac/bes-cov/)

Similarly, a 2014 report from a Secretary of Energy Advisory Board Task Force found that:

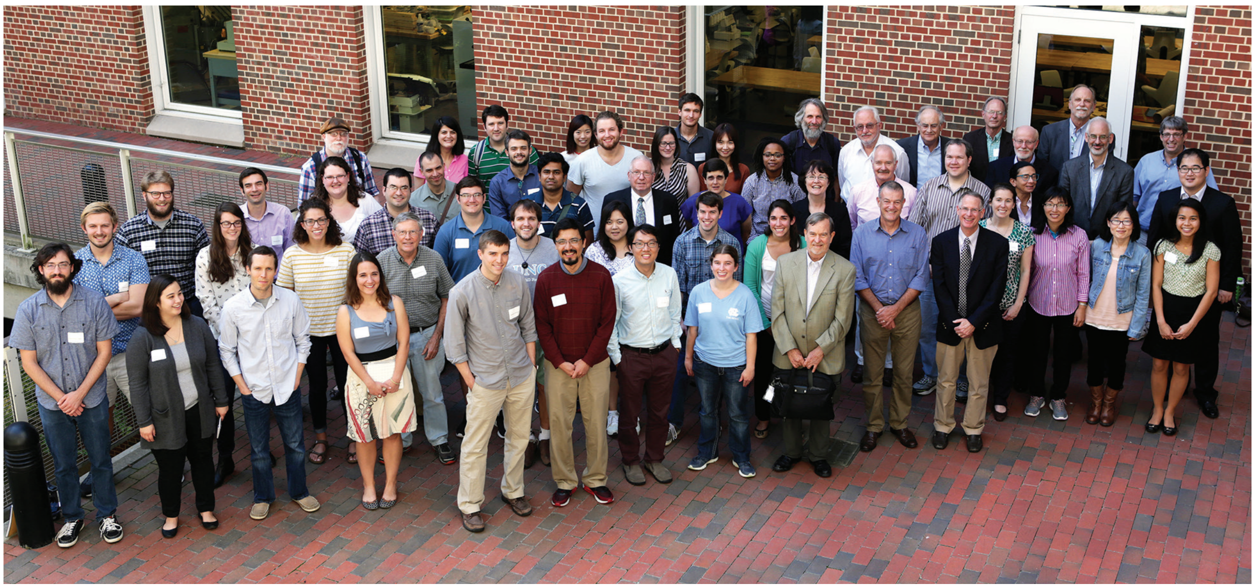
> "The EFRCs have been very successful in bringing the academic community together with the national labs to enable high-quality collaborative science with relevance to energy science and/or industry" (energy.gov/seab/downloads/report-hubs-task-force).

Plenary Session at the 2015 Energy Frontier Research Centers Principal Investigators' Meeting.

To strengthen connections within the EFRC community, BES has held biennial scientific meetings in Washington, D.C., since 2011 for EFRC researchers (more information at energyfrontier.us under Meetings). More than 500 energy researchers and policymakers typically

Energy Frontier Research Centers and Energy Innovation Hubs



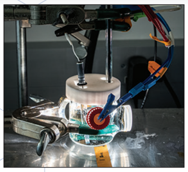
Multidisciplinary Teams for Energy-Relevant Basic Research. The Energy Frontier Research Centers (EFRCs) are large-team efforts as shown here from the all-hands meeting for the Center for Solar Fuels. Each EFRC holds an annual meeting with its team of researchers and advisory board members to review and plan research activities. [Courtesy University of North Carolina]

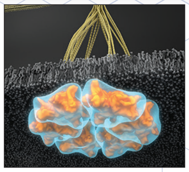
attend these meetings, which include plenary talks, scientific oral and poster presentations from all EFRCs, and a student and postdoctoral competition. In an effort to encourage the EFRCs to communicate their science and impact to a broad audience, each meeting includes an optional communications challenge:

