

Basic Energy Sciences Summary Report



U.S. DEPARTMENT OF
ENERGY

Office of
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Cover Images

Left to right beginning on the back cover: (1) Ferromagnetic nanostructures (scanning electron microscope image) of MnSi microcrystal grown using chemical vapor deposition. [Image courtesy Oak Ridge National Laboratory] **(2)** Hierarchically porous, graphene-based electrodes for a high-capacity lithium-air battery made of self-assembled functionalized graphene sheets. [Image courtesy Jun Liu, Pacific Northwest National Laboratory. Reprinted by permission from Xiao, J., et al. 2011. "Hierarchically Porous Graphene as a Lithium-Air Battery Electrode," *Nano Letters* **11**, 5071–78. DOI:10.1021/nl203332e. Copyright 2011: American Chemical Society.] **(3)** Calculated structure of covalently bound thiophene molecules on a methyl-terminated silicon surface. [Image courtesy Joint Center for Artificial Photosynthesis. Reprinted by permission from Yu, M., et al. 2013. "Theory of Covalent Adsorbate Frontier Orbital Energies on Functionalized Light-Absorbing Semiconductor Surfaces," *The Journal of Physical Chemistry Letters* **4**, 1701–06. DOI:10.1021/jz400601t. Copyright 2013: American Chemical Society.] **(4)** Scanning tunneling microscope image showing atomically dispersed palladium atoms on a copper surface (see p. 25). **(5)** Tell-tale trail of water's passage left by modified amino acid residues on the way to and from the active site of Photosystem II (see p. 26). **(6)** Electron microscope image depicting the emergence of silicon nanostrands from indium droplets (orange spheres) during a plasma-assisted physical vapor deposition growth process. When growth is completed, the nano silicon/indium assembly is used as negative electrodes in lithium-ion batteries. [Image courtesy Argonne National Laboratory] **(7)** Cylinder-forming, self-assembled diblock copolymers (schematic illustration; see p. 18).

Acronyms

2D, 3D	two, three dimensional	JCESR	Joint Center for Energy Storage Research
AFM	atomic force microscope	LANL	Los Alamos National Laboratory
ANL	Argonne National Laboratory	LBNL	Lawrence Berkeley National Laboratory
APS	Advanced Photon Source	LCLS	Linac Coherent Light Source
ARPA-E	Advanced Research Projects Agency-Energy	MEG	multiple exciton generation
BES	Basic Energy Sciences	MSE	Materials Sciences and Engineering
BESAC	Basic Energy Sciences Advisory Committee	nm	nanometer
BNL	Brookhaven National Laboratory	NOMAD	Nanoscale-Ordered Materials Diffractometer
CIGS	copper indium gallium(di)selenide	NSRC	Nanoscale Science Research Center
COV	Committee of Visitors	ORNL	Oak Ridge National Laboratory
CSGB	Chemical Sciences, Geosciences, and Biosciences	PI	principal investigator
DOE	Department of Energy	PNNL	Pacific Northwest National Laboratory
EBMC	Electron-Beam Microcharacterization Center	PSII	Photosystem II
EERE	Energy Efficiency and Renewable Energy	R&D	research and development
EFRC	Energy Frontier Research Center	SEM	scanning electron microscope
EPSCoR	Experimental Program to Stimulate Competitive Research	SLAC	SLAC National Accelerator Laboratory
FEL	free-electron laser	SNAP	Spallation Neutrons and Pressure (Diffractometer)
FOA	funding opportunity announcement	SNS	Spallation Neutron Source
HFIR	High Flux Isotope Reactor	SUF	Scientific User Facilities
IP	intellectual property	UIUC	University of Illinois at Urbana-Champaign
JCAP	Joint Center for Artificial Photosynthesis		

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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.

Director's Letter

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

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

BES core research areas have produced exciting discoveries along a broad spectrum of science: catalysis, superconductivity, magnetism, solar energy conversion, and many more. The Energy Frontier Research Centers completed their fourth year of operation and continue to demonstrate scientific and technological impact with over 4,000 peer-reviewed publications as of August 2013. Having completed its third year of operation, the Fuels from Sunlight Energy Innovation Hub is producing important new science toward its goal of a scalable, manufacturable solar-fuels generator that uses earth-abundant elements to robustly produce fuel from sun, water, and carbon dioxide. The Batteries and Energy Storage Energy Innovation Hub was awarded in November 2012 and focuses on understanding and overcoming critical performance limitations of electrochemical energy storage while enabling the next generation of technologies.

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

Harriet Kung

Associate Director of Science
for Basic Energy Sciences

Overview of Basic Energy Sciences

science.energy.gov/bes/

Mission and Research Portfolio

The mission of Basic Energy Sciences (BES) is to support fundamental research to understand, predict, and ultimately control matter and energy at the level of electrons, atoms, and molecules. This research provides the foundation for new energy technologies and supports Department of Energy (DOE) missions in energy, environment, and national security. To accomplish this objective, BES in 2013 invested approximately \$670M in some 1,400 core research projects, 46 Energy Frontier Research Centers (EFRCs), the Fuels from Sunlight Energy Innovation Hub, and the Batteries and Energy Storage Energy Innovation Hub. These investments span diverse sectors across the country, including research at more than 170 academic, nonprofit, and industrial institutions in all 50 states and at 15 DOE laboratories. BES also supports world-class, open-access, and complementary scientific user facilities such as intense x-ray sources, neutron scattering facilities, electron beam characterization centers, and research centers for nanoscale science. The total annual operating budget of these facilities is about \$780M.

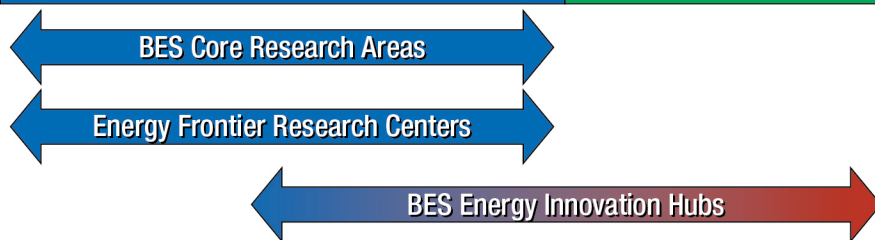
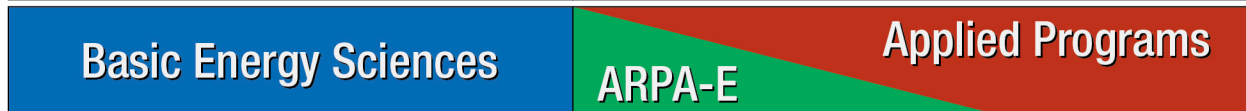
BES investments in basic science are critical for providing the technological breakthroughs needed to address the energy challenges facing the United States in the 21st century. Working closely with the research community, BES has developed a research classification that identifies the role its portfolio plays in the progression from basic research to technology maturation and deployment. The figure on p. 3 illustrates this research and development (R&D) continuum and shows that the bulk of BES's portfolio lies in three categories of basic research: grand

challenge, discovery, and use-inspired. Grand challenge research addresses the most fundamental questions about matter and energy and challenges and refines the basic understanding of physical and chemical phenomena. Discovery research seeks new understanding of materials or processes related more directly to transformative energy technologies. Use-inspired research, while still addressing fundamental issues, is directed more toward scientific “show-stoppers” 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 that can be pursued; instead, alternative approaches must be adopted to achieve the milestone and deliver the product. The two Energy Innovation Hubs are unique in the BES portfolio because they intentionally integrate both basic and 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

Basic Research			Applied Research	Technology Maturation and Deployment	
Grand Challenge Discovery Use-Inspired					
<ul style="list-style-type: none"> • Goal: New Knowledge and Understanding • Focus: Phenomena • Metric: Knowledge Generation 			<ul style="list-style-type: none"> • Goal: Practical Targets • Focus: Performance • Metric: Milestone Achievement 		
<ul style="list-style-type: none"> • Addresses fundamental limitations of current theories and descriptions of matter in the energy range important to most energy technologies. 	<ul style="list-style-type: none"> • Seeks fundamental new understanding of materials or processes that may revolutionize or transform future energy technologies. 	<ul style="list-style-type: none"> • Pursues fundamental new understanding, usually focused on scientific showstoppers, to advance energy technologies. 	<ul style="list-style-type: none"> • Establishes proof of new, higher-risk concepts. • Prototypes new technology concepts. • Explores the feasibility of scaling up demonstrated technology concepts in a “quick hit” fashion. 	<ul style="list-style-type: none"> • Conducts research to meet technical milestones, emphasizing the development, cost reduction, and durability of materials and components or the efficiency of processes. 	<ul style="list-style-type: none"> • Scales up research. Demonstrates small-scale and at-scale technology. • Reduces costs. • Involves manufacturing R&D. • Includes deployment and support activities leading to market adoption. • Shares cost with industry partners.



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

number of group awards. Research conducted at DOE national laboratories primarily consists of large, multi-investigator projects. All BES-funded DOE labs are owned by the federal government and operated by contractors who manage the laboratories and their research activities. BES requires laboratory research to be managed as synergistic, multi-investigator programs rather than collections of projects by individual investigators. This ensures that DOE laboratory projects supported by BES are structured to take unique

advantage of national 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 46 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. With approximately 50 senior investigators, JCAP is a partnership primarily

between the California Institute of Technology and DOE's Lawrence Berkeley National Laboratory, with additional university and laboratory participants. Headquartered at Argonne National Laboratory, JCESR brings together many of the world's leading battery researchers around a common objective of overcoming fundamental challenges to improving energy storage systems. The large scale of the Hubs is required to address the tremendous breadth of their scientific and engineering challenges.

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

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

Strategic Planning and Research Community Involvement

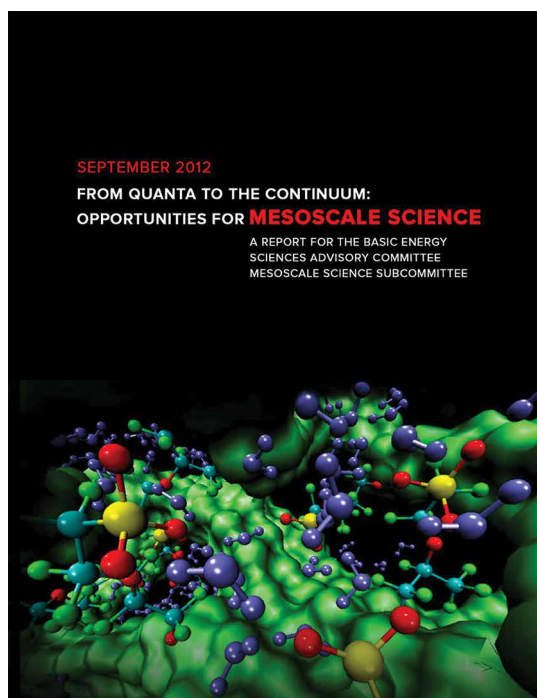
BES actively engages the research community in strategic planning. The Basic Energy Sciences Advisory Committee (BESAC) is chartered under the Federal Advisory Committee Act to advise BES on its research areas and user facilities (science.energy.gov/bes/besac/). The 2003 BESAC report, *Basic Research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

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

opportunities and identify ways that critical needs for advanced energy technologies can inspire new science (science.energy.gov/bes/news-and-resources/reports/). Most recently, BESAC completed the report *From Quanta to the Continuum: Opportunities for Mesoscale Science*. This report explores the opportunity and defines the research agenda for mesoscale science—discovering, understanding, and controlling interactions among disparate systems and phenomena to reach the full potential of materials complexity and functionality. In July 2013, BESAC also completed a report on future light sources, which included performance specifications for light-source concepts that would maximize impact on grand science challenges.

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 portfolio follow, along with representative

research accomplishments (see p. 11). Additional information about BES research projects can be found on the BES website (science.energy.gov/bes/). This site includes summary abstracts of all projects supported by BES core research areas (science.energy.gov/bes/research/) and detailed descriptions of the 46 EFRCs (science.energy.gov/bes/efrc/), the 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

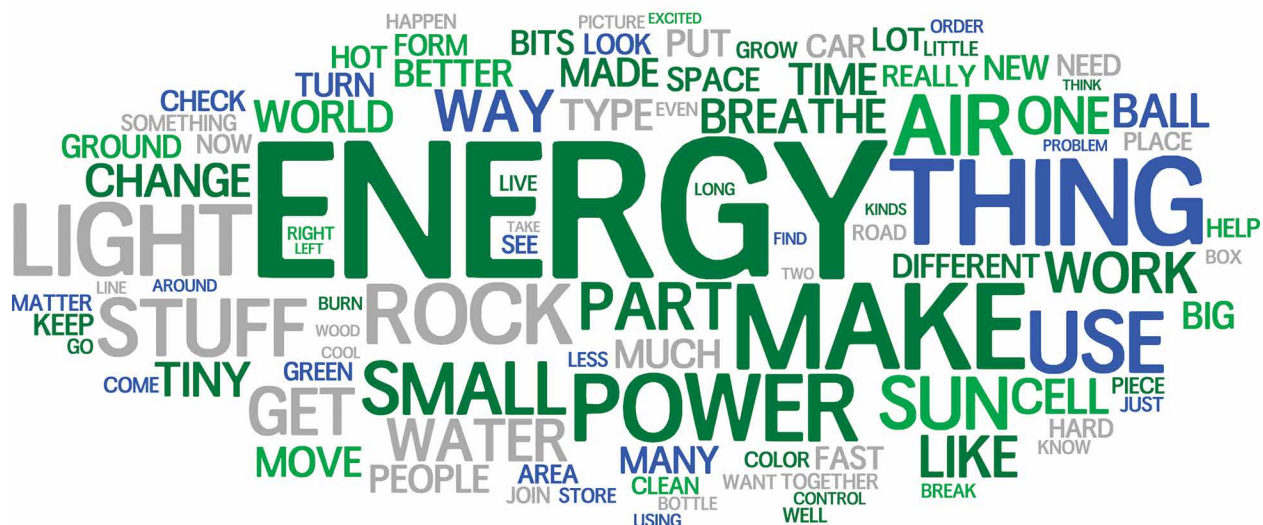
Basic Energy Sciences (BES) is organized into three divisions: Materials Sciences and Engineering (MSE); Chemical Sciences, Geosciences, and Biosciences (CSGB); and Scientific User Facilities (SUF). BES staffing includes about 35 federal program managers who oversee an annual research investment of approximately \$670M and manage scientific user facility operations with an annual operating budget of about \$780M (see current BES organization chart at science.energy.gov/~media/bes/pdf/about/BES_Org_Chart.pdf). As Ph.D. scientists, these program managers have research experience well beyond the postdoctoral level in the scientific areas covered by the portfolios they manage. Many come to BES with previous experience in scientific program or facility management at DOE laboratories or other governmental agencies.

The MSE, CSGB, and SUF divisions support about 1,400 research projects organized into 23 core research areas. Each area is overseen by one or two program managers and has a clearly defined scientific emphasis often spanning multiple scientific and engineering disciplines. In addition to the core research areas, 46 Energy Frontier Research Centers (EFRCs) are managed by a senior technical advisor and a committed team of BES program managers, most of whom also have duties in the core programs. Similarly, a team of program managers also oversees the Fuels from Sunlight and the Batteries and Energy Storage 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). Major examples include FOAs for the EFRCs in FY 2009, the Fuels from Sunlight Energy Innovation Hub in FY 2010, and the Batteries and Energy Storage Energy Innovation Hub in FY 2012. Another example is the annual FOA for the Early Career Research Program, which is administered across the DOE Office of Science and has special requirements. Although each FOA contains specific eligibility requirements regarding teaming arrangements, FOAs typically are broadly open to universities, nonprofits, industry, DOE laboratories, and other federal laboratories. Renewal applications for eligible BES research projects are received prior to 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



Engaging the Public in Understanding of BES Research. This “word cloud” is a combination of words used in the 31 entries for the “Ten Hundred and One Word Challenge” (www.energyfrontier.us/1001-word-challenge-winners), which invited the 46 Energy Frontier Research Centers (EFRCs) to represent their science in images, cartoons, photos, words, and original paintings. Entries could use only the 1,000 most commonly used words in the English language, with the addition of the one word important to the mission of DOE and each EFRC: energy.

