Basic Energy Sciences Program Update

U.S. DEPARTMENT OF ENERGY | Office of Science

BES BY THE NUMBERS

FY 2016

BES supports fundamental research to understand, predict, and ultimately control matter and energy at the electronic, atomic, and molecular levels.

BES RESEARCH SPANS

MORE THAN **150** ACADEMIC, NONPROFIT, AND INDUSTRIAL INSTITUTIONS

17 DOE NATIONAL LABORATORIES | **47** STATES AND WASHINGTON, D.C.

25 CORE RESEARCH AREAS

SUPPORTED RESEARCHERS

~5,400 Ph.D. SCIENTISTS | **~1,700** STUDENTS

36 ENERGY FRONTIER RESEARCH CENTERS

~$717 MILLION RESEARCH BUDGET

MORE THAN **15,000** USERS AT **12** BES FACILITIES

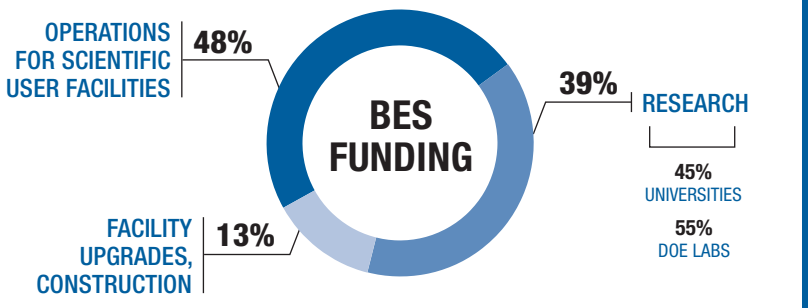
~$897 MILLION SCIENTIFIC USER FACILITY OPERATING BUDGET

OVER **1,000** CORE RESEARCH PROJECTS

~15% AVERAGE NEW GRANT SUCCESS RATE

2 ENERGY INNOVATION HUBS

~$236 MILLION FACILITY UPGRADES, CONSTRUCTION BUDGET



BES Mission

The U.S. Department of Energy's (DOE) Office of Basic Energy Sciences (BES) supports fundamental research to understand, predict, and ultimately control matter and energy at the electronic, atomic, and molecular levels to provide the foundations for new energy technologies and to support DOE missions in energy, environment, and national security. BES research disciplines—including condensed matter and materials physics, chemistry, geosciences, and aspects of physical biosciences—emphasize discovery of new materials and phenomena and design of new chemical processes. These disciplines intersect virtually every aspect of energy resources, production, conversion, transmission, storage, efficiency, and waste mitigation.

BES also plans, constructs, and operates world-class scientific user facilities that provide outstanding capabilities for imaging and spectroscopy, characterizing materials of all kinds ranging from hard metals to fragile biological samples, and studying the chemical transformations of matter. Researchers use these facilities to correlate the microscopic structure of materials with their macroscopic properties and to study chemical processes. Such experiments provide critical insights into electronic, atomic, and molecular configurations, often at ultrasmall length and ultrafast time scales.

Program Updates

Energy Frontier Research Centers

In fiscal year (FY) 2016, BES announced four new Energy Frontier Research Center (EFRC) awards to accelerate the scientific breakthroughs needed to support DOE's environmental management and nuclear cleanup missions. The four multi-institutional centers are led by Florida State University, The Ohio State University, the University of South Carolina, and DOE's Pacific Northwest National Laboratory.

DOE's Office of Environmental Management is responsible for the Department's core mission to clean up hazardous waste resulting from decades of nuclear weapons research and production during the 20th century—a process that will take many years to complete. Fundamental scientific advances from the new EFRCs will provide the foundation for safe, efficient, and cost-effective waste cleanup and storage technologies of the future.

The new centers were competitively selected based on a comprehensive merit review process and were collectively awarded $10 million per year for up to 4 years. The awards are subject to available appropriations, annual reports, and the outcome of a formal progress review in the second year of the 4-year performance period.

Computational Materials Sciences

BES supported two additional computational materials sciences awards in FY 2016, complementing the three awards made in FY 2015. These 4-year awards, totaling $12 million per year, focus on creating computational codes and associated experimental and computational databases for the design of functional materials. The new awards are led by Oak Ridge National Laboratory (quantum Monte Carlo methods) and Lawrence Berkeley National Laboratory (excited state, many body theory).

Integrated, multidisciplinary teams are essential for this research, combining expertise in materials theory, modeling, computation, synthesis, characterization, and processing and fabrication. The projects will develop new *ab initio* theory, mine data from both experimental and theoretical databases, perform advanced *in situ* and *operando* material characterization to generate the specific parameters needed to validate computational models, and conduct well-controlled material synthesis to confirm code predictions.