- Life at the Frontiers of Energy Research Video Contest (energyfrontier.us/video-contest/)
- Ten Hundred and One Word Challenge (energyfrontier.us/1001-word-challenge-winners/)
- Poetry of Science Contest (energyfrontier.us/poetry-winners/)

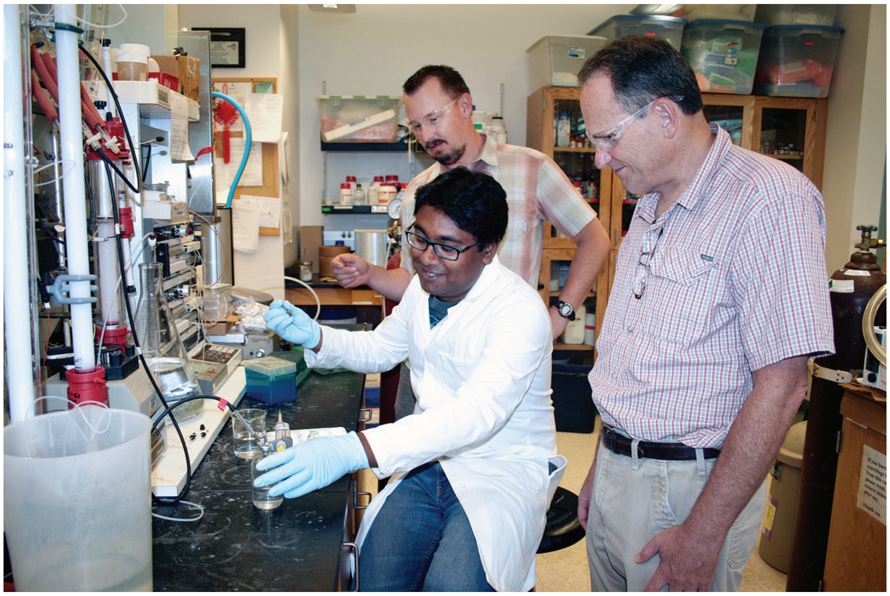
Planned for July 2017, the next Principal Investigators' meeting will be expanded to include representatives from BES's two Energy Innovation Hubs (JCAP and JCESR), as well as the recently initiated Computational Materials Sciences projects.

The EFRCs have established effective collaborations among themselves and with the larger scientific community. Activities include the EFRC Community Website (energyfrontier.us/), which facilitates the sharing of research highlights and meeting information and also serves as a repository for BES communications with the EFRCs. A grassroots effort by early-career scientists working within the EFRCs has resulted in the *Frontiers in Energy Research* newsletter (energyfrontier.us/newsletter/). 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. The EFRC Early



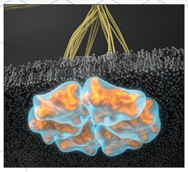
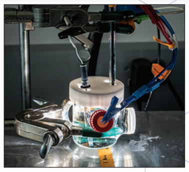
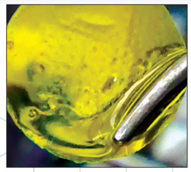


Career Network, established in 2015 and coordinated by a committee of student and postdoctoral representatives from each EFRC, plans informal gatherings at national scientific meetings and "virtual events" on topics of broad interest to students and postdocs across the EFRCs. In 2017, the Early Career Network was expanded to include representatives from the Energy Innovation Hubs and Computational Materials Sciences projects. The group is also planning activities around the 2017 Principal Investigators' Meeting. Finally, each EFRC receives technical advice from a scientific advisory board made up of science and technology leaders in their research area. Currently, there are approximately 220 scientific advisory board members, including representatives from more than 40 companies.