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

BES implements peer review in several forms, optimizing this process for the type and number of research proposals under consideration. For single-investigator or small-group research in the core research areas, an individual peer review process is used to evaluate new and renewal applications, which often arrive in small numbers. In such cases, an application is sent to a set of reviewers who return their individual reviews to the appropriate program manager. For multi-investigator activities at DOE laboratories or universities, renewal reviews often are conducted by a panel of reviewers during a site visit to the host institution. These onsite reviews are

excellent ways to critically examine group synergy and use of the host institution’s unique capabilities. When onsite panel reviews are infeasible or inappropriate, BES may conduct “reverse-site visit” reviews, during which applicants present their research to a review panel at a neutral site. Finally, solicitations or expressions of interest that generate large volumes of applications require the use of review panels to effectively and efficiently complete the peer review process. These panels can be convened in person to evaluate a set of proposals or conducted “virtually” using modern communications tools. Each panel assesses a set of proposals without the applicant present.

Peer review is not the only aspect of a complete merit review process in BES. Another important component is evaluating how well the proposed research fits with a particular BES core research area or responds to the stated objectives of an FOA. These programmatic assessments are made by BES program managers, whose expertise, vision, and judgment are critically important in the development of mission-relevant research programs. Program managers combine these assessments with an analysis of the peer reviews to form a funding recommendation for the

application that then is presented to BES management for approval or rejection. BES management may request additional information or justification from the recommending program manager(s) before finalizing the funding decision(s).

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

User facilities 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

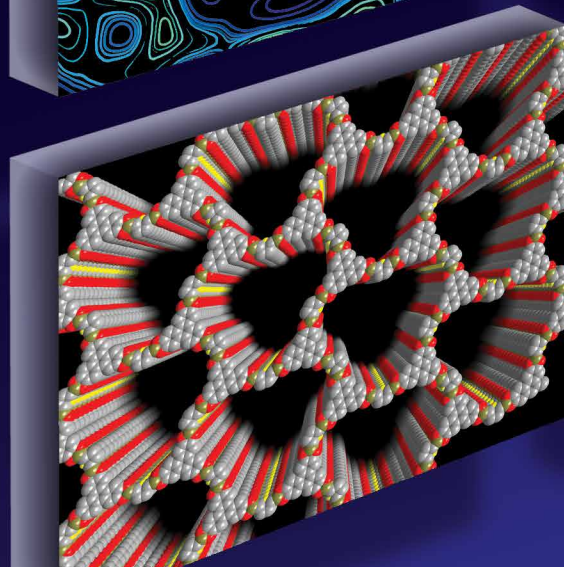
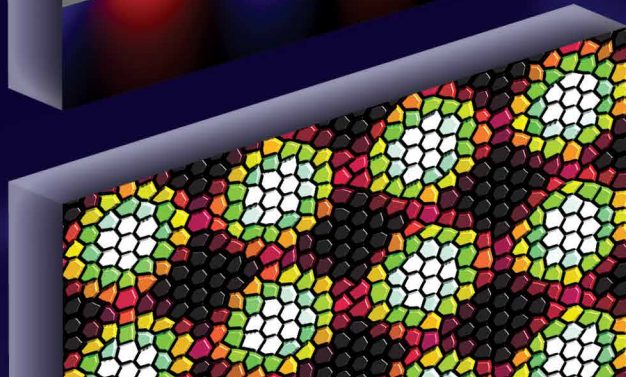
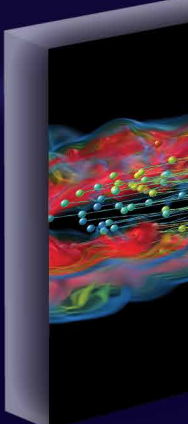
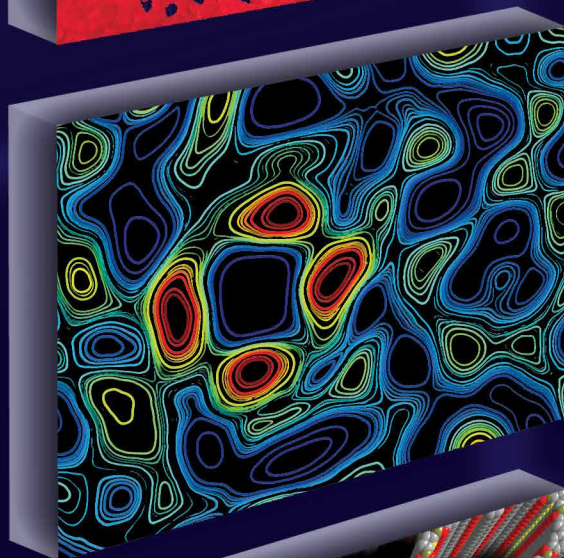
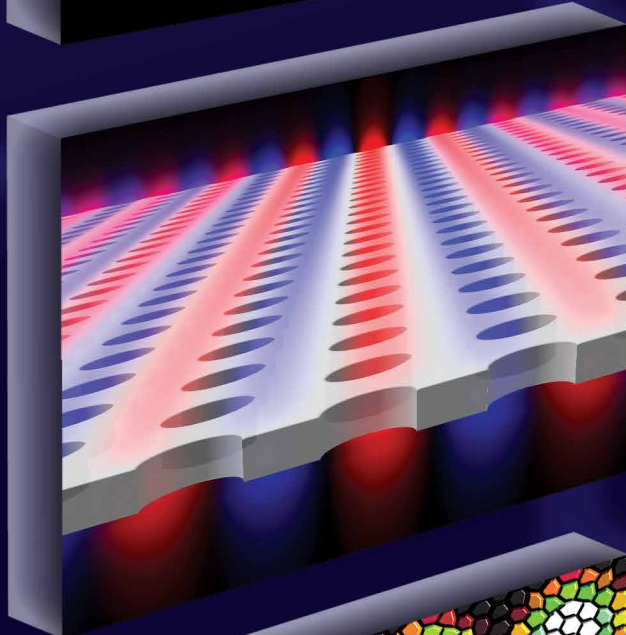
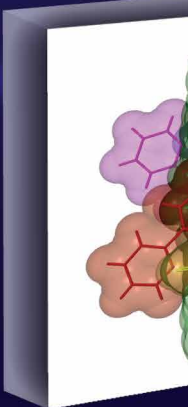
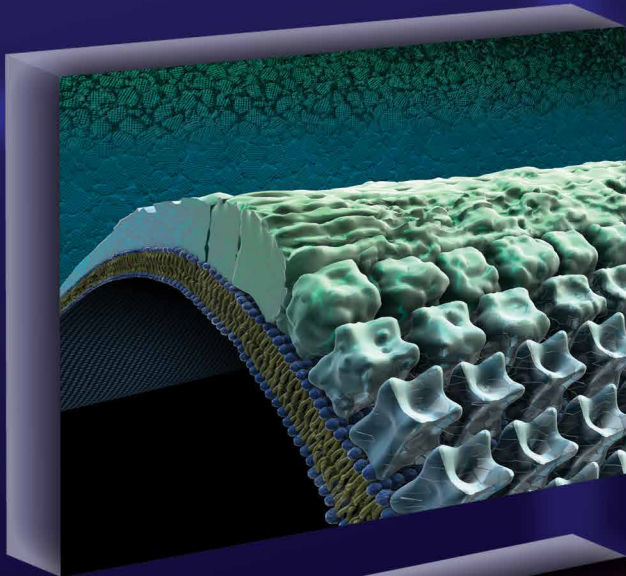
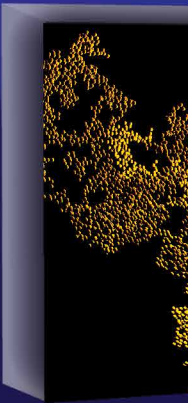
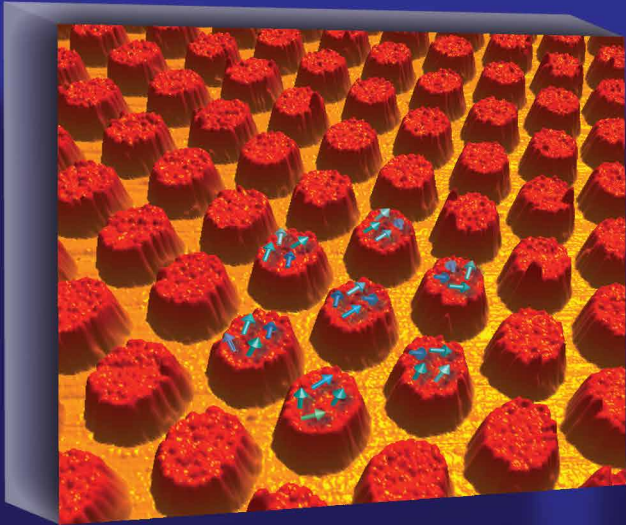
Using several mechanisms, BES program managers actively monitor all research awards during the award period to ensure progress toward the proposed research objectives. Generally, program managers engage in discussions with lead investigators and project directors through regularly scheduled or informal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

publications generated from BES funding. BES program managers review these requests before approving continued funding.

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

Finally, BES program managers organize and conduct PI meetings within a particular research or topical area to foster collaboration,

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





Research Portfolio and User Facilities

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

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



Materials Sciences and Engineering Division

science.energy.gov/bes/mse/

Materials are critical to nearly every aspect of energy generation and use. 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 these wide-ranging 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.

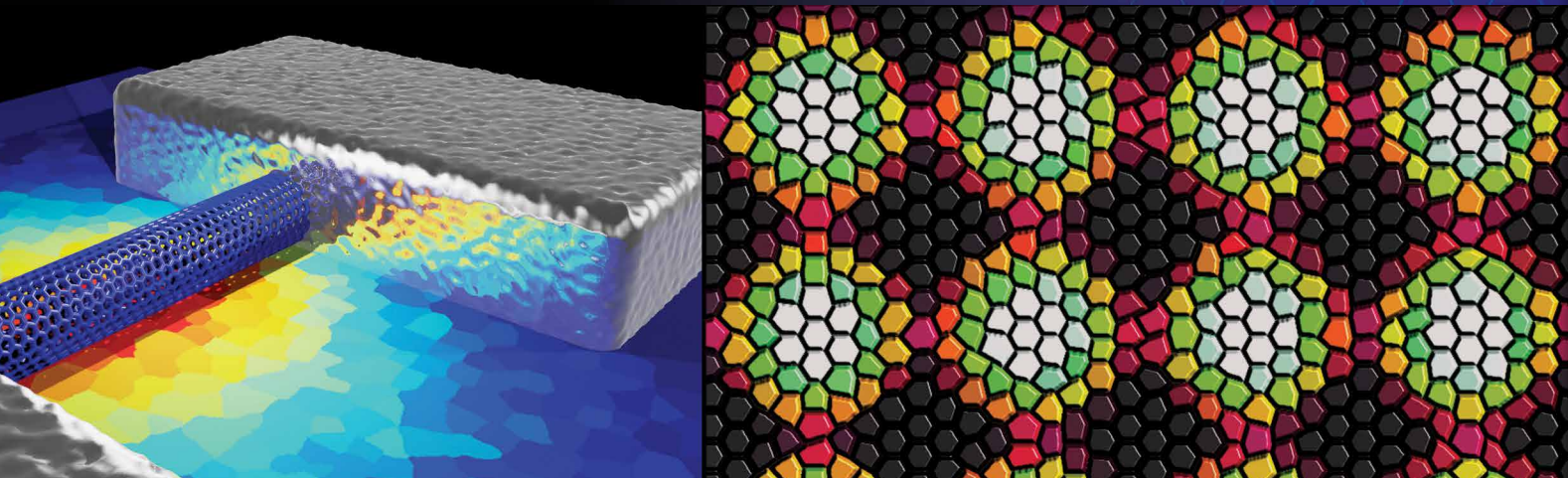
To accomplish these goals, MSE supports the following basic research activities:

- **Materials Discovery, Design, and Synthesis** to design and precisely assemble structures for controlling material properties

and discovering new materials with 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 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 multiple 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

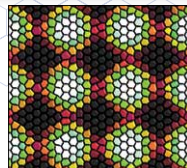
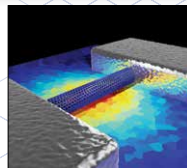
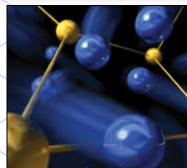
The discovery and development of new materials have long been recognized as the engines advancing science frontiers and driving technology innovations. Predictive discovery of new types of matter with tailored properties—critical to world leadership scientifically, technologically, and economically—depends on understanding how materials form. The Materials Discovery, Design, and Synthesis activity aims to grow and maintain U.S. leadership in materials discovery by investing in advanced synthesis capabilities and by coupling synthesis with state-of-the-art user facilities and advanced computational capabilities. A key part of the portfolio is biomimetic materials research, which translates biological processes into impactful approaches for designing and synthesizing materials with remarkable properties found only in nature (e.g., self-repair and adaptability to changing environments). Research includes activities in *Materials Chemistry and Biomolecular Materials* and in *Synthesis and Processing Science*. These activities underpin many energy-related technological areas such as batteries and fuel cells, catalysis,

solar energy conversion and storage, friction and lubrication, and membranes for advanced gas separations and storage.

Materials Chemistry and Biomolecular Materials research emphasizes chemistry- and biology-based approaches to material synthesis and assembly. Major research directions include (1) the controlled synthesis and assembly of functional nanoscale and mesoscale materials with desired properties; (2) mimicking biology's



Engineering Biomimetic Materials. Sarah Heilshorn (right) at SLAC National Accelerator Laboratory (SLAC), shown here with Kelly Huggins, leads an interdisciplinary research program that characterizes and exploits the tailored molecular interactions inherent in biological systems to engineer dynamically responsive, reversibly assembled biomimetic materials exhibiting self-healing and self-regulating capabilities. [Image courtesy SLAC]



Materials Sciences and Engineering

energy-efficient synthesis approaches to generate new, advanced materials for use under harsher, nonbiological conditions; (3) bioinspired materials that assemble autonomously and dynamically; and (4) adaptive and resilient materials that possess self-repairing capabilities.

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

Scattering and Instrumentation Sciences

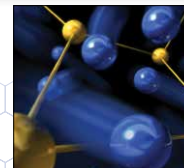
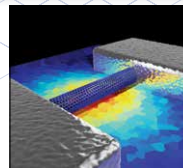
Advanced characterization tools with very high structural and temporal precision are essential for understanding, predicting, and ultimately controlling matter and energy at the level of electrons, atoms, and molecules. The Scattering and Instrumentation Sciences activity supports the science that utilizes 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. 28). Revolutionary advances in these techniques will enable

transformational research on advanced materials for DOE missions in energy, environment, and national security.

Understanding complex materials and phenomena requires combinations of tools to determine the roles of individual species and interfaces in multicomponent systems. Because electrons, neutrons, and x-rays interact uniquely with matter, they offer a range of complementary tools with different sensitivities and resolutions for characterizing materials at length and time scales spanning several orders of magnitude. Furthermore, investigations of dynamic phenomena in real time under natural (or operating) conditions provide insights into the real-world functioning of a material. New capabilities for ultrafast science will investigate dynamics related to electronic, catalytic, magnetic, and other transport processes at very fast time scales.

Condensed Matter and Materials Physics

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



Sputtering System Configured for Metal Oxide Deposition. John Rogers (right), director of the Frederick Seitz Materials Research Laboratory at the University of Illinois at Urbana-Champaign (UIUC), explains the workings of a sputtering system configured for metal oxide deposition. [Image courtesy UIUC]



Novel Thermoelectric Materials. Rachel Segalman [beside an atomic force microscope at Lawrence Berkeley National Laboratory (LBNL)] leads a multi-investigator project focused on using controlled interfaces and nanostructures to drive heat flow and energy generation in novel thermoelectric materials. [Image courtesy LBNL]



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 studies of electronic properties under extreme conditions, such as ultralow temperatures and extremely high magnetic fields. Research relevant to energy technologies includes understanding the elementary energy conversion steps in photovoltaics and electron spin phenomena and basic semiconductor physics related to next-generation information technologies and electronics. Fundamental studies of the interactions of atomic particles and energy (quantum physics) will lead to improved understanding of electrical and thermal conduction in a wide range of material systems. Critically needed is the ability to couple theories describing phenomena at the atomic scale to material properties at the macroscale where the connection between these properties and a material's size, shape, and composition is poorly understood.