New computational codes will advance the predictive capability for functional materials, use DOE's

leadership-class computational resources, and leverage these computers at the petascale today and exascale tomorrow. This research will result in publicly accessible databases of experimental and computational data as well as open-source, robust, validated, user-friendly software that captures the essential physics and chemistry of relevant materials systems. The ultimate goal is use of these codes and data by the broader research community and by industry to dramatically accelerate the design of new functional materials.

Sustainable Ammonia Synthesis

The 2016 Consolidated Appropriations Act (Public Law 114-113) provided $3 million for a university solicitation on nanostructured catalysts to synthesize fertilizer and ammonia without generating secondary greenhouse gases. BES awarded six grants (two of them through the Experimental Program to Stimulate Competitive Research) in FY 2016 that cover a wide range of feasible approaches to solving this grand challenge in catalysis.

Five of the new projects address two primary issues: reducing the reaction temperature and pressure compared to today's dominant process (Haber-Bosch) and avoiding carbon dioxide release into the atmosphere. These projects will investigate electrochemical and photochemical excitation and reduction of dinitrogen from air utilizing hydrogen obtained from sources other than hydrocarbons. Using detailed mechanistic understanding of the elementary steps involved in this chemistry, researchers will rationally design catalysts that function under low-temperature and low-pressure conditions.

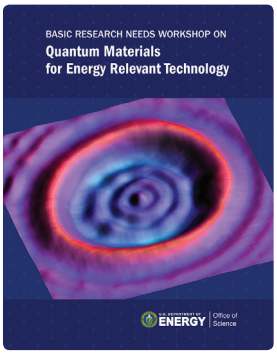
In a totally different approach, another project will heat a very high-temperature material with solar energy and cycle it repeatedly by oxidizing it with dinitrogen in one step and then reducing it with hydrogen in a second step to produce ammonia, thus using the material as a catalyst for the overall reaction. Understanding the elementary processes leading to selective reactivity and structural stability of materials under extreme conditions will advance innovative catalyst design for ammonia synthesis.

Strategic Planning

In FY 2016, BES conducted three strategic planning workshops to identify the basic research needed in the areas of quantum materials, synthesis science, and transformative experimental tools. These Basic Research Needs workshops followed the model established by BES in 2001 to engage the basic research community in the problems associated with our Nation's energy future. The reports summarize the current state of technology and define a set of priority research directions for basic research investment. The three workshops held in FY 2016 were based on opportunities identified in the 2015 Basic Energy Sciences Advisory Committee report, Challenges at the Frontiers of Matter and Energy: Transformative Opportunities for Discovery Science. The workshop reports are available at science.energy.gov/bes/community-resources/reports.

Quantum Materials for Energy Relevant Technology

Imagine computers that can perform calculations a million times faster than today's most powerful supercomputers at a fraction of the energy cost, or picture the generation, storage, and transport of power across the national grid with nearly no loss. What if ultrasensitive sensors could monitor and give updates on what is happening at home or provide warnings when something goes wrong? The key to attaining these technological possibilities is a new class of materials largely



unknown to the public but destined to become as familiar as silicon.

Quantum materials—those in which the extraordinary effects of quantum mechanics give rise to exotic and often incredible properties—have the potential to revolutionize energy, energy-related technologies, and data storage and processing, with possible staggering economic ramifications. Even now new quantum materials are emerging with unprecedented capabilities. One such material is graphene, a sheet of carbon just one atom thick. Not only is graphene 200 times stronger than steel while weighing less than paper, but electrons race through its two-dimensional (2D) plane 100 times faster than they move through silicon.

Beyond graphene, researchers are discovering new quantum materials with even greater potential. For example, 2D transition metal dichalcogenides (TMDCs) are more device-ready than graphene and offer other advantages for high-speed, low-power electronics. Additional breakthroughs in materials known as topological insulators are revealing properties found in electronic states that exist only on the material's surface. These two material classes—along with others that display extraordinary effects such as quantum spin liquids and high-temperature superconductivity—signal the dawn of a new era of quantum materials.

To accelerate the progress of quantum materials research, BES sponsored a Basic Research Needs Workshop on Quantum Materials for Energy Relevant Technology near Washington, D.C., on February 8–10, 2016. More than 100 national and international experts in quantum materials synthesis, characterization, and theory attended the workshop. Four priority research directions were identified that will lay the foundation for better understanding these materials and harnessing their rich technological potential:

- Control and exploit electronic interactions and quantum fluctuations for design of bulk materials with novel functionality.
- Harness topological states for groundbreaking surface properties.
- Drive and manipulate quantum effects (e.g., coherence and entanglement) in nanostructures for transformative technologies.
- Design revolutionary tools to accelerate discovery and technological deployment of quantum materials.

Much basic research is needed to realize the potential of quantum materials. Recognizing this potential, nations around the world already are investing in quantum materials research. For the U.S., learning how to tailor the properties of these materials to address pressing technological needs is critical, along with dramatically improving the ability to synthesize, characterize, and control quantum materials.