Directing Bacterial Conversion of a Greenhouse Gas. From left, Utah State University biochemists Sudipta Shaw, Derek Harris, and professor Lance Seefeldt conduct work as part of the Center for Biological Electron Transfer and Catalysis. The multi-institution team used a phototrophic bacterium to generate methane from carbon dioxide in one enzymatic step. [Courtesy Utah State University]

Dissemination of scientific results through peer-reviewed publications is the primary measure of EFRC success. However, the EFRCs have also impacted energy technology research and industry through licensing of patented inventions, transfer of scientific results to technology development projects, and collaborations between the EFRCs and industry. As of May 2016, EFRC researchers had authored over 7,500 peer-reviewed publications. Centers have generated nearly 500 invention disclosures, more than 380 U.S. and 250 foreign patent applications (from which over 50 patents have been issued), and at least 100 associated licenses. The EFRCs report that about 90 companies have benefited from the results of EFRC research, including a mix of startups (33 percent), mid-size companies (23 percent), and large firms (44 percent).

Energy Innovation Hubs

DOE's Energy Innovation Hubs are multidisciplinary, 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 Energy Innovation Hubs:

- **Fuels from Sunlight**
- **Batteries and Energy Storage**

Fuels from Sunlight Hub

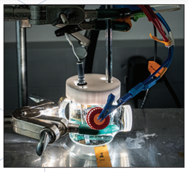
solarfuelshub.org

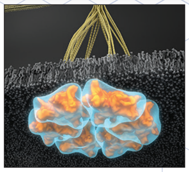
The sun is one of our most remarkable and durable energy resources. Although enough sunlight strikes Earth each hour to power human energy needs for an entire year, only a tiny fraction of this enormous energy potential is being tapped. Scientists have long sought to emulate photosynthesis, nature's 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 been devoted to 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. 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 commercially 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.

The Fuels from Sunlight Energy Innovation Hub was initiated in 2010 as one of DOE's first three Hubs and renewed for a second 5-year term in 2015. Called the Joint Center for Artificial Photosynthesis (JCAP), this Hub is led by the California Institute of Technology with partners at Lawrence Berkeley National Laboratory (LBNL), SLAC National Accelerator Laboratory, and the Universities of California at Irvine and San Diego.

Through a combination of scientific, engineering, and theoretical modeling approaches, JCAP has discovered novel materials and developed solar water-splitting systems that exhibit performance characteristics inconceivable just 5 years earlier, including complete hydrogen-generating solar fuels prototypes. JCAP is now capitalizing on its scientific achievements and sophisticated technology development from the first award period and is focusing on basic science to enable artificial photosynthetic systems that produce carbon-based fuels by consuming carbon dioxide.

The scientific barriers to reducing carbon dioxide are significant, and no currently known catalyst can achieve this conversion with high energy efficiency and selectivity. The solar hydrocarbon-based fuels resulting from this fundamental



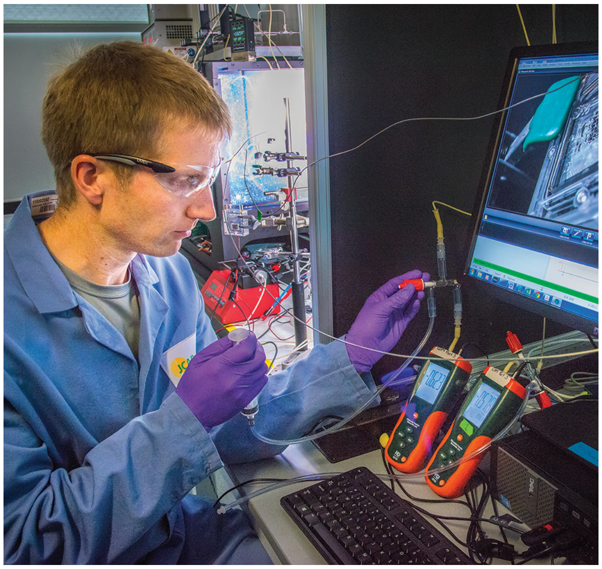


research could potentially be used with existing transportation technologies, thus providing a solar-driven alternative to current fuels.