Another focus area is learning how materials respond to varying temperature, electromagnetic fields, radiation, and chemical environments. Understanding the influence of material defects 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.

Selected Accomplishments

The following pages describe MSE-supported research on (1) the discovery of a new class of magnetic materials, (2) a novel strategy enabling the use of superconductors in high-magnetic fields, (3) design principles for a new class of protein-polymer functional biomaterials, and (4) observations of ion hopping in battery materials on a femtosecond time scale. These accomplishments represent only a small portion of the science supported by MSE.

MSE Research Accomplishment

A New Class of Magnetic Materials with Novel Structural Order

Discovery of the first binary magnetic quasicrystals could help unravel the fundamental relationship between structure and magnetism in aperiodic materials

The Science: A new class of binary alloys made from rare earth elements and cadmium has been discovered. These materials manifest the unique 5-fold symmetry and structural characteristics of quasicrystals and possess magnetic properties, providing the first step toward answering a much-debated question as to whether or not long-range magnetic order can be achieved in a quasicrystalline material.

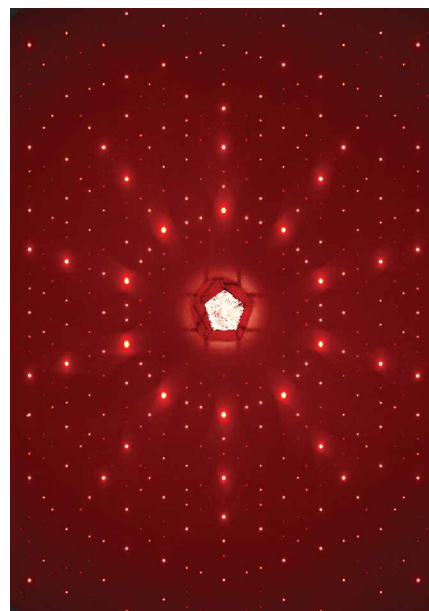
The Impact: This discovery will enable detailed studies of the effect of aperiodicity on magnetism in quasicrystals, in particular, and complex systems, in general, allowing comparison to the properties of related crystalline materials whose atomic compositions are close to those of quasicrystals.

Summary: Quasicrystals are fascinating solids whose atomic arrangements are not periodic but have long-range positional order and 5-fold, 8-fold, and higher rotational symmetries that are forbidden in conventional crystals. Three decades after their discovery in 1984—with over a hundred alloys synthesized and one naturally occurring alloy identified—quasicrystals are now considered a new class of stable materials. Their original discovery led to the 2011 Nobel Prize in Chemistry. Quasicrystals exhibit some novel mechanical properties (e.g., low surface friction) that are different from properties of their related crystalline and glassy alloys. Hence, the search for quasicrystals with new physical properties continues. Scientists at Ames Laboratory have discovered a new family of binary, rare earth-containing quasicrystals in the R-cadmium binary alloy where R = gadolinium, terbium, dysprosium, holmium, erbium, thulium, and yttrium, all of which (except yttrium) have localized magnetic moments. For this family of magnetic quasicrystals, there exist crystal-line compounds, known as crystal approximants, with atomic compositions and arrangements close to those of quasicrystals. Comparisons between quasicrystals and related crystal approximants will help to unravel the relationships among the structure, dynamics, and magnetism in these materials and pave the way to new designer materials for future technologies.

Reference

Goldman, A. I., et al. 2013. "A Family of Binary Magnetic Icosahedral Quasicrystals Based on Rare Earths and Cadmium," *Nature Materials* **12**, 714–18. DOI:10.1038/NMAT3672.

High-Energy X-Ray Diffraction Pattern. A single grain of a gadolinium-cadmium alloy (shown in center) displays the novel 5-fold rotational symmetry characteristic of an icosahedral quasicrystal. Diffraction images were obtained using the recently developed high-energy x-ray precession camera on a high-brilliance superconducting undulator x-ray beam line at the Advanced Photon Source. [Image courtesy Adam Goldman and Paul Canfield, Ames Laboratory. Reprinted by permission from Macmillan Publishers Ltd: From Goldman et al. 2013. Copyright 2013.]



MSE Research Accomplishment

A Breakthrough for High-Field Superconductors

Nanostructuring may help superconductors overcome a decades-long barrier to use in more powerful motors and magnets

The Science: Increasingly high magnetic fields lower performance and eventually destroy superconductivity altogether in superconductors of all types. A recent finding demonstrates, however, that in ultra-thin wires or in thin sheets perforated by an array of nanosized holes, high magnetic fields do not inhibit superconductivity but actually protect it.

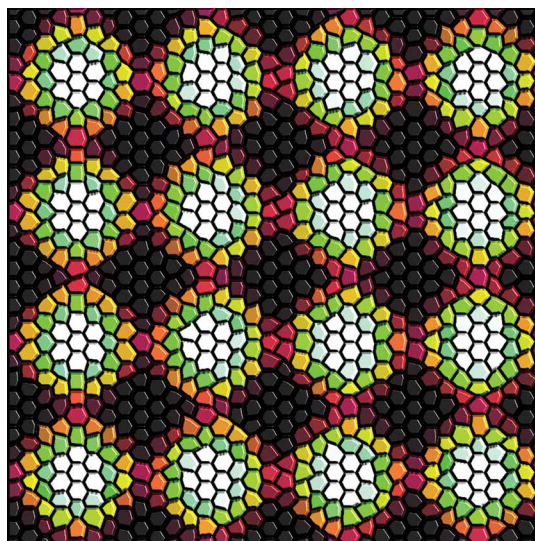
The Impact: Extension of this finding to high-temperature superconductors would enhance the use of superconducting wires in energy-relevant applications that involve high magnetic fields, as well as lower a decades-long barrier to wider technological applications of superconductors, including high-performance motors and generators.

Summary: Magnetic fields can penetrate into technologically useful (Type-II) superconductors by creating thin filaments called magnetic vortices. Only the area between the vortices remains superconducting. However, minute vortex motion can create electrical resistance, which eliminates the remaining superconductivity. Immobilizing these vortices and retaining zero resistance at high fields have been areas of emphasis in superconductor research for decades. Until recently, all the known mechanisms of vortex immobilization or pinning have worked efficiently only at moderate magnetic fields and temperatures, thereby restricting technological and industrial applications of superconductors. An international collaboration including theory research at Argonne National Laboratory has now found a completely new approach to the pinning problem. The team demonstrated that a wire so narrow it can accommodate only one row of vortices, or a film perforated by an array of holes (i.e., physical voids) so close together that only a few vortices can fit between them, turns high magnetic fields into healers of superconductivity rather than destroyers. At high fields, superconducting channels at the edges of the wires or holes squeeze vortices so tightly that they overlap and form clusters that can no longer move.

Reference

Córdoba, R., et al. 2013. "Magnetic Field-Induced Dissipation-Free State in Superconducting Nanostructures," *Nature Communications* 4, 1437. DOI:10.1038/ncomms2437.

Distribution of Superconductivity in a Thin Sheet of Superconducting Film. White regions indicate holes (physical voids), and green regions indicate strong superconductivity. Farther away from the holes, the superconductivity decreases (yellow, red, and finally black) where the material is so densely packed with vortices that they cannot move in high magnetic fields. [Image courtesy Valerii Vinokur, Argonne National Laboratory]



MSE Research Accomplishment

Design Principles Revealed for a New Class of Functional Biomaterials

Ordered arrays of functional proteins with designed molecular properties are created through self-assembly by combining proteins and synthetic polymers

The Science: Synthetic polymers with defined molecular properties (chemical structure and molecular weight) are designed to form block copolymers with globular proteins. The self-assembly is driven by the chemical incompatibility between the proteins and the chemically linked polymers. In aqueous solution at high concentrations, these designed block copolymers exhibit a rich phase behavior that is dependent on the chemical structure of the polymer, polymer volume fraction in the block copolymer, block copolymer concentration, and temperature. By controlling these variables, a variety of protein arrays with different architectures can be created.

The Impact: This discovery represents a significant step forward in controlling nanostructures in protein-based materials, with important applications in biocatalysis, energy conversion, and nanotechnology.

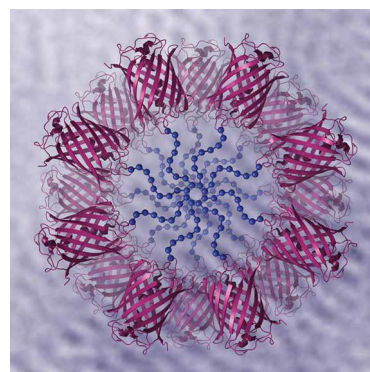
Summary: If functional proteins could be organized into nanostructured arrays such as cylinders (one dimensional), lamellae (two dimensional), and other three-dimensional architectures, this discovery could usher in a new class of materials with unprecedented higher or even new functionality. Working toward this goal, scientists at the Massachusetts Institute of Technology designed a set of block copolymers consisting of proteins covalently bonded with synthetic polymers and explored their solution phase behavior as a function of polymer molecular weight, block copolymer composition, concentration, and temperature in the high-concentration regime. The incompatibility between the protein and polymer and their chemical interaction with the solvent (water in this case) leads to novel self-assembly properties that can be controlled with rational design of the block copolymers. Neutron scattering experiments show that water distribution within the nanostructures drives transitions between ordered phases. Since proteins have incipient aggregating tendency in solutions, especially at higher concentrations, new routes are needed to exploit their unique function. The ability to organize functional biomaterials at high concentrations without aggregation through the block copolymer route offers new ways for the rational design of novel materials for potential applications in catalysis, sensors, nanotechnology, and renewable energy.

References

Lam, C. N., and B. D. Olsen. 2013. "Phase Transitions in Concentrated Solution Self-Assembly of Globular Protein–Polymer Block Copolymers," *Soft Matter* **9**, 2392–402.

Thomas, C. S., et al. 2012. "Kinetically Controlled Nanostructure Formation in Self-Assembled Globular Protein–Polymer Diblock Copolymers," *Biomacromolecules* **13**, 2781–92.

Cylinder-Forming Diblock Copolymers. Schematic illustration of self-assembled diblock copolymers where the first block is a protein at the surface and the second block is the covalently attached synthetic polymer at the interior. [Image courtesy Bradley Olsen, Massachusetts Institute of Technology. Reprinted by permission of The Royal Society of Chemistry: From Lam and Olsen 2013.]



MSE Research Accomplishment

Watching Ions Hop in Next-Generation Battery Materials

Measurements at the atomic-length scale and femtosecond time scale unravel the atomistic pathways and speed limits for copper migration through a nanocrystal

The Science: Time-resolved measurements can decipher the movement of copper ions and the simultaneous change in the sulfur sublattice through which the ions travel. Being able to discern these two key features opens the door to designing energy-relevant materials such as batteries based on electrochemical storage and switching devices.

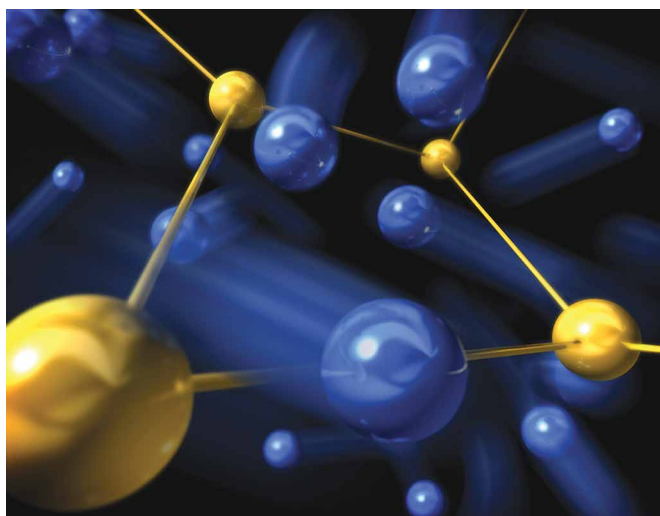
The Impact: Measurements indicate how a class of phase transitions with relevance to materials for next-generation electrochemical energy storage occur, and they show that switching speed at the nanoscale is determined by the process by which copper ions are transported through the nanocrystal.


Summary: Ultrafast x-ray scattering and spectroscopic measurements were used to probe the phase transition of a type of binary nanocrystal where one atomic element becomes mobile (like a liquid) and the other atomic element remains in a crystalline lattice. The crystal class—specifically copper sulfur (Cu S), or copper sulfide in this particular case—is called “superionic” because the Cu ionic sublattice “melts,” allowing the Cu atoms to move more freely while the S sublattice maintains the solid crystalline container. The research confirmed that very little Cu movement is needed to disorder the Cu sublattice, while expanding the interatomic distances between the S atoms and making the S lattice more symmetric. The key finding is that the phase transition occurs on the time scale of a single “hopping event,” defined as the time needed for Cu to move from one local sweet spot to another. This insight is useful because ion transport is a key aspect of battery function and ionic phase transition materials can be used in electrochemical switching devices.

Reference

Miller, T. A., et al. 2013. “The Mechanism of Ultrafast Structural Switching in Superionic Copper (I) Sulphide Nanocrystals,” *Nature Communications* 4, 1369. DOI:10.1038/ncomms2385.

Watching Ions Hop in Battery Materials. Depiction of the superionic phase of copper (blue) diffusing through the sulfur (yellow) sublattice. [Image courtesy Aaron Lindenberg, SLAC National Accelerator Laboratory]





Chemical Sciences, Geosciences, and Biosciences Division

science.energy.gov/bes/csgeb/

The transformation of energy between types (e.g., optical, 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, such as catalysis, that can contribute significantly to new energy technologies.

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

Knowledge of the quantum mechanical behavior of electrons, atoms, and molecules is being translated into the ability to control and direct chemical behavior to achieve a desired result. Such results include, for example, optimal conversion of solar energy into excited electronic states and then into separation of electrical charge in macromolecular

assemblies. This unprecedented degree of control represents a new era for chemical science, which CSGB research seeks to expand further by enabling the tailoring of chemical transformations with atomic and molecular precision. The challenge is to predictively assemble and manipulate large, complex chemical, geochemical, and biochemical systems at the same level of detail now possible for simple molecular systems.