Synthesis Science

Technology is becoming more powerful each day. Smartphones instantly connect individuals around the globe; provide access to a limitless stream of information; control the heating in homes; and serve as cameras, calculators, flashlights, music players, boarding passes, and occasionally phones. Cars are increasingly fuel-efficient, safer, and semi-autonomous and have more computing power than the systems that guided humankind to the moon. LED lighting and solar panels are becoming commonplace, replacing less-efficient technologies and expanding the energy options available worldwide. Novel polymers and nanoparticles are playing a crucial role in enhanced oil recovery.

None of these advances would have been possible without the discovery, development, and ability to create new materials and chemical processes. Envision a world where those discoveries were accelerated a thousand-fold. What if the limit to synthesizing new matter was set by the speed of the imagination? Scientists could build complex assemblies of atoms and molecules with architectures and capabilities far exceeding materials found in nature. Examples include development of catalysts that turn garbage into fuels, solar cells that power homes directly from sunlight, and batteries with the energy density of gasoline. Imagine one- and two-dimensional solids that transport electrical charge hundreds of times faster than silicon or enable construction of quantum bits based on electron spin or photons to realize the promise of "beyond Moore's law" computing.

Advances in synthesis science are required to bring about this future. Not only is knowledge needed to design new molecules and materials with desired functions and properties through theory and computational techniques, but so are capabilities to make these materials. Innovations in the approaches used to discover unimagined matter are also critical. Chemical and materials sciences have traditionally focused on understanding structure-function relationships with the goal of predicting *the placement of atoms* necessary to achieve a targeted property or functionality. Much less effort has been directed toward a predictive science of synthesis, that is understanding *how to get the atoms where they need to go* to achieve the desired structure.

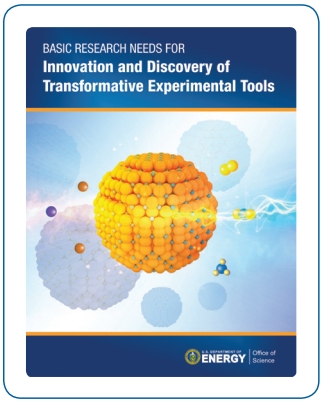
To lay out the scientific challenges and opportunities in synthesis science, BES sponsored a workshop on Basic Research Needs for Synthesis Science for Energy Technologies near Washington, D.C., on May 2–4, 2016. More than 100 national and international scientific experts attended the workshop. Four priority research directions were identified for realizing the vision of predictive, science-directed synthesis:

- Achieve mechanistic control of synthesis to access new states of matter.
- Accelerate materials discovery by exploiting extreme conditions, complex chemistries and molecules, and interfacial systems.
- Harness the complex functionality of hierarchical matter.
- Integrate emerging theoretical, computational, and *in situ* characterization tools to achieve directed synthesis with real-time, adaptive control.

The historical impact of new molecules and materials on society makes a compelling case for developing a foundational science of synthesis. Such research will enable the quick prediction and discovery of new systems and the mastery of their synthesis for rapid deployment in new technologies, especially those for energy generation and use. These priority research directions hold promise for enabling the synthesis of new molecules and materials on-demand by underpinning a long-held goal: linking predictive design to predictive synthesis.

Innovation and Discovery of Transformative Experimental Tools

Scientific discoveries that expand the frontiers of human understanding and lead to technological innovations require scientific tools and instrumentation to enable observation and manipulation of the physical world. As science advances, so too must its tools. The quest for deeper scientific insights and the drive to control chemistry and materials at the atomic and molecular levels demand increasingly powerful and sophisticated instruments.



The vision of an affordable, abundant, and secure energy future will require entirely new technologies that use existing resources more efficiently, harness renewable resources, and store different types of energy. This urgent demand for new energy technologies has ushered in a new era of scientific pursuit to tackle the complexity found at the core of chemical and materials processes. Historically, novel experimental tools and methods have been foundational in both scientific and technological innovations ranging from high-resolution microscopes that enable "seeing" atomic structures to lithography-based advances in semiconductors and computing. Today, pushing the frontiers of basic research requires new generations of instrumentation to understand (1) complex materials and chemical systems; (2) energy systems in realistic working environments; and (3) systems that are dynamic, far from equilibrium, and extremely heterogeneous. A concerted effort to invent, design, and build scientific instrumentation will expand fundamental scientific understanding and ultimately enable transformative technology solutions to the most pressing energy challenges of the 21st century.