To create the scientific foundation for a scalable technology that relies only on energy from the sun to convert carbon dioxide into renewable transportation fuels, JCAP's research objectives address three primary areas:

- **Mechanisms:** Discovery and understanding of highly selective catalytic mechanisms for carbon dioxide reduction and oxygen evolution that can operate at mild temperatures and pressures.
- **Materials:** Accelerated discovery of electrocatalytic and photoelectrocatalytic materials and useful light-absorber photoelectrodes for the selective, efficient reduction of carbon dioxide into hydrocarbon fuels.
- **Prototypes:** Demonstration, in JCAP test-bed prototypes, of the components for artificial photosynthetic carbon dioxide reduction and oxygen evolution that exceed natural photosynthesis in efficiency and rival it in selectivity.

JCAP's current staff comprises more than 150 principal investigators, postdoctoral researchers, technical and administrative staff, and graduate students. The center's research is augmented by collaborations with scientists and engineers from EFRCs, other DOE programs, and foreign countries. Video and telecommunications networks link every laboratory within JCAP so that ideas and data can be freely exchanged. JCAP's management model generally follows that of a startup company, so the center 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.

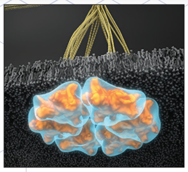
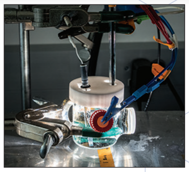
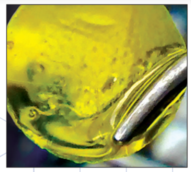


Examining a Solar Fuels Generator Prototype. JCAP scientist Karl Walczak tests and evaluates the performance of a hydrogen solar fuels generator under simulated sunlight. [Courtesy Lawrence Berkeley National Laboratory]

BES oversight of JCAP has included monthly teleconferences between JCAP management and BES staff, quarterly and annual written reports, and informal site visits.

JCAP research has produced numerous scientific publications and invention disclosures, including:

- Discovery of new methods to protect light-absorbing semiconductors from corrosion in aqueous solutions. These methods maintain excellent electrical charge conduction to the surface, enabling the use of photovoltaic materials like silicon in solar fuels generators that split water.
- Creation of an innovative high-throughput experimentation facility with a coordinated pipeline for the rapid preparation, processing,

screening, characterization, and data analysis of light absorbers and electrocatalysts. This facility enabled numerous advances, including the discovery of Earth-abundant copper and manganese vanadate complex oxides that meet highly demanding requirements for water-splitting photoanodes.

- Design, construction, and testing of versatile, fully integrated test beds to facilitate the evaluation and optimization of new components and assemblies for solar fuels generators. Several prototype designs that use only Earth-abundant catalysts have achieved safe, robust hydrogen production from sunlight and water with an efficiency over 10 percent.

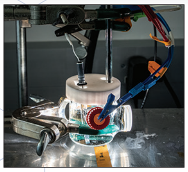
Batteries and Energy Storage Hub

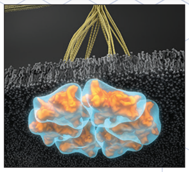
jcesr.org

Batteries and energy storage are key to the nation’s energy future. The need for a strong, secure, and resilient grid, coupled with increasing use of electric transportation vehicles, has greatly enhanced the demand for advanced energy storage solutions. Progress in battery and electrical energy storage technologies over the past decade has been impressive, aided by research sponsored by DOE’s Office of Science, Office of Energy Efficiency and Renewable Energy, Office of Electricity Delivery and Energy Reliability, and, most recently, Advanced Research Projects Agency-Energy (ARPA-E). However, extensive scientific hurdles must be overcome to define a route to revolutionary, next-generation technology solutions. The Hub concept integrates individual efforts into a cross-disciplinary R&D program that spans scientific exploration of new materials, electrochemistry, and system designs to leap beyond existing technology. Success means translating impactful scientific results into innovations that overcome current technical limits for electrochemical energy storage to the point that the risk level is low enough for industry to develop and deploy these new advances into the marketplace.