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

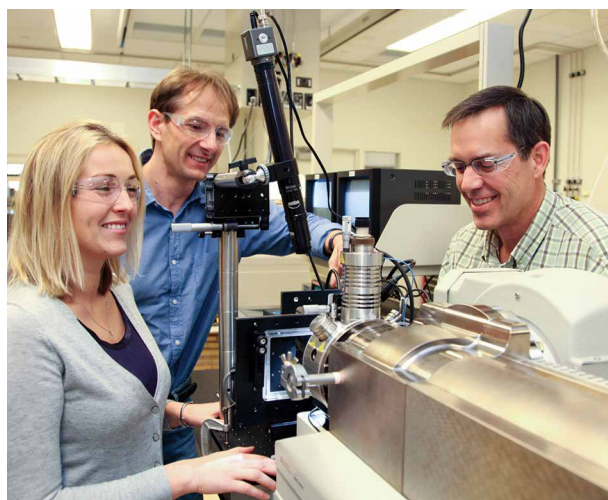
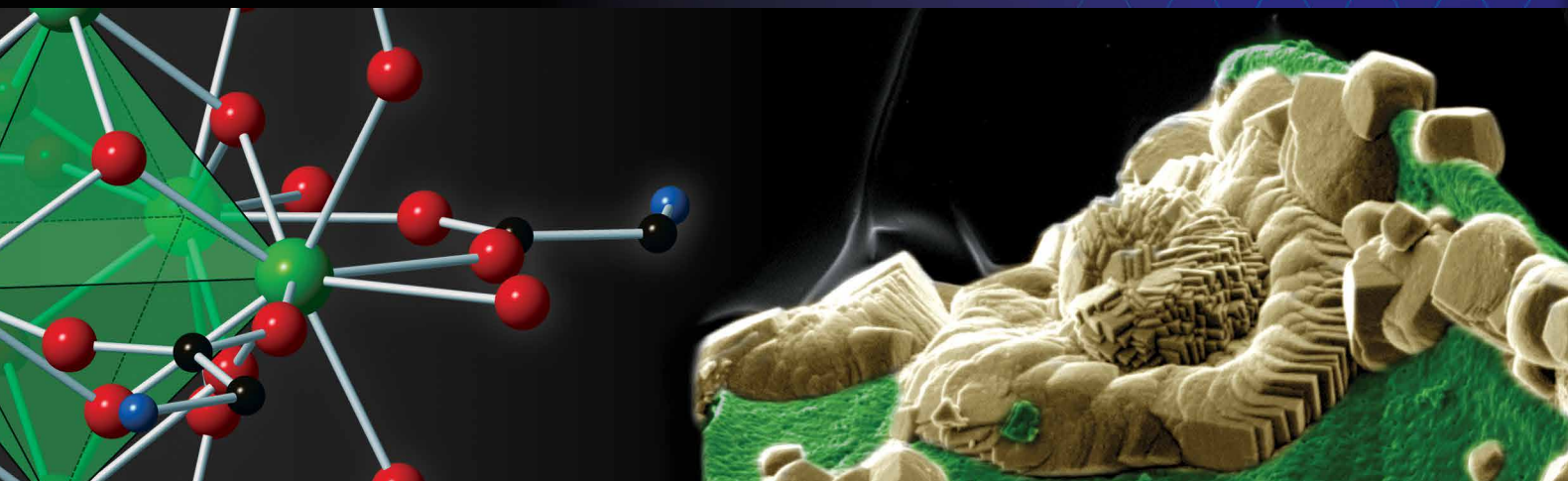
- **Fundamental Interactions**
- **Chemical Transformations**
- **Photochemistry and Biochemistry**

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

CSGB Research Activities

Fundamental Interactions

This activity builds the fundamental science basis essential for technological advances in a diverse range of energy processes. Research emphasizes structural and dynamical studies of atoms, molecules, and nanostructures to provide complete knowledge and rigorous understanding of reactive chemistry in gas and condensed phases. These studies also investigate the chemistry occurring

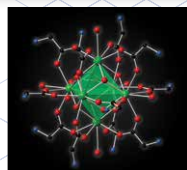
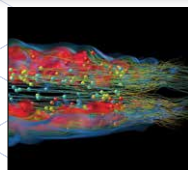


Mass Spectrometry Award. Oak Ridge National Laboratory (ORNL) scientists (from left) Olga Ovchinnikova, Vilmos Kertesz, and Gary Van Berkel were awarded the 2013 Rapid Communications in Mass Spectrometry Beynon Prize for their paper, “Combining Transmission Geometry Laser Ablation and a Non-Contact Continuous Flow Surface Sampling Probe/Electrospray Emitter for Mass Spectrometry Based Chemical Imaging” [*Rapid Communications in Mass Spectrometry* **25**, 3735–40 (2011)]. [Image courtesy ORNL]

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

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

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



Chemical Sciences, Geosciences, and Biosciences

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

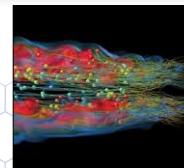
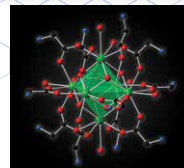
Research in this activity emphasizes the design, synthesis, characterization, and optimization of chemical processes underpinning current and emerging technologies that support DOE missions in energy, environment, and national security. Encompassing the areas of catalysis, separations and analysis, heavy element chemistry, and geosciences, this effort seeks to inform advanced technical solutions in fuel production, nuclear energy, and energy-production byproduct disposal. A wide breadth of novel chemistry is supported including nanostructured surfaces; electrochemistry; nanoscale membranes; bioinspired chemistry; inorganic, organic, and hybrid molecular complexes; and analytical and physical geochemistry. This activity also supports the development of unique tools needed for chemical analysis and molecular detection, emphasizing the imaging of chemically distinct species.

Catalysis science research in this portfolio comprises basic studies to unravel mechanisms by which catalysts accelerate and direct chemical conversions. Such knowledge guides the

rational synthesis of new or vastly re-engineered catalysts to exploit renewable resources and increase energy efficiency and chemical selectivity. Since many fuel and chemical production processes rely on catalysts, improving catalytic efficiency and selectivity has enormous economic and energy consequences. The grand challenge is to rationally design and synthesize durable catalysts that perform as predicted from first principles, particularly for converting uncommon feedstocks. 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.

Exploring the fundamental chemistry at the extreme end of the periodic table, primarily the energy-significant actinides, is a unique focus of this portfolio. Knowledge about the chemical characteristics of actinide and 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, focused on their solution chemistry, interfacial and solid-state bonding, and chemical reactivity.

Research is also pursued in this portfolio to obtain a predictive understanding, at molecular- and nanoscale dimensions, of the basic chemical and physical principles involved in separations systems including the removal of combustion byproducts. Activities also focus on the development of chemical analysis tools so that innovative solutions to DOE mission-related problems may be discovered and advanced.



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 transduction, including processes beyond primary photosynthesis (e.g., carbon reduction and deposition of reduced carbon 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.

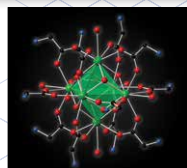
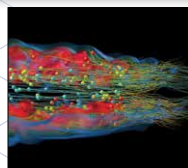
Research in natural photosynthesis emphasizes intersections between the biological sciences and energy-relevant chemical sciences and physics. Such studies explore self-assembly of photosynthetic components, natural mechanisms of photon capture and charge separation, and self-regulating and -repairing properties of the



Revealing Molecular Structures of Actinides. Richard Wilson at Argonne National Laboratory (ANL) prepares a single-crystal x-ray diffraction measurement of an inorganic actinide complex. Such measurements reveal the molecular structures of these elements, knowledge critical to understanding their physical and electronic properties. [Image courtesy ANL]

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



Chemical Sciences, Geosciences, and Biosciences

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.

Selected Accomplishments

The following pages describe a few of the numerous CSGB-supported research projects that are leading to transformational scientific advancements. These selected projects highlight (1) ultra-selective reactions that can be catalyzed by single atoms isolated on a substrate, a novel approach that may lead to new catalysts and efficient chemical conversions; (2) a possible channel that conducts water molecules through the photosynthetic protein complex known as Photosystem II to deliver them to its active site; and (3) a new technique for obtaining detailed structural information on individual aerosol particles in flight.

CSGB Research Accomplishment

Ultra-Selective Hydrogenation Reactions Catalyzed by Individual, Isolated Palladium Atoms

Single palladium atoms convert the surface of an inexpensive metal into an ultra-selective hydrogenation catalyst

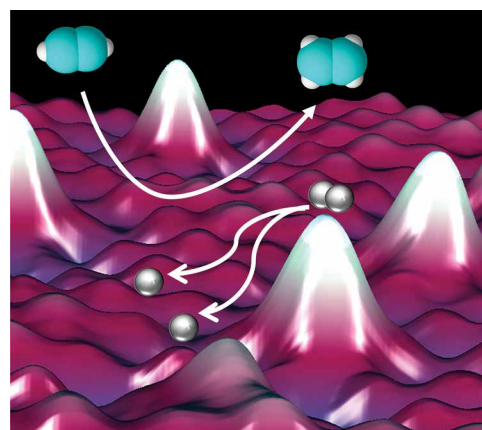
The Science: High-resolution imaging was used to characterize the active sites in single-atom bimetallic surfaces, and the chemistry was studied via temperature-programmed reaction spectroscopy. The mechanism involved facile dissociation of molecular hydrogen (H) at individual palladium (Pd) atoms, followed by spillover onto the copper (Cu) surface. This weak binding of H and acetylene to Cu enabled the ultra-selective hydrogenation of both alkenes and alkynes. The reaction selectivity was much higher than that measured on pure Pd, illustrating the unique synergy of the bimetallic system.

The Impact: Single metal atoms strongly bound onto crystalline surfaces of a different metal offer a general strategy for designing novel bifunctional heterogeneous catalysts. Catalytic selectivity and activity can be fine-tuned with ultimate precision by controlled changes to the electronic structure of the atomically dispersed metal.

Summary: Catalytic hydrogenations are critical to many industries, including fuels, agricultural chemicals, foods, and pharmaceuticals. In the petroleum-refining industry, for instance, catalytic hydrogenations are performed to produce light and hydrogen-rich products like gasoline. Typical heterogeneous hydrogenation catalysts involve nanoparticles composed of expensive noble metals or alloys based on platinum, Pd, rhodium, and ruthenium. Demonstrated for the first time is how single Pd atoms can convert the otherwise catalytically inert surface of an inexpensive metal, Cu, into an ultra-selective catalyst. High-resolution imaging was used to characterize the active sites in the bimetallic surfaces, and temperature-programmed reaction spectroscopy was used to probe the chemistry. This surface science and kinetics experimentation unambiguously shows that atomic dispersion of transition metals onto other metal surfaces may lead to novel catalysts or efficient chemical conversions.

References

- Kyriakou, G., et al. 2012. "Isolated Metal Atom Geometries as a Strategy for Selective Heterogeneous Hydrogenations," *Science* **335**, 1209–12.
- Boucher, M. B., et al. 2013. "Single Atom Alloy Surface Analogs in Pd_{0.18}Cu₁₅ Nanoparticles for Selective Hydrogenation Reactions," *Physical Chemistry Chemical Physics* **15**(29), 12187–196.



Scanning Tunneling Microscope Image Showing Atomically Dispersed Palladium Atoms on a Copper Surface. The Pd atoms activate H, and the Cu sites insert it into acetylene, thus allowing the industrially important conversion of acetylene to ethylene to proceed with 100% selectivity. [Image courtesy Charles Sykes, Tufts University]

CSGB Research Accomplishment

Following the Trail of Water Molecules Through Photosystem II During Photosynthesis

Researchers have identified a possible channel that enables substrate water molecules to travel to the active site of Photosystem II

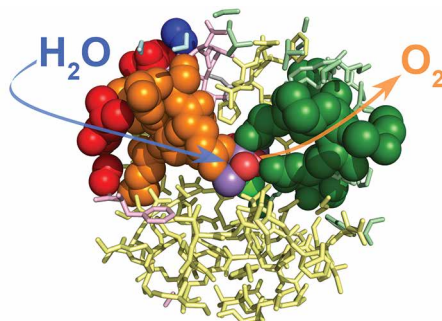
The Science: To map the pathway that water travels to and from the active site of Photosystem II (PSII), water was exposed to short bursts of high-energy radiation to generate highly reactive compounds. These compounds, in turn, chemically reacted with amino acids that were in close proximity to the water in the PSII protein complex. Using sophisticated mass spectroscopic techniques, researchers “mapped” these modified amino acids to their locations in the protein structure. By performing these studies over time, the researchers were able to propose a “water channel” through the protein, identifying at least one possible channel in PSII that directs water to the active site.

The Impact: Several computational studies by other researchers have suggested possible water channels in the PSII complex, but these studies reached differing conclusions. This research is the first study to provide direct experimental evidence of the specific amino acids that may line the channel involved in delivering water molecules to the active site of PSII, the key enzyme complex that splits water molecules in photosynthesis. Identification of the pathways used by the substrate (water) and the product (oxygen) provides new insights into PSII’s function and may suggest new approaches for solar fuels production using natural or artificial photosynthesis.

Summary: Photosynthesis uses large, multiprotein complexes called photosystems to capture solar energy and convert it to chemical energy. PSII specifically uses light energy from the sun to extract electrons from water, resulting in the oxidation or “splitting” of water to form oxygen and hydrogen. Water “channels” have been proposed to allow surface water to get to PSII’s active site, which is “buried” deep within the protein complex. Researchers at Louisiana State University used a combination of induced water radiolysis followed by mass spectrometry to identify possible water and oxygen pathways within PSII. Their direct experimental results were compared to earlier computational studies suggesting putative water and oxygen channels in PSII. While this study examined only a subset of the proteins in PSII, the results were consistent with one of the computational models. Identification of the paths taken by the substrate (water) and its product (oxygen) provides important new knowledge on how natural photosystems work. Such insights may lead to new strategies for developing artificial photosynthetic systems for solar fuels production.

Reference

Frankel, L. K., et al. 2013. “Radiolytic Mapping of Solvent-Contact Surfaces in Photosystem II of Higher Plants: Experimental Identification of Putative Water Channels Within the Photosystem,” *The Journal of Biological Chemistry* **288**, 23565–72. DOI:10.1074/jbc.M113.487033.



Trail of Water to PSII. Modified amino acid residues leave a tell-tale “trail” of water’s passage through the photosynthetic protein complex known as PSII. Proposed pathways to the PSII active site for the substrate (water) and the product (molecular oxygen) are shown superimposed on a PSII model. [Image courtesy Terry Bricker, Louisiana State University]

CSGB Research Accomplishment

X-Ray Vision Exposes Aerosol Structures

Detailed images of airborne soot particles are recorded using ultrafast x-rays at the Linac Coherent Light Source

The Science: Soot particles were entrained in carrier gas and fed into the path of Linac Coherent Light Source (LCLS) x-rays. Diffraction patterns were measured from single particles, and mass spectroscopy probed the particles' composition. A long-term goal is to monitor particles as they change shape in response to their environment.

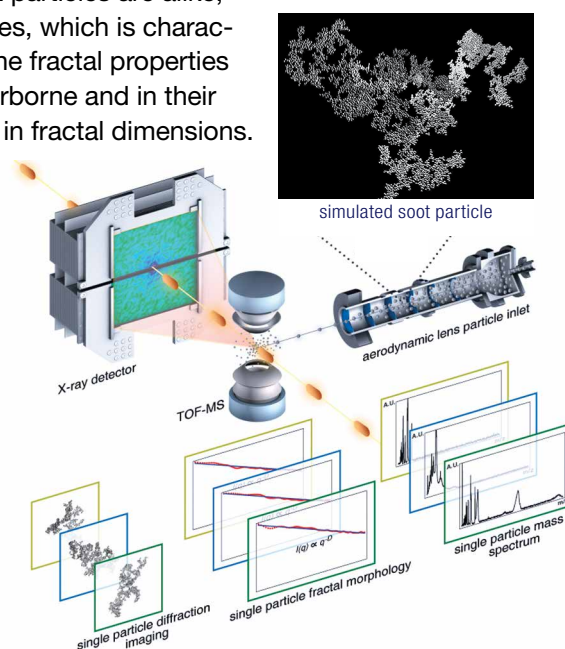
The Impact: Understanding the structure of airborne particulates smaller than 2.5 microns is important in fields ranging from toxicology to climate science.

Summary: The most detailed structural information to date on individual airborne soot particles in flight, a key contributor to global warming and a health hazard, reveals surprisingly complex structures. This information will improve the understanding of atmospheric processes important to climate change, as well as enable the design of cleaner combustion sources, from car engines to power plants. Soot and similar particles—especially those 2.5 microns or less in diameter, which are the most dangerous to human health—are difficult to image while airborne. When placed on a surface for examination with a microscope, they tend to clump together and change shape. In this experiment, researchers wafted individual soot particles up to 3.25 microns in diameter into the path of the LCLS laser beam. With extraordinarily short and tremendously intense laser pulses, it is possible to capture information about the particles, only millionths of a meter across, in the quadrillionths of a second before they are blown apart. This research pioneers a method for studying a broad range of individual particles, such as cells or proteins, and opens up exciting possibilities for the study of aerosol dynamics using highly focused x-ray lasers, such as those at LCLS. The researchers found that although no two soot particles are alike, they exhibit similar patterns of complexity at different scales, which is characteristic of fractals. Other research methods have probed the fractal properties of soot, but the examination of individual soot particles, airborne and in their natural state, revealed surprising diversity and complexity in fractal dimensions. Such observations can help validate various theoretical models used to describe soot particles.

Reference

Loh, N. D., et al. 2012. "Fractal Morphology, Imaging and Mass Spectrometry of Single Aerosol Particles in Flight," *Nature* **486**, 513–17.

Schematic of Concurrent Imaging, Morphology, and Spectroscopy of Single Soot Particles in Flight. Coherent x-ray free-electron laser pulses (orange) intersect a particle stream, producing a diffraction pattern and ion fragments whenever a pulse and particle coincide. [Image courtesy N. D. Loh and A. Freeberg, SLAC National Accelerator Laboratory. Adapted by permission from Macmillan Publishers Ltd: From Loh et al. 2012. Copyright 2012.]