To identify the highest priorities for instrumentation innovation and development needed to address grand challenges in energy sciences, BES sponsored a workshop on Basic Research Needs for Innovation and Discovery of Transformative Experimental Tools near Washington, D.C., on June 1–3, 2016. More than 100 national and international scientific experts attended the workshop. Four priority research directions were identified:

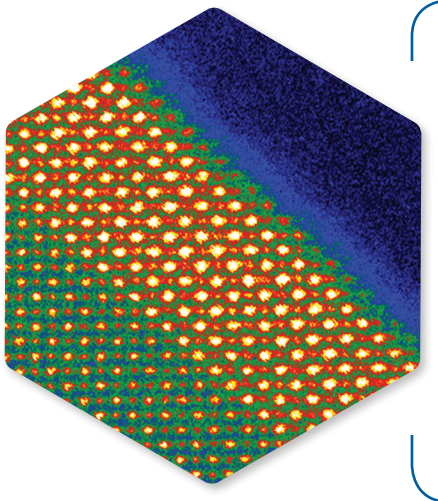
- Establish new frontiers in time, space, and energy resolution for characterization and control.
- Create innovative experimental methods for investigating real-world systems.
- Simultaneously interrogate form and function, bridging time, length, and energy scales.
- Drive a new paradigm for instrumentation design through integration of experiment, theory, and computation.

Investments in these research directions will yield breakthroughs in the ability to characterize, understand, and control critical energy processes. Inventing and developing transformative tools that enable unprecedented insight into complex systems will be a game-changing capability across all fields of basic energy sciences.

Research Highlights

The remaining pages describe select research highlights from across the three divisions in BES.

- **The Materials Sciences and Engineering Division** supports fundamental experimental and theoretical research to provide the knowledge base for the discovery and design of new materials with novel structures, functions, and properties.
- **The Chemical Sciences, Geosciences, and Biosciences Division** supports experimental, theoretical, and computational research to provide fundamental understanding of chemical transformations and energy flow in systems relevant to DOE missions.
- **The Scientific User Facilities Division** supports the R&D, planning, construction, and operation of scientific user facilities for the development of novel nanomaterials and for materials characterization through x-ray, neutron, and electron beam scattering.



New See-Through Material for Electronics

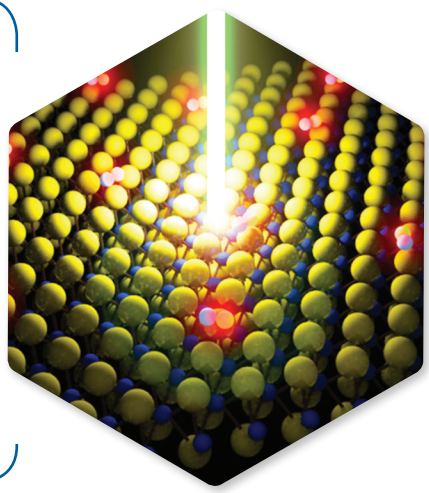
A low-cost, stable oxide film is highly conductive and transparent

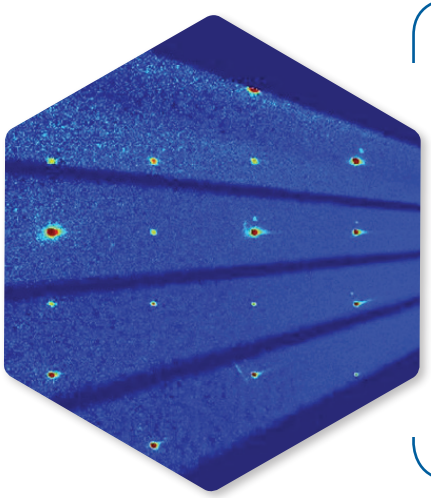
Numerous applications from flat-panel displays to solar cells require high-performance transparent conducting oxides. When these systems absorb light, negatively charged electrons and positively charged holes are generated and move into different layers of the system. Transparent oxides that conduct electrons have been commercialized, but their counterparts that conduct holes have not because of low conductivity. Scientists discovered a new material with a perovskite structure that efficiently conducts both electrons and holes, and retains most of its transparency to visual light. This new material could lead to more efficient solar cells, light-emitting diodes, light detectors, and other transparent electronics.

Superacid Repair and Enhancement of Thin Films

New semiconductor treatment could lead to flexible LED displays

Defects, such as missing atoms, are believed to severely limit the light emission (photoluminescence) efficiency in semiconductors. Researchers treated a monolayer of molybdenum disulfide (MoS_2) by dipping it in a superacid, which repaired defects and removed contamination that limited the emission efficiency. The treated films exhibited a dramatic increase in photoluminescence efficiency, increasing the percentage of emitted light to nearly 100 percent of the energy absorbed. These perfect monolayer semiconductors could lead to the development of highly efficient light-emitting diodes, lasers, and solar cells based on two-dimensional materials.





