Science for Energy Technologies

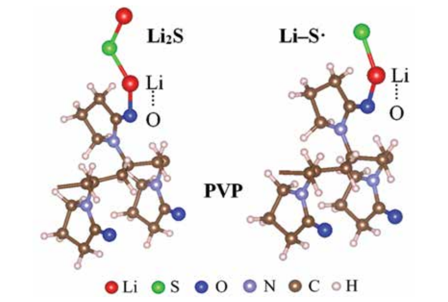
BES supports use-inspired research to accelerate the innovation of clean energy technologies. Use-inspired research, while still addressing fundamental issues, is directed more toward scientific "show-stoppers" that limit the development of new energy technologies. Select highlights from the BES research portfolio in the areas of energy generation, storage, and efficiency follow below.

Semiconductors Stabilized for Incorporation in Photoanodes for Solar Fuel Generators. Highly light absorbing semiconductors, such as silicon and gallium arsenide, corrode when submerged in the aqueous solutions used in solar fuel production. A new transparent titanium dioxide coating protects components, paving the way for use of these semiconductors in solar fuel generators.

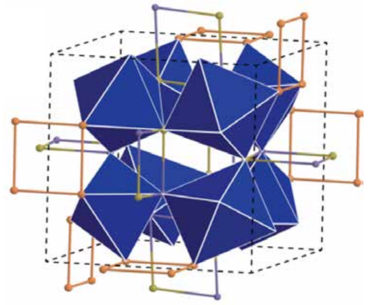
Next-Generation Energy Storage Systems. Emerging battery technologies have the potential to increase battery life, lower battery cost, and increase energy storage capacity. A novel molecular design for lithium-sulfur (Li_2S) cathodes has demonstrated record performance, with a 40% increase in storage capacity and only half the polysulfide loss compared with that of conventional technologies.

Electricity from Waste Heat. Heat loss is a major source of inefficiency in energy conversion processes, from home heating to transportation applications and large-scale power generation facilities. Recent experiments with $CoSb_{3(1-x)}Ge_{1.5x}Te_{1.5x}$ confirmed that substituting Ge/Te atoms reduces thermal conductivity, leading to more efficient thermoelectric materials that can reclaim lost energy as electrical power.

Creating Fuels from Sunlight. An artificial photosynthesis system would generate usable fuels directly from sunlight, carbon dioxide, and water. To address one of many scientific and engineering challenges for such a system, a new transparent, yet electronically conducting, titanium dioxide coating was devised to protect materials from corrosion in water while maintaining excellent electrical charge conduction to the surface. [DOI:10.1126/science.1251428]



Rational Battery Electrode Design. Using *ab initio* simulations, the polyvinylpyrrolidone (PVP) binder was found to possess strong affinity for both Li_2S and lithium polysulfides. Illustration shows density functional calculations of the stable configurations and binding energies of Li_2S and Li-S functional groups in the PVP binder. [Yi Cui, SLAC National Accelerator Laboratory. DOI: 10.1039.C3SC51476E]



Reducing Thermal Conductivity in Skutterudites. Dominant heat-carrying modes in skutterudites are associated with pnicogen ring vibrations. Disrupting the ring structure has proven effective in reducing the lattice thermal conductivity in this cobalt arsenide mineral. Shown is a typical crystal structure with an energetically favorable ring configuration at x = 0.5. [Ctirad Uher, University of Michigan. DOI: 10.1103/PhysRevB.86.195209]

BES Research at a Glance

Total investments span diverse research sectors, including more than 170 academic, nonprofit, and industrial institutions in all 50 states and at 15 DOE laboratories.

In FY 2014, BES invested some $670M in research across all funding modalities:

- 998 core research projects in 23 core research areas
- 32 Energy Frontier Research Centers
- Fuels from Sunlight Energy Innovation Hub
- Batteries and Energy Storage Energy Innovation Hub

BES supports worldclass, open-access, and complementary scientific user facilities with the FY 2014 operating budget of about $780M, including:

- Intense x-ray sources
- Neutron scattering facilities
- Research centers for nanoscale science
- Electron beam characterization centers