Scientific User Facilities Division

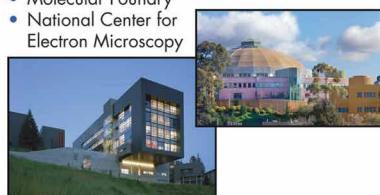
science.energy.gov/bes/suf/

Basic Energy Sciences (BES) operates a suite of scientific user facilities through its Scientific User Facilities (SUF) Division. These facilities provide unique technical tools—including x-ray light sources, neutron scattering facilities,

Nanoscale Science Research Centers (NSRCs), and Electron-Beam Microcharacterization Centers (EBMCs)—for advancing science in basic and applied energy-related disciplines. Research conducted at the facilities involves characterizing

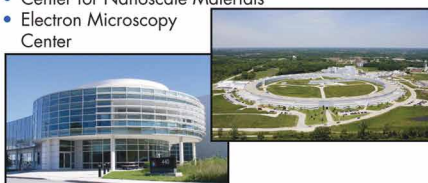
Lawrence Berkeley National Laboratory

- Advanced Light Source
- Molecular Foundry
- National Center for Electron Microscopy



Argonne National Laboratory

- Advanced Photon Source
- Center for Nanoscale Materials
- Electron Microscopy Center



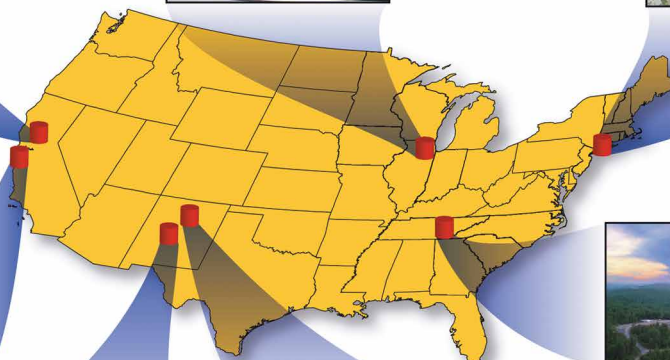
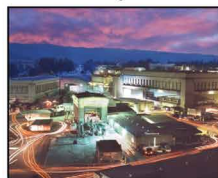
Brookhaven National Laboratory

- Center for Functional Nanomaterials
- National Synchrotron Light Source
- National Synchrotron Light Source II



SLAC National Accelerator Laboratory

- Linac Coherent Light Source
- Stanford Synchrotron Radiation Lightsource



Oak Ridge National Laboratory

- Center for Nanophase Materials Sciences
- High Flux Isotope Reactor
- Shared Research Equipment Facility
- Spallation Neutron Source



Sandia National Laboratories

- Core Facility for Center for Integrated Nanotechnologies

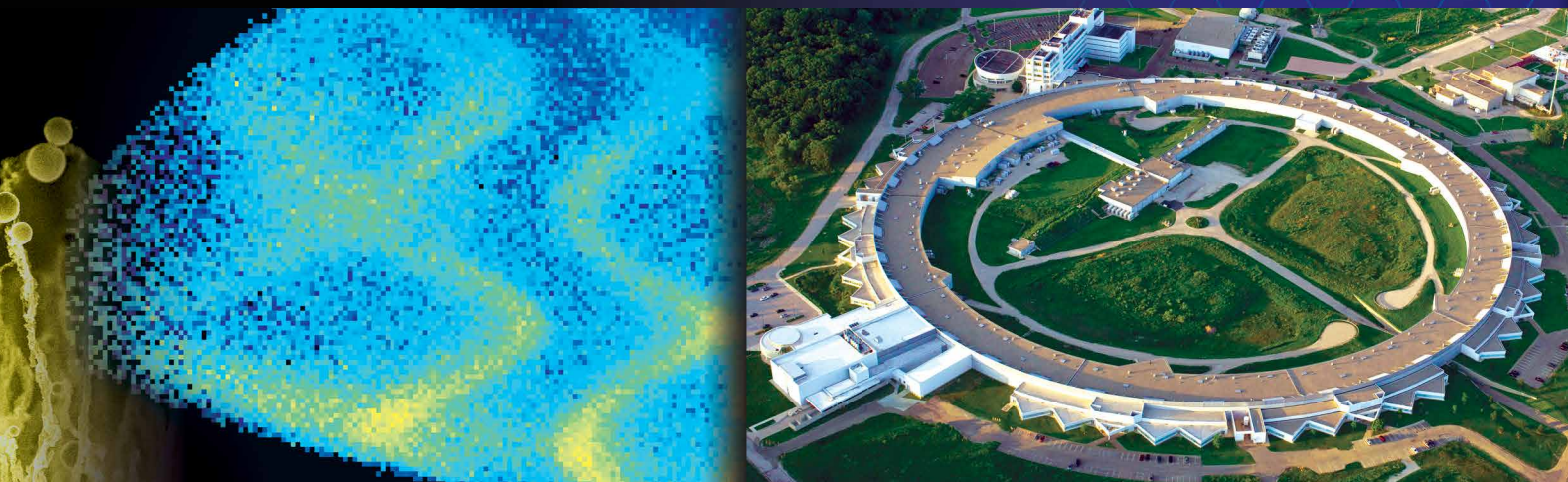


Los Alamos National Laboratory

- Gateway Facility for Center for Integrated Nanotechnologies
- Lujan Neutron Scattering Center



BES Scientific User Facilities



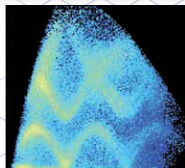
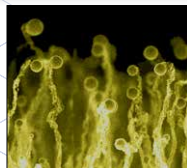
materials at the highest level of spatial, spectral, and temporal resolution. The breadth of instrumentation available across the facilities enables complementary evaluations of material structure, composition, and function and the evolution of such properties over time in a variety of operating conditions.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

These premier scientific facilities are open access, based on acceptance of user proposals through a competitive merit review process, allowing scientists from academia, federal laboratories, and industry to use the unique capabilities and sophisticated instrumentation of the facilities. In FY 2013, 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.

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

Breakdown of Scientific Users in FY 2013	
Facility	Users
X-Ray Light Sources	11,400
Advanced Light Source	2,222
Advanced Photon Source	4,542
National Synchrotron Light Source	2,367
Stanford Synchrotron Radiation Lightsource	1,675
Linac Coherent Light Source	594
Neutron Scattering Facilities	1,329
High Flux Isotope Reactor	395
Lujan Neutron Scattering Center	208
Spallation Neutron Source	726
Nanoscale Science Research Centers	2,258
Center for Nanoscale Materials	454
Center for Functional Nanomaterials	439
Molecular Foundry	451
Center for Nanophase Materials Sciences	467
Center for Integrated Nanotechnologies	447
Electron-Beam Microcharacterization Centers	581
National Center for Electron Microscopy	209
Electron Microscopy Center for Materials Research	162
Shared Research Equipment User Facility	210
Total Users in FY 2013	15,568

next-generation x-ray and neutron sources. In addition, construction activities support new and upgraded facilities and beamlines.



Scientific User Facilities

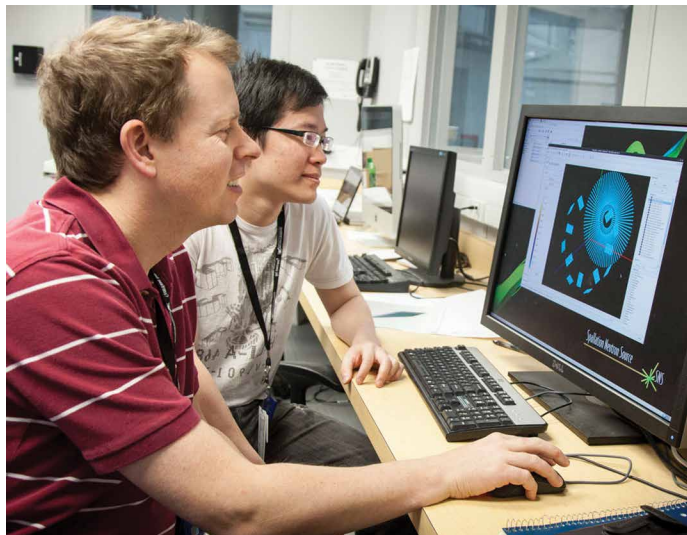
X-Ray Research

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.

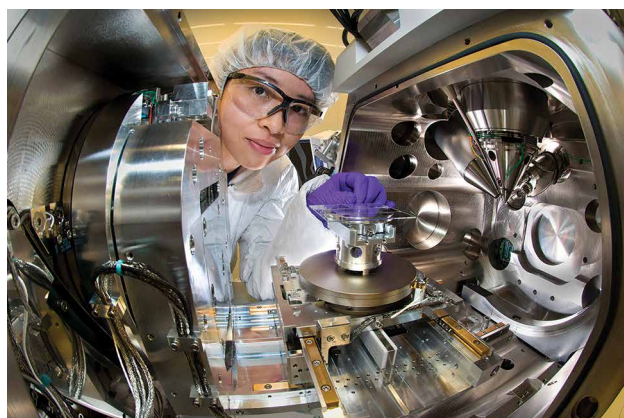
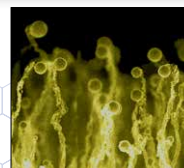
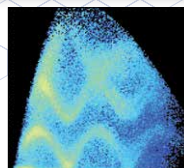
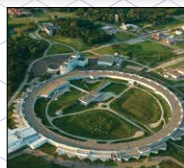
Synchrotron radiation has vastly enhanced the utility of x-ray techniques including diffraction, spectroscopy, and imaging. Moreover, the broad energy range of x-rays allows researchers to tailor characterization techniques to the individual materials and functions to be analyzed. Finally, the ability 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 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 a 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.



Users Review Spallation Neutron Source (SNS) Data. Carsten Sievers and Guo Shiou Foo of the Georgia Institute of Technology review data from the VISION vibrational spectrometer at SNS. [Image courtesy Oak Ridge National Laboratory]



State-of-the-Art Clean Room for Fabricating Devices. Devices include those for nanoelectronics, nanophotonics, biomedical engineering, photovoltaics, x-ray optics, nanomagnetism, and beyond. [Image courtesy Brookhaven National Laboratory]

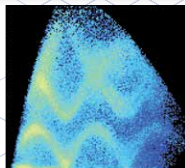
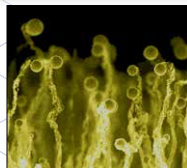
Neutron Scattering

A goal of BES science is to understand the factors that determine the properties of matter on the atomic scale and then use this knowledge to optimize those properties or develop new materials and functionality. With expanding applications in 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.

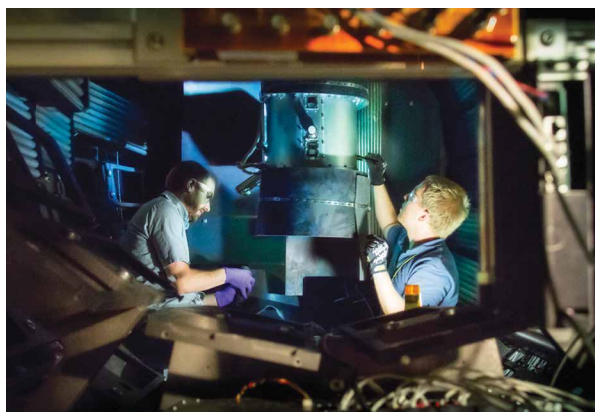
Neutrons have several unique advantages among the different probes used to investigate atomic-scale structure and dynamics. For studying structure with atomic resolution, neutrons have a wavelength similar to the spacing between atoms, and for investigating dynamics, they have energies similar to those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

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. Since accelerators are generally pulsed, the resulting neutron source also is pulsed, enabling highly efficient time-of-flight neutron scattering techniques used in studying material systems. The Lujan Neutron Scattering Center (Lujan Center) at Los Alamos National Laboratory (LANL) and the Spallation Neutron Source (SNS) at ORNL are pulsed spallation neutron sources. Each year more than 1,300 scientists, engineers, and industrial



Scientific User Facilities



Nanoscale-Ordered Materials Diffractometer (NOMAD) at the Spallation Neutron Source. Scientific associates Luke Heroux (left) and John Carruth work on the NOMAD instrument. [Image courtesy Oak Ridge National Laboratory]

researchers from across the United States conduct their research at HFIR, Lujan Center, and SNS.

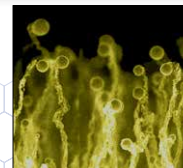
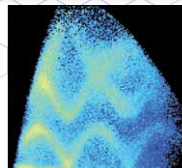
Nanoscale Science and Electron Microscopy

Nanoscale science 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 LANL. Each NSRC has particular expertise and capabilities in selected theme areas such as nanomaterial synthesis and characterization; catalysis; theory, modeling, and simulation; electronic materials; nanoscale photonics; soft and biological materials; imaging and spectroscopy; and nanoscale integration.

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

As important components of the user facility portfolio, BES's three EBMCs seek to develop next-generation electron-beam instrumentation and conduct corresponding research. The net results are unsurpassed spatial resolution with a world-record 50 picometers (0.05 nm) and the ability to simultaneously obtain structural, chemical, and other types of information from subnanometer



regions. Such capabilities allow study of the fundamental mechanisms of catalysis, energy conversion, corrosion, charge transfer, magnetic behavior, and many other processes. Moreover, they are critical for understanding and improving materials for energy applications and the associated physical characteristics and changes governing material performance. These EBMCs are the National Center for Electron Microscopy at LBNL, the Electron Microscopy Center for Materials Research at ANL, and the Shared Research Equipment User Facility at ORNL.

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

Accelerator and Detector Research

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

This research activity was a major supporter of the theoretical and experimental studies leading to rapid development of LCLS, the world's brightest light source. These studies addressed many of the fundamental physics questions concerning FELs and high-brightness beams, resulting in remarkably successful experiments and demonstrating that high peak beam brightness is possible with a very low average current, as realized at LCLS. This activity also is investing in research to develop 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 (3D) detectors that adapt to beam quality and perform initial analysis of data as it is received at the detector.

Selected Accomplishments

The following pages describe examples of how DOE scientific user facilities have been used to (1) understand the behavior of ice under high pressure, (2) develop new superconducting undulator technologies, (3) help industry develop new products such as Dow's Powerhouse™ Solar Shingles, and (4) create new nanomaterials that could play a prominent role in the future of computing. These accomplishments highlight only a few of the scientific advances enabled by BES user facilities.

SUF Research Accomplishment

Disruption of the Water Molecule in Ice Under High Pressures

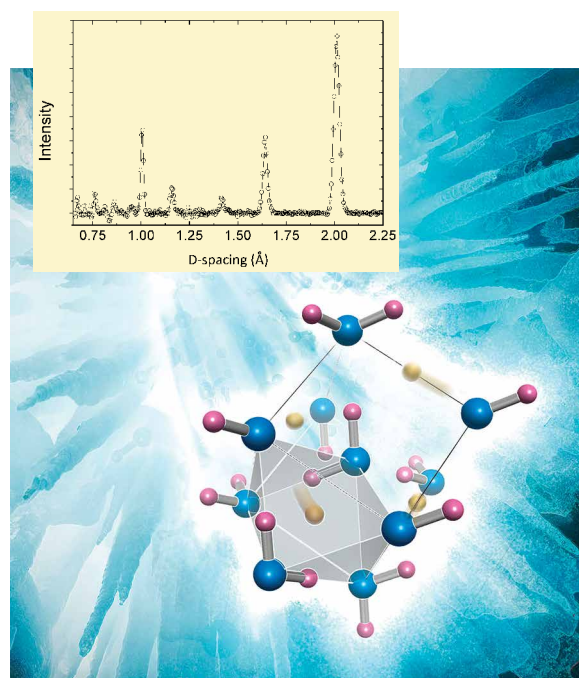
Results may aid understanding of icy planets and have implications for energy science

The Science: When water (H_2O) freezes into ice, it takes on unique properties under high pressures and at low temperatures. Researchers combined recently developed high-pressure techniques with the newly commissioned high-pressure neutron scattering instrument (SNAP) at Oak Ridge National Laboratory's Spallation Neutron Source to investigate the structure of ice under pressures as high as 52 GPa. They found that at these pressures about 25% of the protons were dissociated from their water molecules and located in octahedral voids in the oxygen lattice.