Defects, Electrons, and an Old Controversy

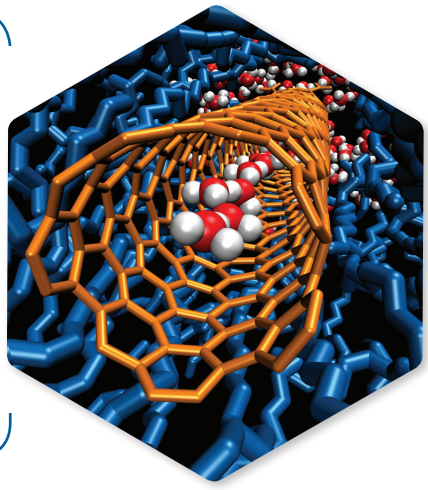
Study explains data variation in topological insulator properties

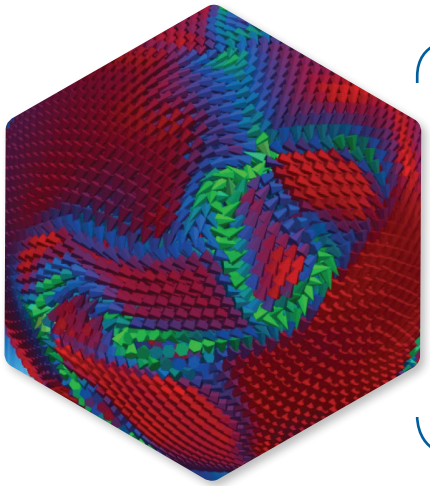
A topological insulator is a material that carries an electrical charge on its surface while the interior acts as an insulator. Recent research linked such a material's structure and chemistry with its unusual low-temperature electronic properties, answering long-standing questions about variations in these properties' measurements. Careful control and monitoring of chemical changes in a sample revealed that aluminum defects suppress the topological behavior, among other insights. This research establishes a systematic relationship between the material's bulk chemistry and surface topological properties and advances efforts to leverage such materials in quantum computers and energy-efficient electronics.

Fast and Furious Bucket Brigade

Confining water in a nanotube confirms predicted rapid proton transport

The movement of protons (hydrogen atoms with the electrons stripped away) through a membrane is critical to efficiently producing electricity in a fuel cell. A decade ago, theory predicted that confining water in a one-dimensional chain would achieve rapid proton transport, with the protons hopping down a chain of hydrogen-bonded water molecules similar to a bucket brigade passing along a water pail. Scientists used carbon nanotubes to validate this prediction and achieved proton transfer rates an order of magnitude faster than in bulk water and faster than in state-of-the-art fuel cell membranes.





Tunable Ferroelectric Nanoparticles

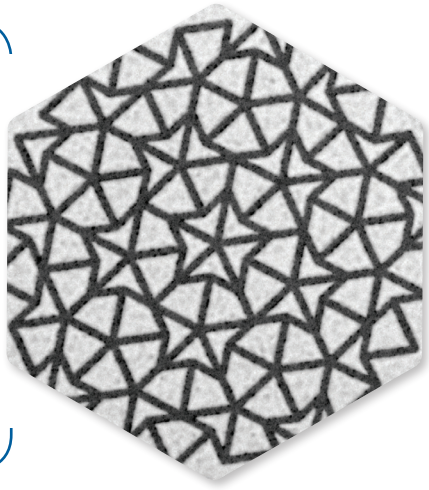
Particle size, properties, and surroundings influence behavior

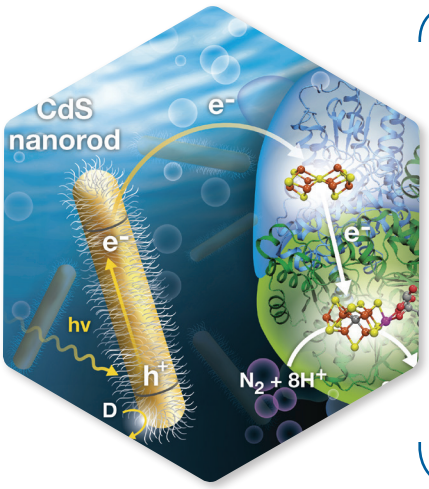
A ferroelectric material creates a spontaneous electric polarization that can be reversed by applying an external electric field. Scientists modeled spherical ferroelectric nanoparticles in a dielectric medium to understand how specific properties, such as the nanoparticle's diameter and the dielectric strength, affect the ferroelectric behavior. Three-dimensional modeling showed highly tunable dielectric properties that could be used to develop next-generation electronic materials.

Energy Cascades in Artificial Quasicrystals

Nonrepeating structure controls energy transport across the network

Researchers created two-dimensional (2D) nanoscale magnetic networks patterned as artificial quasicrystal lattices—irregular alloys with short range order but no periodicity—and showed that their novel magnetic behavior is related to their non-repeating pattern. By comparing experimental results and simulations, energy was mapped at points across the network. They found that magnetization reversal occurs via branching 2D avalanches, distinct from that seen for periodic lattices. Such networks can propagate and store information based on their magnetic state and may have potential for low-power computers based on artificial neural networks.