The Batteries and Energy Storage Hub was awarded in November 2012 to the Joint Center for Energy Storage Research (JCESR), one of four Energy Innovation Hubs currently supported by DOE. JCESR is led by Argonne National Laboratory (ANL) in partnership with four other DOE national laboratories, 10 universities, and five private firms. Joining ANL on the JCESR team are Lawrence Berkeley National Laboratory, Pacific Northwest National Laboratory, Sandia National Laboratories, and SLAC National Accelerator Laboratory. Partner universities include Harvard University, Massachusetts Institute of Technology, Northwestern University, Notre Dame University, University of Chicago, University of Illinois at Chicago, University of Illinois at Urbana-Champaign, University of Michigan, University of Utah, and University of Waterloo. Private firms contributing to the effort are Dow Chemical Co.; Applied Materials, Inc.; Johnson Controls, Inc.; Clean Energy Trust; and United Research Technology Center.

JCESR’s core task is basic research to create game-changing, next-generation battery technologies, and its overarching strategy is to use new nanoscience tools that allow scientists to observe, characterize, and control matter down to the atomic and molecular scales. This enhanced ability to understand materials and chemical processes at a fundamental level is enabling innovation in electrical energy storage. By integrating discovery science with novel battery designs and research-stage, pre-commercial prototyping



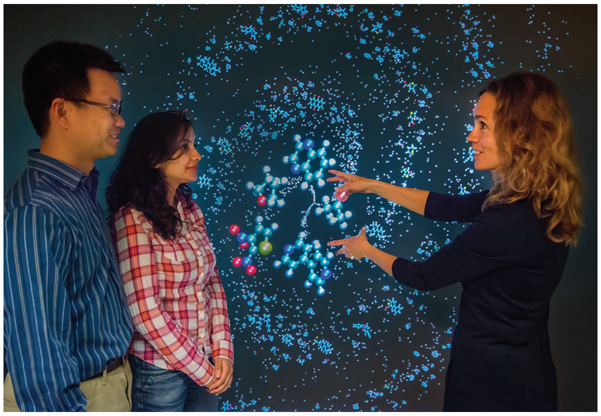


in one interactive organization, JCESR's results are accelerating scientific advances to understand and provide routes to resolve technological problems. The center's goal is to demonstrate scientific advances in research prototypes whose performance indicates that scale up by industry will result in commercial batteries that are five times more powerful and five times cheaper. Industrial partners help guide JCESR's efforts to ensure that the research retains awareness of practical concerns that will be critical to competitiveness in the marketplace.

JCESR's discovery science activities are motivated by three primary technical challenges related to the next generation of rechargeable batteries beyond lithium ion:

- **Store energy in liquids for the grid:** Replace solid battery electrodes with energy-dense liquids that charge and discharge as they flow through the battery.
- **Store energy in chemical bonds:** Discover and stabilize new materials that store and release energy by making and breaking chemical bonds.
- **Increase energy storage capacity:** Create high-capacity, high-voltage batteries using doubly or triply charged ions, such as magnesium or aluminum, rather than the singly charged lithium ion.

JCESR's advanced computational tools are key to streamlining next-generation materials discovery and guiding battery design and development. Materials genome techniques are being used to discover and evaluate tens of thousands of advanced battery materials. Technoeconomic modeling translates these materials discoveries to systems-level operation, projects the performance and cost of candidate battery systems before they are prototyped.

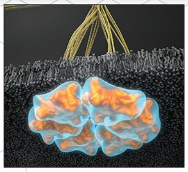


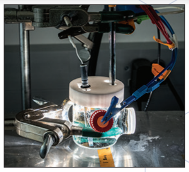
Accelerating Discovery of New Electrolytes for Batteries. Kristin Persson (right), Nav Nidhi Rajput, and Xiaohui Qu (left) work with a three-dimensional visualization of molecular interactions simulated as part of JCESR's Electrolyte Genome, a computational tool that rapidly screens thousands of molecules for desirable properties. [Courtesy Lawrence Berkeley National Laboratory]

With more than 250 published scientific journal articles, JCESR is well on its way to providing the energy storage research community a library of fundamental scientific knowledge for batteries beyond lithium ion. JCESR publicly released a database of its simulated material properties in May 2016, including 1,500 compounds investigated for multivalent intercalation electrodes and 21,000 organic molecules relevant for liquid electrolytes. Along with the database, JCESR made available a number of data analysis tools to enable discovery of systematic trends in electrochemical behavior.