The Impact: This new and completely unpredicted finding is expected to have a broad impact for understanding bonding in H_2O under extreme pressure conditions, with major implications for modeling ice-rich planets such as Uranus and Neptune. This discovery could also yield greater understanding of methane-containing clathrate hydrates and even hydrogen storage materials that could one day power cars.

Summary: When water freezes into ice, its molecules are bound together in a crystalline lattice held together by hydrogen bonds, which are highly versatile. As a result, crystalline ice reveals a striking diversity of at least 16 different structures. The H_2O molecule is the universal building block in all these ice forms. Due to the strong sensitivity of neutrons to hydrogen atoms, neutron scattering techniques can be used to investigate the water molecule's characteristics. This neutron study provided the first glimpse of the hydrogen atoms themselves in ice at unprecedented pressures. Results indicate that some of the molecules begin to dissociate at much lower pressures and via a different path than previously predicted.

These findings could alter scientists' understanding of how the water molecule responds to conditions found deep within planets and have implications for energy science.



Reference

Guthrie, M., et al. 2013. "Neutron Diffraction Observations of Interstitial Protons in Dense Ice," *Proceedings of the National Academy of Sciences (USA)* **110**, 10552–56.

Ice Under High Pressure. Neutron diffraction data obtained from a 30 μg sample at 43 GPa shows dissociated protons (gold) locating in voids in the oxygen lattice (blue). Both water molecules and hydroxyls may coexist (inset). [Images courtesy Oak Ridge National Laboratory and Malcolm Guthrie, Carnegie Institution for Science (inset)]

SUF Research Accomplishment

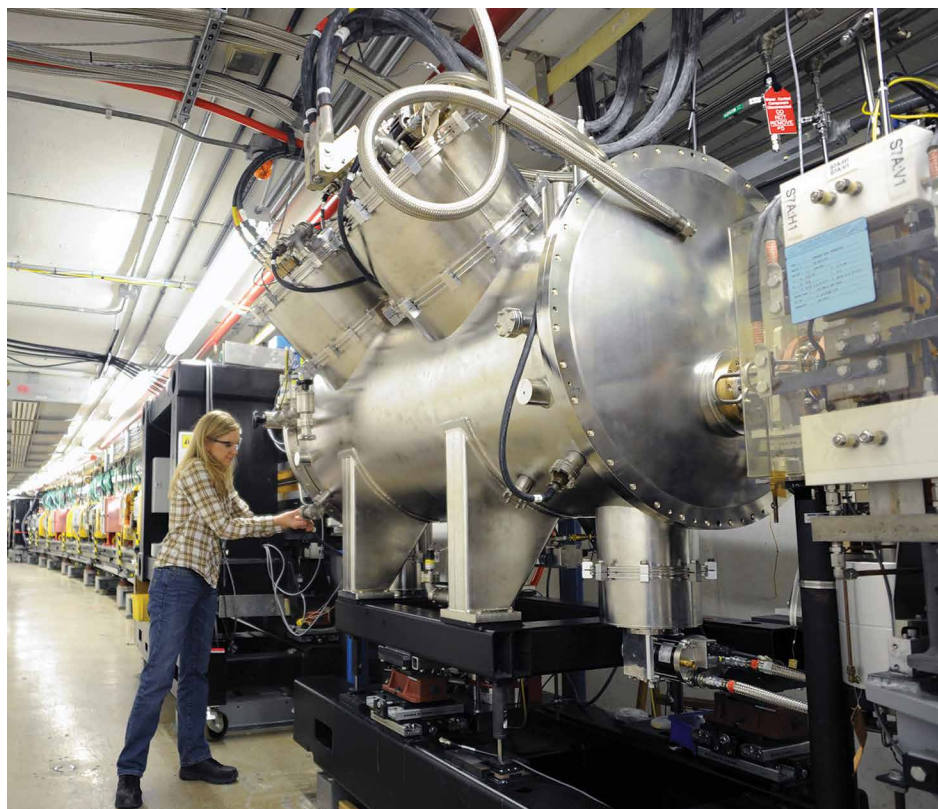
First Light from the First High-Energy Superconducting Undulator

New technology advancement boosts synchrotron x-rays, improving the performance of high-energy light sources

The Science: Superconducting technology in magnetic devices for synchrotron light sources offers superior performance in higher peak field over the same distance compared, for example, to conventional permanent magnetic devices.

The Impact: The successful development of the superconducting undulator at the Advanced Photon Source (APS) will provide current and future light sources with superior undulators, advancing the performance of those facilities.

Summary: Superconducting technology has been utilized before at synchrotron radiation facilities for building powerful wigglers or bending magnets, devices that also produce synchrotron x-rays. Making small-period (short), strong-magnetic-field undulators that meet stringent field quality requirements has been a long-standing objective for accelerator science. On Jan. 21, 2013, after more than 8 years of effort by physicists, engineers, and technicians, the first x-rays were produced from a novel superconducting undulator at the APS electron accelerator and storage ring at Argonne National Laboratory. This



is the first such superconducting undulator operated at a third-generation synchrotron x-ray facility. About 0.35 m long, this prototype device is superior to the standard 2.4-m-long permanent magnetic devices used at APS in producing high-energy x-rays.

Superconducting Undulator at the Advanced Photon Source. [Image courtesy Argonne National Laboratory]

SUF Research Accomplishment

DOE Light Source Helps Reinvent the Roof

X-ray research leads to manufacturing process for first solar shingles

The Science: Using *in situ* x-ray diffraction and scanning techniques, Dow Chemical scientists conducted numerous synchrotron experiments at the Advanced Photon Source (APS) at Argonne National Laboratory to study the chemical and structural composition of copper indium gallium (di) selenide (CIGS), the active material in Powerhouse™ Solar Shingles.

The Impact: This research led to the development of synthesized CIGS materials used in first-of-its-kind solar shingles for electricity generation. Dow has been manufacturing the solar shingles in Midland, Michigan, and will create more than 1,200 jobs when its new factory there is fully operational. Additional plant space will be added as needed to meet demand.

Summary: An overarching challenge in developing innovative energy systems is the ability to observe material behavior in real time during synthesis processing or under functional conditions. Using *in situ* x-ray diffraction at the APS, Dow researchers investigated and mapped the process-structure-property relationships in CIGS materials. This study led to the development of a successful process to form a semiconductor phase with optimal solar photovoltaic properties in the four-component system. The research has since been scaled up into a manufacturing process for the first commercial solar shingles, Powerhouse™ Solar Shingles, in which photovoltaics are built into the roofing materials. The product is currently available in 12 states nationwide including California, Texas, and New York.



Solar Shingles. With help from a DOE light source, Dow Powerhouse™ Solar Shingles advanced from research to manufacturing to installation of new roofs for U.S. homes in less than 5 years. [Images courtesy Dow Chemical Company]

SUF Research Accomplishment

Putting Light to Work at the Quantum Scale

Using artificial nanostructures to control the properties of light could play a prominent role in the future of computing

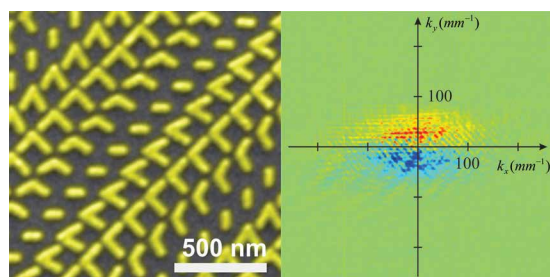
The Science: A 2D array of nanosized gold antennas with various geometries positioned on a silicon surface (i.e., a metamaterial) can generate and amplify a usually minute, quantum-level property of light (called the photonic spin Hall effect) sufficiently for observation with a simple camera.

The Impact: The ability of metamaterials to tailor and control measurable changes in quantum properties of light can be exploited for optical information processing and communication. Moreover, metamaterials with nanosized antennas have the potential to shrink such photonic devices to the nanometer range.

Summary: Combining quantum-based optics with artificial nanostructures has resulted in a breakthrough that could play a prominent role in the future of computing by manipulating photon spin and orbital momentum energy transfer, which can encode quantum information. One possible route involves the use of metamaterials—artificial materials comprising precisely controlled assemblies of multiple structural elements. Collectively, these elements have properties unachievable with conventional materials, in part by incorporating structural elements that are smaller than the wavelength of the light they affect. Researchers from Lawrence Berkeley National Laboratory and the University of California–Berkeley designed a metamaterial surface consisting of an array of V-shaped, nanosized gold antennas engineered to generate an effect on the quantum particles of light (photons). The photons making up the beam are somewhat akin to a spinning baseball passing through the air, thereby curving it to the left or right, depending on the spin. The photonic spin Hall effect is very weak and, until now, has been notoriously difficult to observe. This metamaterial system, however, enhances the photonic spin Hall effect enough for it to be observed using a simple camera. Future prospects are promising for deploying this type of material system in photon-based information processing and communication.

Reference

Yin, X., et al. 2013. “Photonic Spin Hall Effect at Metasurfaces,” *Science* **339**, 1405–07. DOI:10.1126/science.1231758.



Silicon Surface Hosting Nanoscale Array and Circular Polarization. **Left:** Scanning electron microscope image of a silicon surface hosting a nanoscale array of V-shaped gold antennas (metasurface) with different lengths, orientations, and angles. **Right:** The antenna array forces linearly polarized light traveling through it into a curved trajectory, resulting in components with different circular polarization (red and blue) to move in opposite directions, a quantum-optical phenomena called the photonic spin Hall effect. [Image courtesy Lawrence Berkeley National Laboratory]

The background of the top section features a complex arrangement of molecular models. In the foreground, there are large, semi-transparent spheres in shades of orange, red, and blue. Behind them, several ball-and-stick molecular models are visible, showing atoms in white, grey, blue, and yellow. The overall aesthetic is scientific and high-tech, with a gradient from white to red and blue across the top.

Energy Frontier Research Centers and Energy Innovation Hubs

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

Energy Frontier Research Centers

Basic Energy Sciences (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 research challenges identified in the Basic Research Needs and Grand Challenges reports (see p. 5). The EFRCs support energy-relevant, basic research that will lay the groundwork for transformative energy technologies of the future. There are currently 46 EFRCs involving some 850 senior investigators, with an additional 2,000 postdoctoral associates, students, and technical staff participating on a full- or part-time basis at more than 115 institutions in 35 states and the District of Columbia.

The EFRCs address scientific grand challenges described in the report *Directing Matter and Energy: Five Challenges for Science and the Imagination* and span the range of energy research challenges described in the BES *Basic Research Needs* series of workshop reports (science.energy.gov/bes/news-and-resources/reports/). These workshops solicited community input to define the basic research needed to enable advances related to 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, and superconductivity.

The EFRCs bring together the skills and talents of multiple investigators to enable fundamental research of a scope and complexity not possible with standard individual investigator or small group research 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 and Joint Center for Energy Storage Research. 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 new, 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 regular and frequent interactions with the EFRCs, including annual progress reports, monthly phone calls, site visits, and



meetings with the EFRCs as a group. To facilitate communication of research advances and technology needs and ensure that research activities are not duplicated, the EFRC management team (science.energy.gov/bes/efrc/contact/) coordinates EFRC research within BES and with the DOE technology offices. In 2012, the research productivity and progress of each EFRC were assessed by merit review panels of external scientific experts. The midterm assessment found that each EFRC had met or exceeded the expected progress toward its 5-year goals in its first 2 years of operations, and that collectively the EFRCs had demonstrated the potential to substantially impact the scientific understanding underpinning transformational energy technologies. In addition, the review found that the EFRC research teams are synergistic, making progress in ways that would not have been likely through separate support of the individual scientists.

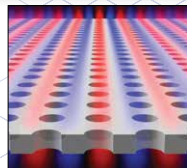
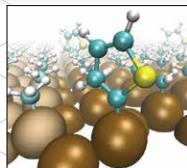
Two major EFRC meetings have been held in Washington, D.C., to strengthen connections within the EFRC community (more information



Poster Session at 2013 EFRC Principal Investigators' Meeting. [Image courtesy Pacific Northwest National Laboratory]

at www.energyfrontier.us/underMeetings). In May 2011, more than 1,000 of America's top energy researchers and policy-makers attended the 3-day Science for Our Nation's Energy Future: EFRC Summit and Forum. This meeting included plenary talks, scientific oral and poster presentations from all 46 EFRCs, and the Life at the Frontiers of Energy Research Video Contest (www.energyfrontier.us/video-contest).

In July, nearly 500 EFRC members and DOE employees attended the 2-day 2013 EFRC Principal Investigators' Meeting. In addition to presentations by senior investigators from all the EFRCs, 22 graduate students and postdoctoral researchers, nominated by their directors, were selected by BES to present their research at this meeting. From the finalists, BES selected six winners based on scientific excellence and how well the research exemplified the opportunities provided by the EFRC funding modality (www.energyfrontier.us/content/student-and-postdoc-competition). BES challenged the EFRCs to creatively communicate the mission and achievements of the program to the public through the



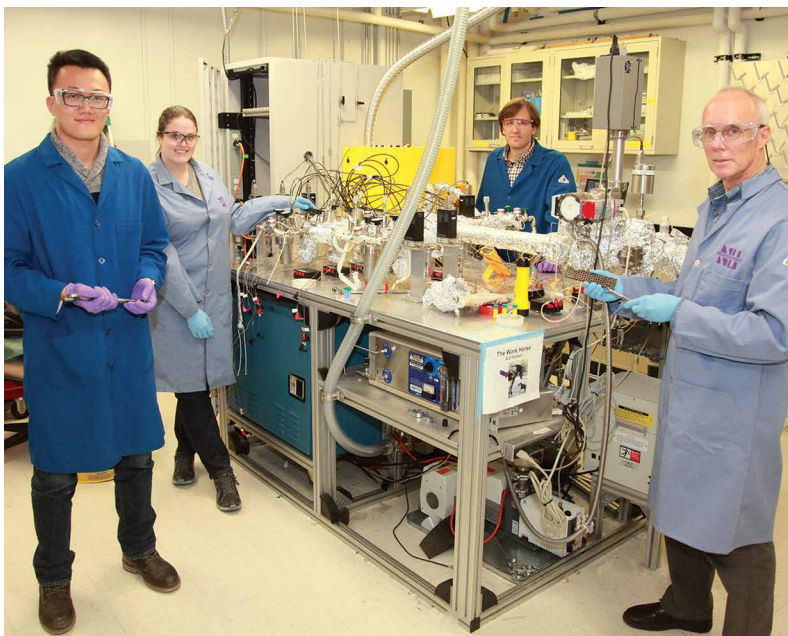
Energy Frontier Research Centers and Energy Innovation Hubs

Ten Hundred and One Word Challenge (www.energyfrontier.us/1001-word-challenge-winners, see also p. 7).

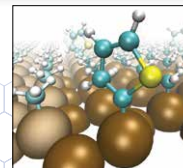
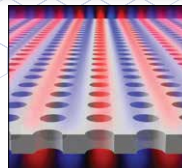
The EFRCs have established effective collaborations among themselves and with the larger scientific community. Activities include the EFRC Community Website (www.energyfrontier.us/), which facilitates the sharing of research highlights and meeting information and also serves as a repository for BES communications with the EFRCs. A grassroots effort by early-career scientists working within the EFRCs has resulted in the *Frontiers in Energy Research* newsletter (www.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. Each EFRC receives technical advice from a scientific advisory board made up of science and technology leaders in their research area. Altogether, there are more than 260 scientific advisory board members, including representatives from more than 40 companies.