Sunlight Powers Ammonia Production

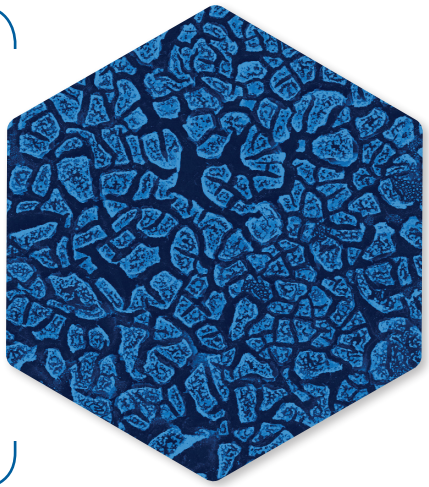
Nanorods provide electrons to enzyme in solar-driven process

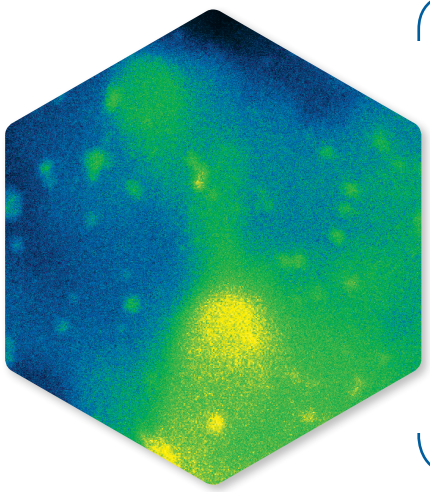
Haber-Bosch—the high-temperature, high-pressure chemical process for making ammonia—accounts for about 1–2 percent of all energy consumption in the world. Using a biohybrid approach, researchers coupled the enzyme nitrogenase to light-harvesting cadmium sulfide nanorods to reduce nitrogen to ammonia under ambient conditions using only light for energy and electrons from an artificial donor. Relatively high rates of nitrogen reduction were achieved: more than 60 percent of the normal enzyme rate. These nanoparticle-protein complexes show the potential for solar-driven ammonia production and provide insights for developing new electrocatalysts for this process.

Bimetallic Materials Do More with Less

Nickel-gallium films surpass copper-based catalysts in fuel production

Guided by theoretical results, researchers discovered that thin films composed of nickel and gallium require less excess energy to electrochemically reduce carbon dioxide to fuels such as ethylene, ethane, and methane than the copper-based materials previously considered the best candidate catalysts. Neither nickel nor gallium alone perform this way, indicating that unique and tunable reactivity results from using the bimetallic catalyst. Because similar chemical reactions are required for the solar-driven production of hydrocarbons or alcohols from carbon dioxide, this information could aid in developing artificial photosynthesis systems that generate renewable transportation fuels.





New View of Catalyst's Structural Dynamics

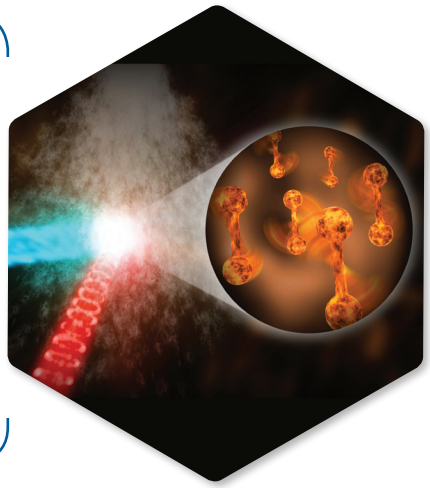
Changes in particle size, shape, and charge seen under working conditions

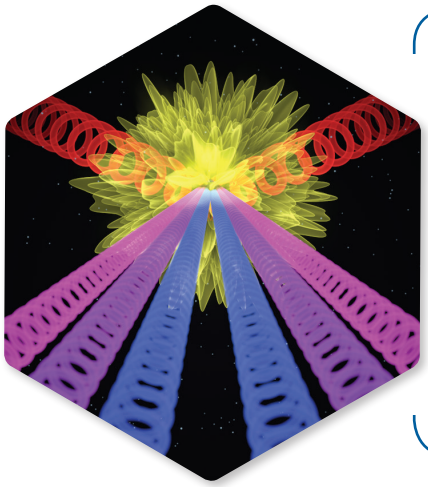
Scientists have confirmed experimentally and with high accuracy the long-held hypothesis that the structure of platinum catalyst nanoparticles supported on alumina changes during the catalytic conversion of ethylene to ethane. They designed a miniature reactor that collects nanoscale structural images simultaneously with synchrotron x-ray absorption spectra and catalyst performance measurements obtained under the same reaction conditions. This approach for structural and kinetic characterization *operando* provides precise atomic-scale dynamic information underpinning model refinement and more effective design of supported metal catalysts optimized for hydrocarbon dehydrogenation.