Significant results from published JCESR research include:

- Developed and studied a series of novel molecular, oligomeric, and polymeric redox materials for use with a size-selective porous membrane in a flow battery for grid applications. The membrane was specially developed





by JCESR to keep materials separated in a flow battery configuration.

- Developed an electron microscopy technique that enables researchers to see what is happening at the nanoscale when a small battery cell undergoes repeated charge-discharge cycles. Using this technique, JCESR obtained the first visual evidence of the initial stages of the formation of unwanted lithium dendrites—microscopic, pin-like fibers that limit the lifetime and safety of rechargeable lithium batteries.
- Developed a computer model able to project future performance and manufacturing cost of beyond-lithium-ion battery systems and applied it to candidate batteries for transportation and grid applications. In a series of papers, the JCESR team reported application of this model to candidates from all three of JCESR's core scientific challenges. These models are broadly available to the community as a research tool.

In addition to journal publications and the more than 20,000 material properties calculations that have been released to the public, the JCESR team has produced over 50 invention disclosures and has filed more than 25 patent applications.

Images

Research Portfolio and User Facilities, pp. 10–11

Row one, from left: (1) Atomic-resolution topographic rendering of the borophene surface, taken in the scanning tunneling microscope. The borophene sheet forms large buckled wrinkles, as seen in the center, in response to the underlying silver crystal. These atomic-scale wrinkles may serve to steer the flow of electrons and could lead to other surprising properties. [Courtesy Center for Nanoscale Materials at Argonne National Laboratory (ANL)] **(2)** Rapid proton transport in water confined to a subnanometer carbon nanotube straw. The illustration shows one such straw (orange) embedded in a lipid membrane (blue). A very tight inner channel in the carbon nanotube squeezes water molecules (red – oxygen atoms and gray – hydrogen atoms) into a one-dimensional chain that allows for rapid proton transport—an order of magnitude faster than in bulk water. [Courtesy Y. Zhang and A. Noy, Lawrence Livermore National Laboratory] **(3)** Scanning electron microscopy image of the hair coating of Saharan silver ants, which shows the triangular cross section of the hairs. The uniquely shaped hair coating strongly reflects sunlight and efficiently dissipates heat through thermal radiation. [Courtesy Norman Nan Shi and Nanfang Yu, Columbia University]

Row two, from left: (4) Photoelectrochemical cell illuminated by a solar simulator. A bismuth vanadate thin-film electrode is being tested in an electrolyte solution to mimic conditions in an artificial photosynthesis device. [Courtesy Lawrence Berkeley National Laboratory] **(5)** Examining the enzyme complex that makes cellulose microfibrils. Center for Lignocellulose Structure and Formation. [Courtesy Nixon, B. T., et al. 2016. "Comparative Structural and Computational Analysis Supports Eighteen Cellulose Synthases in the Plant Cellulose Synthesis Complex," *Scientific Reports* **6**, 28696. DOI:10.1038/srep28696.] **(6)** National Renewable Energy Laboratory researchers demonstrate efficient hydrogen production using the hydrogenase enzyme, a well-known biocatalyst for the hydrogen evolution reaction, immobilized directly onto a nanoporous silicon (black Si) photoelectrode surface. [Reprinted with permission from Zhao, Y., et al. 2016. "Proton Reduction Using a Hydrogenase-Modified Nanoporous Black Silicon Photoelectrode," *ACS Applied Materials & Interfaces* **8**(23), 14481–87. DOI: 10.1021/acsami.6b00189. Copyright 2016 American Chemical Society.]