The EFRCs focus on grand challenge and use-inspired science. Consequently, dissemination of scientific results through peer-reviewed publications is the primary measure of 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 August 2013, EFRC researchers had authored over 4,000 peer-reviewed publications, including more than 135 in *Science* and *Nature*. Centers have generated more than 90 unpatented invention disclosures, 200 U.S. and 130 foreign patent applications, and 50 associated licenses. The EFRCs report that 60 companies have benefited from the results of EFRC research, including small startups. In addition, EFRC staff and students are entering the workforce, with over 215 accepting university faculty and staff positions; 340 taking industrial positions; and 130 working at national laboratories, in



Synthesizing Oxide Nanocavity Catalysts. From right, Peter Stair and Justin Notestein of Northwestern University and Cassie George and Zhenyu Bo of the EFRC Institute for Atom-Efficient Chemical Transformations use an atomic layer deposition reactor to synthesize oxide nanocavity catalysts. [Image courtesy Northwestern University]



government, and for nonprofits. EFRC research highlights include:

- Experimental and theoretical demonstration showing that the vibrations carrying heat across materials can travel in a wavelike fashion through a stack of thin films, suggesting new ways for engineering thermoelectric materials that convert waste heat to electricity.
- Addition of an oxide sieve, a layer containing nanocavities, to a catalyst surface makes existing highly active catalysts selective for specific reactions and increases efficiencies for chemical processes.
- Isolation and characterization of a functioning photosynthetic megacomplex, including the light-harvesting antenna called a phycobilisome and the Photosystem I and II reaction centers. Researchers were able to observe for the first time how energy is transferred within the megacomplex.

Selected Accomplishments

The following pages describe EFRC science that has led to (1) a new material for separating methane from carbon dioxide and (2) the experimental verification of a single photon generating two electrons, a process that could be used to improve the efficiency of organic solar cells. These highlights represent a small fraction of the total research output of the 46 EFRCs. Additional EFRC research highlights can be found at science.energy.gov/bes/efrc/highlights/.

EFRC Research Accomplishment

Discovery of New Materials to Capture Methane

Predicted zeolites could economically produce high-purity methane from natural gas sources and separate it from coal mine ventilation systems

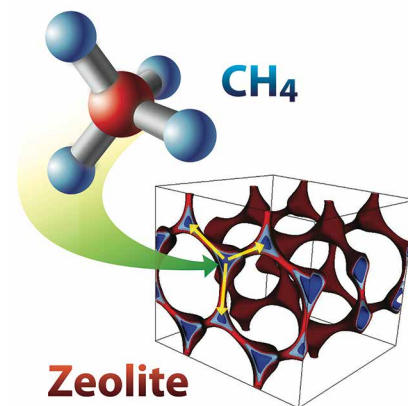
The Science: Computer simulations reveal new zeolites (porous crystalline adsorbents used by oil industries) with sufficient methane (CH_4) adsorption capacity and better methane/carbon dioxide (CO_2) and methane/nitrogen selectivity to be technologically promising for CH_4 capture from dilute and medium-concentration sources.

The Impact: The long-sought-after, low-cost separation of high-purity CH_4 from low-quality natural gas sources could provide a new commercial source of CH_4 for use as a fuel or chemical feedstock. Capturing CH_4 emitted from a variety of low-concentration sources will help reduce its powerful greenhouse gas contribution to global climate change and improve coal mine safety.

Summary: CH_4 , a common gas emitted from natural gas systems, landfills, coal mining, wastewater treatment, and ocean hydrates, is both a source of energy as well as a greenhouse gas with a global warming potential over 20 times that of CO_2 . CH_4 often coexists with CO_2 and nitrogen gas (N_2). Effective techniques are needed for the economical separation of CH_4 from these gases to use as a fuel and reduce its environmental impact. Such techniques have proved challenging, however, because CH_4 molecules are nonpolar, having an overall charge-neutral system with a highly symmetric structure that makes them interact weakly with most materials systems. To address this knowledge gap, a team of Lawrence Berkeley National Laboratory scientists from the Center for Gas Separations Relevant to Clean Energy Technologies, an EFRC led by the University of California–Berkeley, collaborated with scientists at Lawrence Livermore National Laboratory to develop novel computational approaches for screening over 87,000 possible zeolites. This study discovered several technologically promising zeolite structures with sufficient CH_4 sorption capacity and excellent selectivity for separating CH_4 from mixtures with CO_2 and N_2 . Realization of these new zeolite materials could enable the economic production of high-purity CH_4 from natural gas systems. These materials could be used to separate CH_4 from a variety of low-concentration sources, reducing its environmental impact and enhancing safety in closed environments in which high CH_4 concentrations could result in explosions.

Reference

Kim, J., et al. 2013. “New Materials for Methane Capture from Dilute and Medium-Concentration Sources,” *Nature Communications* **4**, 1694. DOI:10.1038/ncomms2697.



Capturing Methane. Calculations predict that the zeolite structure, schematically shown in the figure above, will effectively capture methane (CH_4) from a low-quality natural gas mixture of carbon dioxide (CO_2) and CH_4 . Under medium CH_4 concentrations, CH_4 adsorbs preferentially over CO_2 because the distances (yellow arrows) between adsorption sites (blue) are optimal for favorable CH_4 - CH_4 interactions. [Image courtesy Berend Smit, University of California–Berkeley. Reprinted by permission from Macmillan Publishers Ltd: From Kim et al. 2013. Copyright 2013.]

EFRC Research Accomplishment

Double the Current from Each Absorbed Photon

Two independent studies demonstrate the possibility of generating more than one electron of current from each absorbed photon of light in organic solar cells

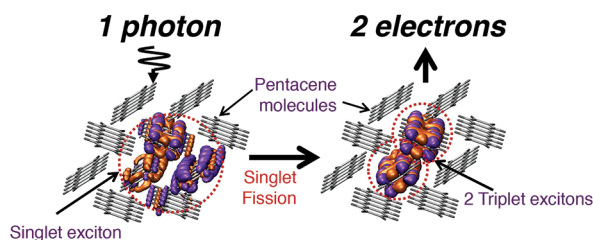
The Science: Two EFRC research teams have identified processes in organic photovoltaic materials that could enable the generation of more than one electron of current per incident photon of light.

The Impact: These results demonstrate the potential for incorporating materials into solar cell designs that can significantly enhance solar cell efficiency beyond the limit imposed by the assumption that each absorbed photon generates only one electron.

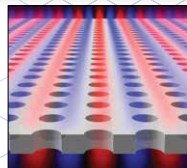
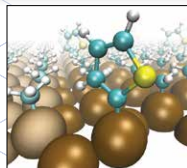
Summary: Conventional solar cells generate a maximum of one electron per incident photon and waste the remaining energy as heat. Multiple exciton generation (MEG) refers to the creation of two or more pairs of charge carriers (electron-hole pairs known as excitons) from the absorption of one photon of light. Although MEG holds great promise for improving the efficiency of organic solar cells, it has proven challenging to implement. Working independently, researchers at two EFRCs—the Center for Re-Defining Photovoltaic Efficiency Through Molecule Scale Control (RPEMSC) at Columbia University and the Center for Excitonics (CE) at the Massachusetts Institute of Technology—showed that singlet fission can reduce losses and produce up to two electrons per absorbed photon. Both groups studied pentacene, a well-known singlet fission material, deposited on carbon fullerene layers to produce a donor/acceptor interface. Using ultrafast spectroscopy techniques, RPEMSC researchers found that the multi-exciton state can decay into two triplet excitons that can subsequently transfer two electrons into the fullerene layer. Under certain conditions, they also found that two electrons can be transferred directly from the multi-exciton state to an adjacent fullerene layer on a subpicosecond time scale. Similarly, studies by CE researchers confirmed a fission yield of two triplet excitons per absorbed photon for pentacene layers larger than 5 nm and demonstrated an electron yield of 1.26 electrons per photons in pentacene-based organic solar cells. Together, these studies point to a new set of solar cell design principles for harvesting energy through multiple exciton generation in organic materials (see figure).

References

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Yield of Two Electrons per Absorbed Photon. A single photon is absorbed by a pair of pentacene molecules to generate an energetically excited state consisting of a bound electron-hole pair (i.e., a singlet exciton) and involving the electron orbitals of both pentacene molecules (left). Fission of the singlet exciton produces two separate triplet excitons (right), each capable of producing an electron of current via charge transfer to an acceptor molecule (not shown). [Image courtesy Shane Yost and Troy Van Voorhis, Massachusetts Institute of Technology]



Energy Frontier Research Centers and Energy Innovation Hubs

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 and 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 viable solar fuels generator has the potential for profound environmental and economic impacts. This development would establish U.S. global leadership in renewable energy, reduce dependence on imported oil, decrease greenhouse gas emissions, and provide new jobs in an emerging high-tech field.

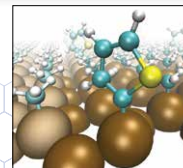
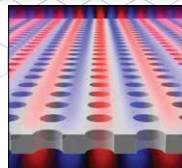
In September 2010, BES initiated the Fuels from Sunlight Energy Innovation Hub as one of DOE's first three Hubs. Called the Joint Center for Artificial Photosynthesis (JCAP), this Hub is led by the California Institute of Technology with partners at Lawrence Berkeley National Laboratory (LBNL), SLAC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



JCAP focuses specifically on the design and development of artificial photosynthetic prototypes for the commercial marketplace. It is organized into eight project areas that support two primary research thrusts:

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

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



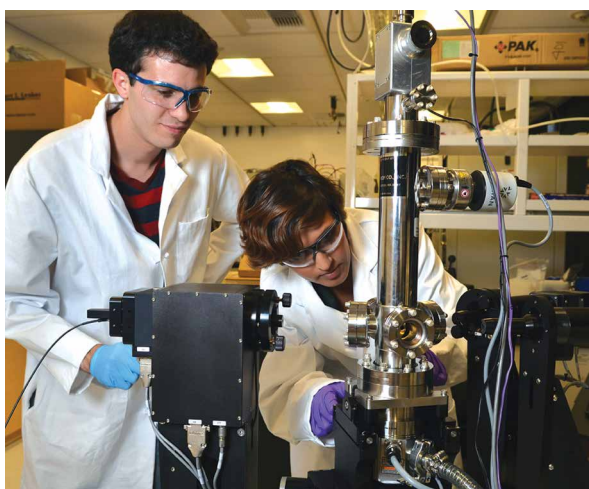
daily, as detailed in the research accomplishment on p. 51.

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

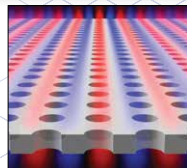
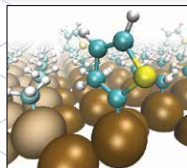
JCAP is currently staffed by some 150 principal investigators, postdoctoral researchers, technical and administrative staff, and graduate students. JCAP research is augmented by collaborations with scientists and engineers from EFRCs, other DOE programs, and foreign countries. Video and telecommunications 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 it has worked diligently to establish formal mechanisms to protect intellectual property, license materials and devices, and secure confidential advice from collaborators and two external advisory boards. BES oversight of JCAP has included monthly teleconferences between JCAP management and BES staff, quarterly and annual written reports, and informal site visits.

Research conducted by JCAP has produced numerous scientific publications and invention disclosures. These include:

- Synthesis and detailed characterization of many earth-abundant semiconductor materials with suitable band gaps for water splitting and carbon dioxide activation. (Current artificial photosynthetic systems use expensive or rare metals unsustainable for large-scale or long-term use.)
- Development of technologies that enable rapid synthesis and in-line characterization of light absorbers and catalysts for artificial photosynthetic systems—scalable to 1 million samples per day.
- Establishment of benchmarking capabilities that evaluate the efficacy and stability of catalysts and light absorbers, including a systematic investigation of published and novel oxygen evolution reaction catalysts.



Characterization of Light-Absorbing Materials. JCAP investigators Erik Verlage (left) and Pri Narang use a spectroscopic ellipsometer to determine semiconductor band gaps. Members of a large scientific team, they are working toward synthesis and characterization of novel light-absorbing materials. [Image courtesy California Institute of Technology]



Energy Frontier Research Centers and Energy Innovation Hubs

Batteries and Energy Storage Hub

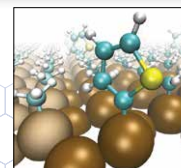
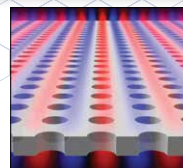
www.jcesr.org

Batteries and energy storage are key to the nation's energy future. Few areas of science and technology are more crucial to developing a fundamentally new energy economy with decisively reduced dependence on imported oil. The expanded use of renewable but intermittent energy sources (e.g., sun, wind, and tide), coupled with increasing demand for electric transportation vehicles, has greatly enhanced the need for advanced energy storage solutions. Progress in battery and electrical energy storage technologies over the past decade has been impressive, and work continues apace, including research sponsored by DOE's Office of Science, Office of Energy Efficiency and Renewable Energy (EERE), and, most recently, Advanced Research Projects Agency-Energy (ARPA-E). However, improvements achieved to date, while meaningful and important, fall short of the genuinely transformational advances in technology needed to usher in a new era of significantly greater reliance on renewable energy and reduced petroleum consumption. To build on and accelerate progress made thus far, individual efforts need to be integrated into a cross-disciplinary R&D program that includes the exploration of new materials, devices, systems, and approaches for transportation and utility-scale storage. Success means producing and translating 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 further develop and deploy these new technologies into the marketplace.

In November 2012, the Batteries and Energy Storage Hub was awarded to the Joint Center for Energy Storage Research (JCESR) as the fourth Energy Innovation Hub established by DOE since 2010. JCESR is led by Argonne National Laboratory (ANL) in partnership with four other DOE national laboratories, five universities, and four private firms. Joining ANL on the JCESR team are LBNL, Pacific Northwest National Laboratory, Sandia National Laboratories, and SLAC. Partner universities include Northwestern University, University of Chicago, University of Illinois at Urbana-Champaign, University of Illinois at Chicago, and University of Michigan. Private firms contributing to the effort are Dow Chemical Co.; Applied Materials, Inc.; Johnson Controls, Inc.; and Clean Energy Trust.



JCESR's goal is to enable rechargeable batteries that are five times more powerful and five times cheaper within 5 years. JCESR's core task is basic research, and its overarching strategy is to use a new generation of 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 will enable JCESR to reinvent electrical energy storage and accelerate major battery performance improvements at reduced cost. JCESR's industrial partners will help guide the Hub's efforts to ensure that the research leads toward practical solutions that are competitive in the marketplace.



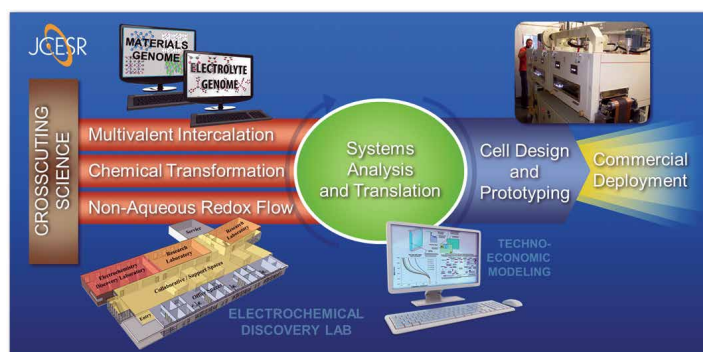
JCESR's discovery science activities are motivated by three primary technical challenges related to the next generation of rechargeable batteries beyond lithium (Li) ion:

- **Increasing Charge Density**
- **Storing Energy in Chemical Bonds**
- **Storing Energy in Liquids**

Increasing Charge Density research explores the use of multiply charged ions. For example, can a singly charged Li ion be replaced with a doubly or triply charged ion such as magnesium or aluminum to double or triple the energy density of batteries? Use of multiply charged ions leads to fundamental questions related to the speed with which they move through liquids, across interfaces between battery materials, and into solids where they store and release energy. Success with this process, called multivalent intercalation, coupled with battery electrode improvements, could lead to high-capacity, high-voltage batteries that store five times more energy in the same space as today's batteries.

The **Storing Energy in Chemical Bonds** activity seeks to discover new electrode materials that can store and release electricity by making and breaking high-energy chemical bonds. Such chemical transformation discoveries can lead to new battery materials and architectures with highly reversible charge and discharge cycles, dramatically increased storage capacities, longer battery lifetimes, and lower system costs.

Storing Energy in Liquids research investigates whether conventional solid electrodes can be replaced with inexpensive liquid solutions or nanoparticle suspensions that charge and

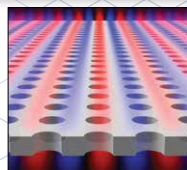
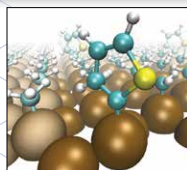


JCESR Battery R&D Paradigm. Researchers from across disciplines and JCESR partner institutions are working together to produce discovery science and predictive models that enable translation of the science into innovative technical approaches to research prototypes of next-generation rechargeable batteries. [Image courtesy JCESR]

discharge as they flow through next-generation batteries. Scientific knowledge of the so-called nonaqueous redox flow cell will help JCESR design new molecules, electrolytes, and membranes that greatly increase battery storage capacity, stability, and power output, while dramatically reducing costs.