Ultrafast Snapshots of Molecular Motion

Instrument uses electron pulses to image nitrogen rotation

An important step in understanding chemical reactivity is determining how molecular structure changes during a reaction. A new instrument with an unprecedented combination of time and spatial resolution can image the ultrafast evolution of chemical reactions with atomic resolution. Researchers aligned nitrogen molecules with a laser pulse and then illuminated the sample with ultrashort electron pulses at different times after the laser pulse. They were able to capture very fast changes in the orientation of the molecules, demonstrating a significant and promising step toward making atomically resolved movies of chemical reactions.





Exquisite Control of X-Ray Light

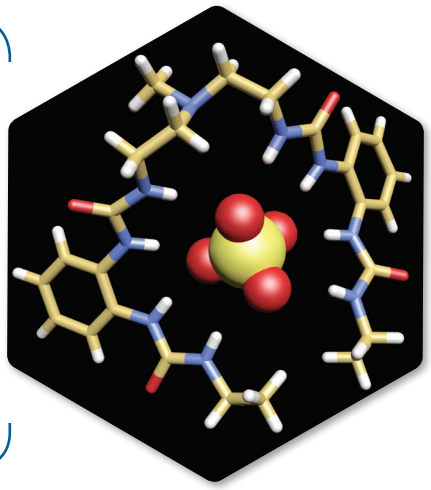
Tabletop setup uses visible lasers for precise manipulation

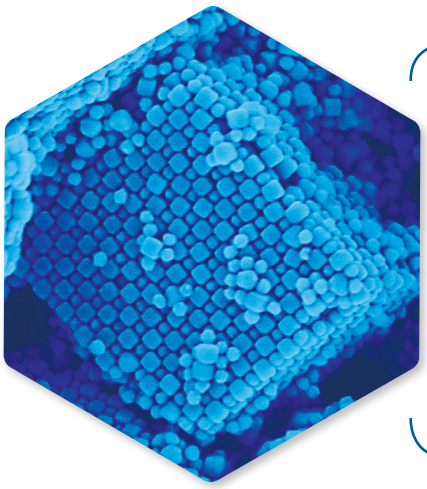
By crossing two counter-rotating ultrafast laser beams in a gas target, scientists controlled the direction and polarization of laser-like beams in the extreme ultraviolet and soft x-ray portions of the spectrum. This technique represents a new ability to manipulate creation of x-ray beams using visible light and obviates the need for inefficient and expensive optics to filter and deliver such beams. This method enables, for example, tabletop measurements of ultrafast dynamics in novel magnetic materials and the study of chiral molecules, such as proteins or DNA, that come in left- and right-handed versions.

Molecules Extract Ions from Nuclear Waste

Synthetic control enables selective binding of target sulfate anions

The long-term resistance to dissolution and degradation of radioactive wastes in subterraneous geologic environments can be improved by removing specific ions before disposal. To extract particular ions from radioactive waste, researchers designed a family of molecular pincers that selectively bind sulfate anions in complex aqueous solutions. The team efficiently separated sulfate using organic frameworks with structures tailored to recognize and tightly latch onto inorganic anions. Sulfate removal is important not only for nuclear waste disposition, but also for other energy and biological applications.





New Strategy for Nanoparticle Self-Assembly

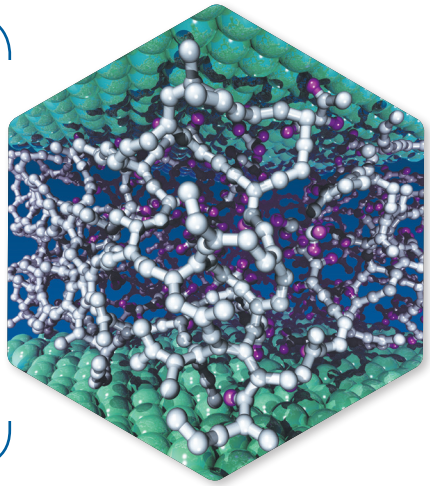
Superlattices form through shape-induced directional binding

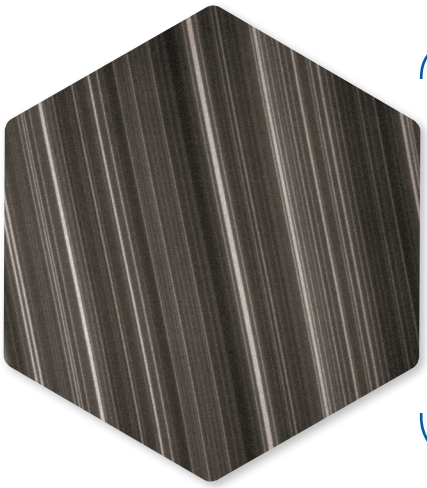
Researchers at the Center for Functional Nanomaterials formed three-dimensional binary crystals with predictable symmetry by combining anisotropic polyhedral blocks (cubes and octahedrons) and spherical nanoparticles through shape-induced directional interactions facilitated by DNA recognition. The spatial symmetry of the facets of the polyhedral blocks determined the structure of the crystals. Introducing directional binding into the field of nanoparticle self-assembly will significantly increase the diversity of achievable structures.