Cover image credits. Extended captions and credits at *Basic Energy Sciences Summary Report*, science.energy.gov/bes/research/. **ROW 1: (1)** Ions hopping in battery materials [Aaron Lindenberg, SLAC National Accelerator Laboratory] **(2)** Remote Joule heating [John Cumings, University of Maryland] **(3)** Superconducting film [Valerii Vinokur, Argonne National Laboratory (ANL)] **(4)** Structure of superconducting state [Ali Yazdani, Princeton University] **(5)** High-energy X-ray diffraction pattern [Adam Goldman and Paul Canfield, Ames Laboratory. Reprinted by permission from Macmillan Publishers Ltd: From Goldman et al. 2013. © 2013.] **ROW 2: (1)** Combustion simulation [Jackie Chen, Sandia National Laboratories] **(2)** Hexanuclear cluster [Reprinted by permission from Knope, K., and L. Soderholm. 2013. "Plutonium(IV) Cluster with a Hexanuclear $[Pu_6(OH)_4O_4]^{12+}$ Core," *Inorganic Chemistry* **52**(12), 6770–72. © 2013: American Chemical Society.] **(3)** Reacted forsterite, indicating magnesite formation [Andrew Felmy, Pacific Northwest National Laboratory] **(4)** Niobium islands [Nadya Mason and Serena Eley, University of Illinois, Urbana-Champaign] **(5)** Atomically dispersed palladium atoms on copper [Charles Sykes, Tufts University] **ROW 3: (1)** Nanowires [ANL] **(2)** Spin dynamics [Reprinted by permission from Ehlers, G., et al. 2013. "Incommensurability and Spin Dynamics in the Low-Temperature Phases of $Ni_3V_2O_8$," *Physical Review B* **87**, 214418. DOI:10.1103/PhysRevB.87.214418.] **(3)** Advanced Photon Source (APS) [ANL] **(4)** Carbon nanotubes [ANL] **(5)** Superconducting undulator at APS [ANL]

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Basic Energy Sciences

Basic Energy Sciences supports fundamental research to understand, predict, and ultimately control matter and energy at the electronic, atomic, and molecular levels. This understanding provides the foundations for new energy technologies that support Department of Energy missions in energy, environment, and national security. Key research areas are described below.

Discover and design new materials with novel structures, functions, and properties by exploring the origin of macroscopic material behaviors and their fundamental connections to a material's atomic, molecular, and electronic structures.

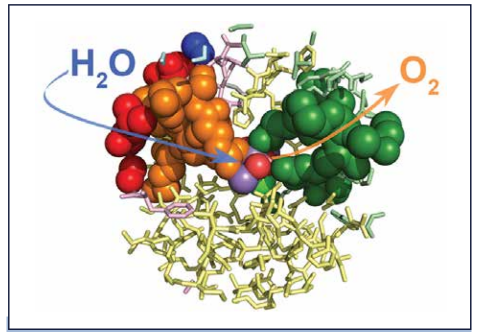
Understand and control complex chemical, geological, and biochemical processes underpinning diverse energy technologies by examining physical and chemical phenomena across vast spatial and temporal scales and at multiple levels of complexity.

Harness x-rays, neutrons, and electrons to reveal structure, composition, and function through open-access scientific user facilities offering sophisticated instrumentation to probe and create materials.

U.S. DEPARTMENT OF ENERGY
ENERGY
Office of Science

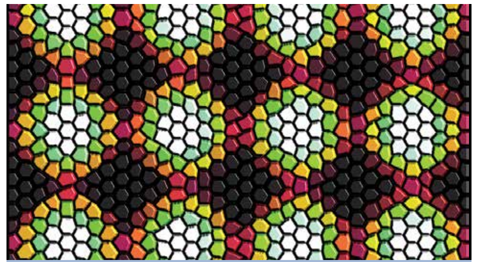
Discovery Science

The energy systems of the future—whether they tap sunlight, store electricity, or make fuel from splitting water or reducing carbon dioxide—will revolve around materials and chemical changes that convert energy from one form to another. BES-supported research helps develop the basic understanding of these processes to enable transformational advances in energy technologies. Select BES research portfolio accomplishments are described below.



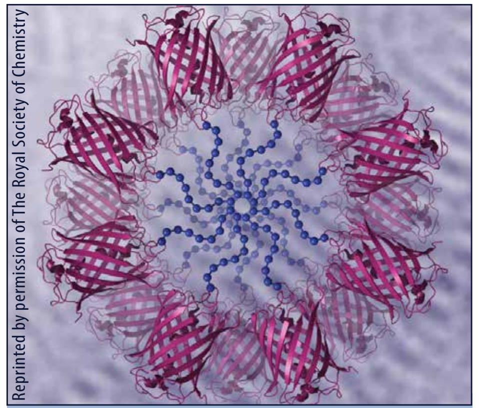
Sophisticated mass spectroscopy techniques mapped amino acids in the channel delivering water to the active site of PSII. Water and oxygen products shown superimposed on a PSII model. [Terry Bricker, Louisiana State University. DOI: 10.1074/jbc.M113.487003]

Tracking Water Molecules During Photosynthesis. Researchers have identified a possible channel that enables substrate water molecules to travel to the active site of Photosystem II (PSII), an enzyme complex used by plants to capture and convert solar energy to chemical energy. Insights may suggest new strategies for solar fuel production using natural and artificial photosynthesis.