Row three, from left: (7) Advanced electronic structure and reaction kinetics calculations explain the rate of redox chemistry on reduced TiO_2 (rutile). Charge transfer between the surface and adsorbed O_2 enables CO oxidation only after an electronic excitation despite an apparently low thermal barrier. Similarly, CO_2 dissociation also requires additional energy from the ground-state pathway (lower band) to the excited state (higher band) to successfully skip over the humps along the way. Center for Lignocellulose Structure and Function. [Courtesy Nathan Johnson and Vassiliki-Alexandra Glezakou, Pacific Northwest National Laboratory; Yoon, Y., et al. 2015. "Impact of nonadiabatic charge transfer on the rate of redox chemistry of carbon oxides on rutile TiO_2 (110) surface," *ACS Catalysis* **5**(3), 1764–71. DOI: 10.1021/cs501873m] **(8)** An X-band radio-frequency transverse deflecting cavity (also called "XTCAV") installed downstream of the undulator at the Linac Coherent Light Source. The XTCAV produces an elongated "streak" of the electron beam and maps its duration, enabling measurements of the time-dependent free-electron laser lasing effects to be captured on every pulse in the camera image at the transverse profile monitor located at the beam dump. [Courtesy Patrick Krejcik, SLAC National Accelerator Laboratory] **(9)** Linear polarization. Electron distributions resulting from the ionization of atoms/molecules using a linearly polarized lasers exhibit complicated holograms due to interferences between electrons that rescatter off the parent ion and those that do not. [Courtesy Kapteyn-Murnane group and Brad Baxley, JILA]

Row four, from left: (10) Negatively charged molecules attract to form two-dimensional (2D) islands. Negatively charged molecules typically repel each other, but this behavior changes when molecules sit on graphene supported by an insulator. Under these conditions, charged molecules attract each other and undergo self-assembly to form 2D islands. [Courtesy Tsai, H.Z., et al. 2015. "Molecular Self-Assembly in a Poorly Screened Environment: F4TCNQ on Graphene/BN," *ACS Nano* **9**, 12168.] **(11)** Building precision nanobatteries by the billions. Nanostructures for Electrical Energy Storage. [Courtesy Liu, C., et al. 2014. "An All-in-One Nanopore Battery Array," *Nature Nanotechnology* **9**, 1031–39. DOI:10.1038/nnano.2014.247.] **(12)** Snapshot from a large quantum molecular dynamics simulation of the production of hydrogen molecules (green) from an aluminum-lithium alloy nanoparticle containing 16,661 atoms (represented by the silver contour of charge density) and dissolved charged lithium atoms (red). [Courtesy Kalia, Nakano, Vashishta, and Shimojo, University of Southern California, at the ANL IBM Blue Gene Q supercomputer with 786,432 processors.]

Materials Science and Engineering

From left, pp. 12–15: (13) See image 10, above. **(14)** See image 12, above. **(15)** See image 2, above.

Chemical Sciences, Geosciences, and Biosciences

From left, pp. 16–19: (16) See image 9, above. **(17)** See image 6, above. **(18)** See image 7, above.

Scientific User Facilities

From left, pp. 20–25: (19) See image 1, above. **(20)** See image 3, above. **(21)** See image 8, above.

Energy Frontier Research Centers and Energy Innovation Hubs

From left, pp. 26–34: (22) See image 5, above. **(23)** See image 4, above. **(24)** Scientists, guided by simulations, have made a selective membrane from a polymer with tailored microporosity for use in a flow battery. This specialized membrane greatly reduced active-material crossover, resulting in improved battery lifetime and efficiency. Reprinted with permission from C. Li, A. L. Ward, S. E. Doris, T. A. Pascal, D. Prendergast, and B. A. Helms. 2015. "Polysulfide-blocking microporous polymer membrane tailored for hybrid Li-sulfur flow batteries," *ACS Nano Letters* **15**, 5724. DOI: 10.1021/acs.nanolett.5b02078. Copyright 2015 American Chemical Society.

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