JCESR's advanced computational tools are key to streamlining next-generation materials discovery and guiding battery design and development. Materials genome techniques will discover and evaluate tens of thousands of advanced candidate electrodes. JCESR's innovative electrolyte genome opens access to broad new classes of "soft" energy storage materials unconstrained by crystal structure. Techno-economic modeling translates these materials discoveries to systems-level operation, projecting the performance and cost of candidate battery systems before they are prototyped.

In its first full year of operation (corresponding roughly to the 2013 calendar year), JCESR completed its startup phase while establishing



Energy Frontier Research Centers and Energy Innovation Hubs

and equipping research facilities, hiring personnel, setting up management and operations procedures, and establishing strategic objectives and milestones.

JCESR already has reached nearly full staffing levels with over 150 scientists, graduate students, postdoctoral researchers, and technical and administrative staff joining the effort in the first year. JCESR management has been building a collaborative research community that can present findings, impediments, and solutions on a real-time basis, so that scientific inspiration and discovery can advance unhindered by time and physical locations. Video and telecommunications networks link personnel and support weekly and biweekly meetings of the various JCESR research teams, and additional software collaboration tools have been added as part of the “JCESR Without Walls” operational strategy. Processes for identifying, protecting, and using intellectual property (IP) are in place as part of an integrated IP management system that features an umbrella nondisclosure agreement for JCESR’s partners. JCESR management receives external guidance from two independent advisory councils: the Strategic Advisory Council, made up of the Science and Technology Panel and the Commercialization Panel, and the Venture Advisory Council. BES oversight of JCESR has included monthly teleconferences between JCESR management and BES staff, quarterly written reports, and an informal site visit in the startup phase. BES also conducted an independent review of JCESR’s management structure and early operations in October 2013.

Initial JCESR research has produced several scientific publications and invention disclosures. Highlights include:

- Characterizing the electrochemical properties of a novel Li metal/polysulfide semi-liquid cell and creating a design for a hybrid flow battery that eliminates the need for a separator membrane. A lab-scale research prototype of the battery cell maintained excellent energy storage performance through more than 2,000 charges and discharges, equivalent to more than 5 years of daily cycles.
- Discovering that activated carbon promotes Li superoxide (Li_2O) formation during discharge of a Li-air battery. Partial conversion of Li_2O to Li peroxide (Li_2O_2) during discharge results in a core (Li_2O_2)–shell (Li_2O) product that is believed to be responsible for a significantly lower overpotential, and thus greater efficiency, in the recharging process.
- Combining theoretical calculations and experimental data to probe sodium (Na) ion transport and deformation behavior in tin oxide nanowires, discovering that Na ion diffuses 30 times slower than Li ion and that pore formation upon Na ion removal leads to poor cycling of this electrode type.

Selected Accomplishments

The following pages highlight DOE Hub research on (1) the high-throughput discovery of solar fuel catalysts and (2) rational design of electrodes for rechargeable batteries. These highlights represent only a small portion of the research output of the two BES-managed Hubs. The latest BES highlights can be found at science.energy.gov/bes/highlights/.

JCAP Hub Research Accomplishment

High-Throughput Discovery of Solar Fuels Catalysts

New technology enables rapid synthesis and in-line characterization of materials for artificial photosynthesis

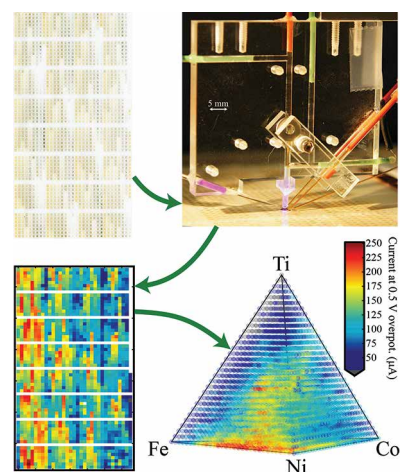
The Science: Researchers at JCAP have developed the capability for creating enormous libraries of materials and quickly evaluating their utility as light absorbers and catalysts for artificial photosynthetic systems. This approach has uncovered novel catalysts that use light to produce oxygen from water and promises to yield other high-performing light absorber–catalyst combinations, a critical step in the pathway toward large-scale production of storable fuels from sunlight.

The Impact: Decades of conventional research have led to the identification of only a small number of materials capable of producing fuels from sunlight, but no assembly of known materials has proven sufficiently efficient for large-scale solar fuel production. This high-throughput technology developed by JCAP enables rapid synthesis and in-line screening of candidate materials, greatly accelerating the discovery rate of artificial photosynthetic light absorbers and catalysts.

Summary: Development of artificial photosynthetic systems requires transformational materials that absorb sunlight and efficiently catalyze chemical reactions that produce fuel. Conventional research approaches have not yet yielded such materials, prompting JCAP researchers to greatly amplify these efforts by developing the technology to make and screen enormous libraries of candidate materials. Similar high-throughput methods have yielded breakthroughs in drug discovery and related fields, but they have not been widely applied to energy science. JCAP has developed unique capabilities to make and characterize potential photocatalytic materials in unprecedented throughput—capabilities that can be scaled to a million samples per day. Initial demonstrations of this technology involved synthesis of new metal oxide compositions and rapid evaluation of their optical and catalytic performance. For example, by screening 5,456 different mixtures of iron, copper, nickel, and tin oxides, the group discovered a new, unpredicted high-performance catalyst. Such newly discovered materials are further investigated by carefully crafted teams of JCAP scientists and engineers, ultimately leading to the creation of new artificial photosynthetic devices. JCAP is applying its high-throughput methods to explore a plethora of materials with other atomic compositions, accelerating the discovery of light absorbers and catalysts needed for large-scale production of solar fuels.

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Catalytic Current Evaluation Tools. Scanning drop electrocatalyst screening is 1 of 10 analytical pipeline tools developed to evaluate large libraries of candidate materials for artificial photosynthesis. Printed using a novel ink-jet method, the (Fe-Ni-Co-Ti) O_x library (top left) is evaluated by a scanning drop electrochemical cell (top right) to produce a map of catalytic current (plot, bottom left) that is rearranged to identify catalytic activity trends in the 3D composition space (plot, bottom right). [Image courtesy California Institute of Technology. Reprinted by permission: From Gregoire et al. 2013b. Copyright 2013: AIP Publishing LLC.]

JCESR Hub Research Accomplishment

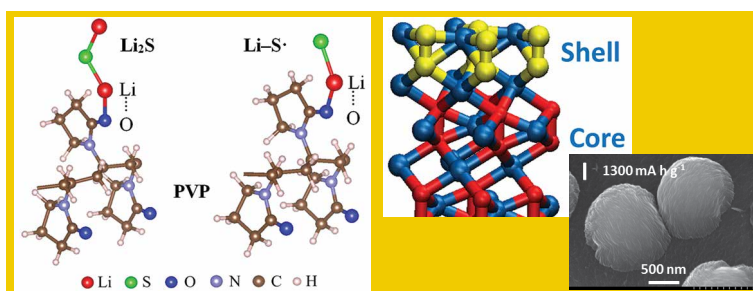
Rational Design of Electrodes for Batteries

Approach could lead to high-performance battery systems for use in emerging applications such as vehicle electrification and grid-scale energy storage

The Science: Rechargeable batteries have three major components—an anode, a cathode, and an electrolyte sandwiched in between the two electrodes. A major limitation of today's rechargeable batteries is the energy capacity limit of the cathode materials used in current Li-ion batteries. Two promising higher-energy cathodes for batteries beyond Li ion are air (O_2) cathodes, when paired with Li-metal anodes, and Li-sulfur (Li_2S) cathodes, when paired with non-Li metal anodes such as carbon or silicon.

The Impact: Understanding the full range of chemical and physical changes that cathode materials undergo during repeated charging and discharging is critical to the rational design of improved cathodes, replacing the less efficient trial-and-error method of searching for better performance. Furthermore, the design of higher energy-density cathodes must be done in conjunction with the development of a suitable anode and electrolyte to produce an integrated battery system that is high performing, safe, and reliable. The corresponding capability to perform system-level modeling, also enabled by the discovery science, supports rational battery design and ensures that the system's components will work together reliably beyond laboratory-scale research prototypes.

Summary: JCESR researchers have combined theoretical calculations and experimental data to elucidate the chemical interactions and changes that occur at O_2 and Li_2S electrode assemblies, which include the cathode material, conductive supports, binders, and additives. Calculations were used to identify specific polymeric binders that possess strong Li-O interaction with both Li_2S and lithium polysulfides, which resulted in reduced Li_2S dissolution and therefore significantly more stable cycling performance in Li_2S cathodes when tested in the laboratory. In similar studies of the electrochemical reduction of O_2 to Li_2O at an air cathode, the porosity of an activated carbon electrode was discovered to provide a nanoscale environment that promotes growth of a core (Li_2O_2)/shell (Li_2O) structure during discharge. The voltage required to recharge the system starting from the composite discharge product is significantly less than from Li_2O itself, demonstrating that activated carbons provide an excellent platform for the rational design of more efficient cathodes for high energy-density Li- O_2 battery systems.



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- Seh, Z. W., et al. 2013. "Stable Cycling of Lithium Sulfide Cathodes Through Strong Affinity with a Bifunctional Binder," *Chemical Science* **4**, 3673–77.
- Zhai, D., et al. 2013. "Disproportionation in Li- O_2 Batteries Based on a Large Surface Area Carbon Cathode," *Journal of the American Chemical Society* **135**, 15364–72.

Battery Electrode Design. **Left:** Using *ab initio* simulations, poly (vinylpyrrolidone) (PVP) binder was found to possess strong affinity for both Li_2S and lithium polysulfides. **Bottom right:** Li_2O (shell)/ Li_2O_2 (core) composite structure grown on an activated carbon electrode at a discharge capacity of 1300 mAh/g. **Top right:** Shell-core illustration shows result from *ab initio* simulations. [Left image courtesy Yi Cui, SLAC National Accelerator Laboratory. Reprinted by permission of The Royal Society of Chemistry: From Seh et al. 2013. Right images courtesy Larry Curtiss, Argonne National Laboratory. Reprinted by permission of the American Chemical Society: From Zhai et al. 2013. Copyright 2013.]

Images

Research Portfolio and User Facilities, pp. 10–11

Row one, from left: (1) Atomic force microscope (AFM) micrograph of arrays of niobium islands (red) on gold underlayer (yellow). Arrows illustrate fluctuating superconducting properties of the niobium islands. Designing geometrical arrays of superconducting islands enables novel, highly tunable superconducting and metallic states, which can be used to enhance understanding of various technologically important materials. [Image courtesy Nadya Mason and Serena Eley, University of Illinois Urbana-Champaign] **(2)** Advanced Photon Source at Argonne National Laboratory (ANL). [Image courtesy ANL] **(3)** Simulated soot particle (see p. 27).

Row two, from left: (4) Schematic of multistage pathway of 2D crystallization by S-layer proteins on a lipid membrane (background constructed from AFM images from different time points; foreground based on cryoelectron tomography images). [Image courtesy Jim DeYoreo, Pacific Northwest National Laboratory (PNNL), with Sungwook Chung, Seong-Ho Shin, and Luis Comolli, Lawrence Berkeley National Laboratory] **(5)** Nanosized particles (composed of copper sulfide) cling to extremely thin threads (single-walled carbon nanotubes). [Image courtesy ANL] **(6)** Encapsulation of the sulfate anion in a urea-functionalized, self-assembled cage. [Image courtesy Radu Custelcean. Custelcean, R. 2014. "Anion Encapsulation and Dynamics in Self-Assembled Coordination Cages," *Chemical Society Reviews* advance article. DOI:10.1039/C3CS60371G.]

Row three, from left: (7) Observation of light trapped without mirrors and confined within a photonic crystal slab with a periodic array of holes, "allowing" light to escape. Blue and red colors indicate amplitude of the light's electric field. [Image courtesy Chia Wei, Harvard University] **(8)** Low-temperature scanning tunneling spectroscopy image of a heavy electron material revealing the structure of the superconducting state. [Image courtesy Ali Yazdani, Princeton University] **(9)** Combustion simulation of a lifted auto igniting turbulent hydrogen/air jet flame by Chung Sang Yoo and Jackie Chen; volume visualization of hydroxyl radical and particle tracks (colored by temperature) by Hongfeng Yu and Kwan-Liu Ma; particle visualization by Ray Grout. [Image courtesy Jackie Chen, Sandia National Laboratories]

Row four, from left: (10) Distribution of superconductivity in a thin sheet of superconducting film (see p. 17). **(11)** Thiophene-based covalent organic framework. [Image courtesy Mircea Dinca; Bertrand, G. H. V., et al. 2013. "Thiophene-Based Covalent Organic Frameworks," *Proceedings of the National Academy of Sciences (USA)* **110**(13), 4923–28. DOI:10.1073/pnas.1221824110.] **(12)** High-performance, solution-processed TIPSE pentacene-polymer blend. [Reprinted by permission from Chen, J., et al. 2013. "Conjugated Polymer-Mediated Polymorphism of a High Performance, Small-Molecule Organic Semiconductor with Tuned Intermolecular Interactions, Enhanced Long-Range Order, and Charge Transport," *Chemistry of Materials* **25**(21), 4378–86. Copyright 2013: American Chemical Society.]

Materials Science and Engineering

From left, pp. 12–13: (13) Watching ions hop in battery materials (see p. 19). **(14)** Artist's rendering of remote Joule heating (palladium plates: silver blocks; carbon nanotube: dark blue). [Image courtesy John Cumings, University of Maryland] **(15)** Distribution of superconductivity in a thin sheet of superconducting film (see p. 17).

Chemical Sciences, Geosciences, and Biosciences

From left, pp. 20–21: (16) See image 9. **(17)** Hexanuclear cluster observed in crystal structure of $\text{Li}_6[\text{Pu}_6(\text{OH})_4\text{O}_4(\text{H}_2\text{O})_6(\text{HGly})_{12}]\text{Cl}_{18}\cdot 10.5\text{H}_2\text{O}$, which was isolated from aqueous solution and characterized using x-ray diffraction. [Reprinted by permission from Knope, K., and L. Soderholm. 2013. "Plutonium(IV) Cluster with a Hexanuclear $[\text{Pu}_6(\text{OH})_4\text{O}_4]^{12+}$ Core," *Inorganic Chemistry* **52**(12), 6770–72. Copyright 2013: American Chemical Society.] **(18)** High-resolution scanning electron microscope (SEM) image of reacted forsterite, indicating formation of magnesite. [Image courtesy Andrew Felmy, PNNL]

Scientific User Facilities

From left, pp. 28–29: (19) Edge-on SEM photograph depicting free-standing, self-aligned silica nanowires supported by a silicon wafer and possessing small indium droplets at their tips. [Image courtesy ANL] **(20)** Spin waves along the $(-1, K, +0.4)$ direction through the Γ and S points. [Reprinted by permission from Ehlers, G., et al. 2013. "Incommensurability and Spin Dynamics in the Low-Temperature Phases of $\text{Ni}_3\text{V}_2\text{O}_8$," *Physical Review B* **87**, 214418. DOI:10.1103/PhysRevB.87.214418.] **(21)** Advanced Photon Source. [Image courtesy ANL]

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From left, pp. 38–39: (22) Calculated structure of covalently bound thiophene molecules on a methyl-terminated silicon surface. [Image courtesy Joint Center for Artificial Photosynthesis. Reprinted by permission from Yu, M., et al. 2013. "Theory of Covalent Adsorbate Frontier Orbital Energies on Functionalized Light-Absorbing Semiconductor Surfaces," *The Journal of Physical Chemistry Letters* **4**, 1701–06. Copyright 2013: American Chemical Society.] **(23)** See image 7. **(24)** ANL battery researcher Javier Bareno Garcia-Ontiveros manipulating an air-sensitive sample inside an inert glove box filled almost entirely with argon gas; thus very little water or oxygen is inside to react with and degrade the special battery materials. [Image courtesy Joint Center for Energy Storage Research]