In this thin sheet of superconducting film, the superconducting annuli surrounding the white holes (physical voids) induce superconductivity in the inter-hole constrictions. This results in a chain-mail-like configuration. [Valerii Vinokur, Argonne National Laboratory. DOI: 10.1038/ncomms2437]

High-Field Superconductors. A nanostructure approach demonstrates that in ultrathin wires or in thin sheets perforated by an array of nanosized holes, high magnetic fields do not inhibit superconductivity but actually protect it. Extension of this approach to high-temperature superconductors would enhance the use of superconducting wires in applications with high magnetic fields, and lower the barrier to wider use of superconductors in high-performance motors and generators.



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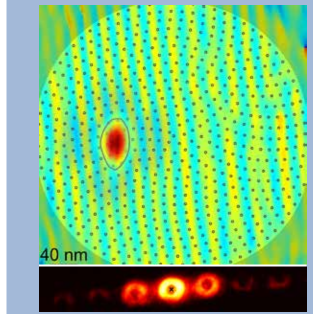
Cylinder-Forming, Self-Assembled Diblock Copolymers. First block: protein at the surface; second block: covalently attached synthetic polymer at the interior. [Bradley Olsen, Massachusetts Institute of Technology. DOI: 10.1039/C2SM27459K]

Self-Assembled Functional Biomaterials. Ordered functional protein arrays with designed molecular properties have been created through self-assembly, which is driven by the chemical incompatibility between the proteins and their chemically linked, designed synthetic polymers. Controlling the chemistry of the polymers and their interaction with water results in formation of materials with novel structures. Controlling these material nanostructures is significant for important applications in biocatalysis, sensors, renewable energy, and nanotechnology.

Enabling Tools for Basic Research

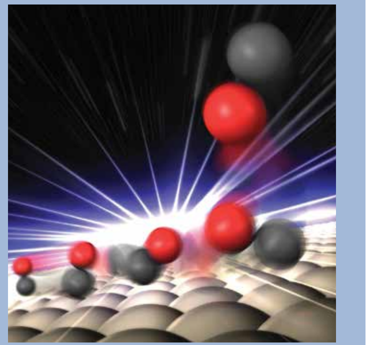
The development of advanced tools often leads to new scientific discoveries. BES invests in important tools for basic research ranging from large facilities like the light sources, to the pairing of theory and experiment to advance understanding of materials and phenomena, to laboratory equipment for the synthesis of new materials. Select highlights focusing on this connection between advanced tools and new scientific discoveries follow.

Towards Understanding Electronic Switching in Magnets. A penetrating, non-destructive, and high-resolution X-ray synchrotron imaging technique revealed key atomic-scale properties in ferroelectric materials. This technique can be used to study material behavior during harsh film-growth conditions or to characterize material below the coatings used in energy-conversion devices. Improved resolution and size of the image provide a unique opportunity to understand and engineer the domain regions that control the electronic properties in magnetic and charge-aligned, thin-film materials.



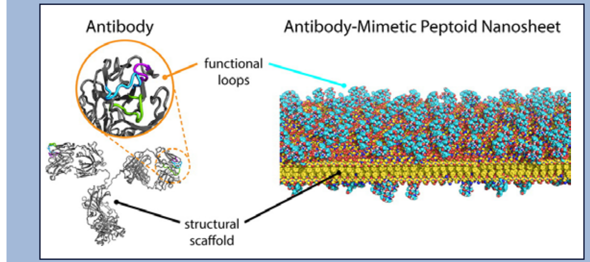
Electronic charge alignment in ferroelectric thin films, shown in alternating yellow and blue "stripes," was reconstructed from X-ray diffraction patterns (e.g., images at bottom). The position of the diffraction measurements are indicated by the open dots. The bright spot shows the shape and intensity of the x-ray nano-beam footprint at a single point. [Argonne National Laboratory; DOI: 10.1103/PhysRevLett.110.177601]

Real-Time Imaging of Catalyst Reaction. Catalysts, which speed up chemical reactions and increase their efficiency and effectiveness, are essential to the industrial production of many chemicals. Understanding how catalysts work, at ultrafast time scales and with molecular precision, is essential to developing lower-cost synthetic fuels as alternative energy sources that reduce pollution. Theoretical calculations predicted a short-lived state of the reactant that transitions so rapidly it could not be observed without a free-electron laser such as the Linac Coherent Light Source (LCLS). Combining theory with experiment helped build understanding about how the catalyst works and could lead to predictive design of new catalysts.



The ultrafast, ultrabright X-ray pulses of the LCLS have enabled an unprecedented view of how carbon monoxide molecules (red and charcoal joined spheres) react with the surface of a ruthenium catalyst. [SLAC National Accelerator Laboratory. DOI: 10.1126/science.1231711]

Functionalized Peptoid Nanosheets for Sensors, Catalysts, Supercapacitors. The synthesis of new materials is essential for advancing energy technologies. Using a custom-built automated synthesis capability, researchers discovered a new class of antibody-mimetic peptoid nanosheets covered in functional peptide loops, which can be programmed to selectively bind certain enzymes or inorganic materials. The new material holds promise for chemical sensing and catalysis and is an important step toward extending the rules of protein folding to the world of synthetic materials. The protein-binding ability of the nanosheets was demonstrated and used to template growth of gold metal; the resulting layered, gold-peptoid-gold composite shows potential as a miniaturized supercapacitor for energy storage.



Architecture of a natural antibody (left) and an antibody-mimetic nanosheet (right) with a high density of loops on a peptoid nanosheet scaffold. [Lawrence Berkeley National Laboratory. DOI: 10.1021/nn403899y]

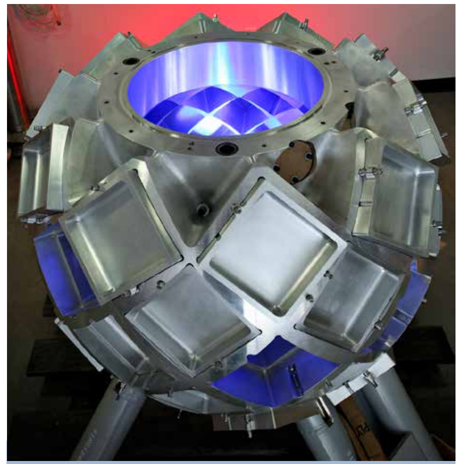
Scientific User Facilities

The scientific user facilities operated by BES provide unique capabilities and sophisticated instrumentation for advancing science in basic and applied energy-related disciplines. These premier facilities provide access based on user proposals submitted through a competitive merit review process by scientists from academia, federal laboratories, and industry.

X-Ray Light Sources. Supporting more than 11,000 users annually, the BES light sources provide incisive probes for advanced research in areas such as materials science, chemical sciences, metrology, geosciences, environmental sciences, biosciences, medical sciences, and pharmaceutical sciences. The fundamental parameters used to perceive the physical world (i.e., energy, momentum, position, and time) correspond to three broad categories of experimental measurement techniques: spectroscopy, scattering, and imaging.

Advanced Photon Source at Argonne National Laboratory.

Neutron Scattering Facilities. The BES neutron scattering facilities house unique and effective tools to probe the structure of matter, supporting more than 1,300 users per year. Neutron scattering is particularly well-suited for determining the atomic positions of both light and heavy atoms in a solid and the thermal fluctuations in those positions. In addition, neutrons scatter from magnetic moments in a material, providing information on magnetic structure as well.



Detector Array for the TOPAZ Single-Crystal Diffractometer at the Spallation Neutron Source at Oak Ridge National Laboratory.

Nanoscale Science Research Centers. The BES Nanoscale Science Research Centers (NSRCs) are premier user facilities for interdisciplinary research at the nanoscale level, serving more than 2,200 users annually. The NSRCs complement each other with different instrumentation and capabilities, thrusts of in-house research programs, and technical expertise of their staffs. The NSRCs contain clean rooms, nanofabrication resources, one-of-a-kind signature instruments, and other instruments not generally available except at major user facilities.

State-of-the-Art Clean Room for Fabricating Devices. Devices include those for nanoelectronics, nanophotonics, biomedical engineering, photovoltaics, x-ray optics, nanomagnetics, and beyond.