Giving Friction the Slip with New Carbon Films

Diamond-like carbon coating could revolutionize lubrication

Tribology—the study of friction, wear, and lubrication—is critical to the efficiency and durability of engines and other moving metal parts. Scientists at the Center for Nanoscale Materials discovered that new self-healing tribofilms containing diamond-like carbon can reduce friction by 25 to 40 percent and wear to nearly zero. Advanced computational simulations traced the origin of the anti-wear properties to new catalytic phenomena possible only under the extreme conditions afforded by friction. Further knowledge about the catalytic mechanisms, coupled with the predictive power of simulation, may enable the design of new mechanical coatings.





Advanced Metrology for High-End Instrumentation

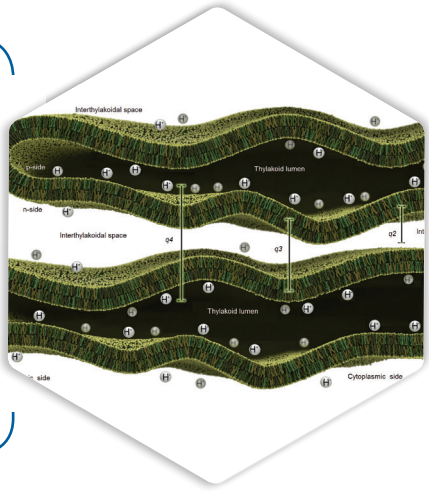
Record-resolution test patterns improve calibration

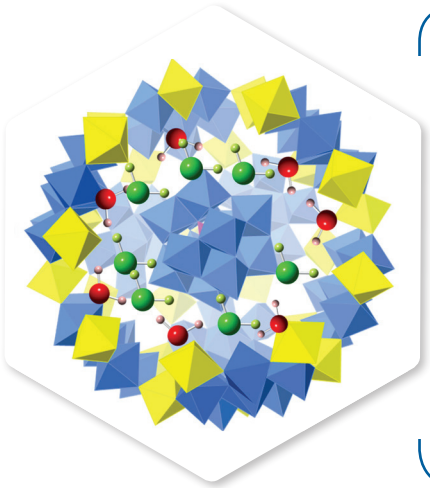
Metrology is a multibillion-dollar business essential for precise fabrication. Researchers developed a turn-key solution to automatically calibrate metrology systems. A variety of test samples were designed and fabricated with a record resolution of 1.5 nanometer minimum linewidth. These samples improved the calibration of a broad spectrum of nanometrology tools, including transmission electron microscopes, atomic force microscopes, scanning electron microscopes, optical microscopes, and interferometers.

Membrane Dynamics in Live Cyanobacteria

Neutron scattering shows light intensity influences membrane motion

Cyanobacteria are a group of photosynthetic, nitrogen-fixing microorganisms. Scientists used capabilities at the Spallation Neutron Source and High Flux Isotope Reactor to directly measure the mobility of photosynthetic membranes in living cyanobacterial cells for the first time. They found that membranes were more relaxed and flexible in the dark compared to those under high light conditions. These results provide a deeper understanding of the relationship between photosynthesis and cellular architecture.





Formation of Metal-Oxide Nanoclusters

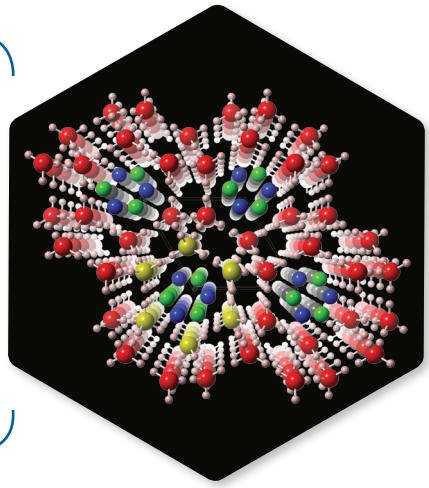
Water molecules bridge and stabilize the structures

Polyoxometalates (POMs) are well-defined nanoscale metal-oxide clusters with applications in catalysis and magnetically and electronically active materials. Scientists recently uncovered the formation mechanism of typical core-shell POMs, observing that two types of water molecules play vital roles in bridging core and shell structures and stabilizing the cluster structures. The Spallation Neutron Source and Advanced Photon Source were essential tools in probing the dynamics of the water molecules, revealing the formation mechanism. These results aid in the design, synthesis, and tuning of physical and chemical properties of novel clusters.

Structure of Hydrogen-Stuffed, Quartz-Like Ice

Interconnected water molecules form tubes filled with hydrogen

Using the Advanced Photon Source, a team of scientists identified the structure of a new type of ice crystal that resembles the mineral quartz. It is stuffed with over 5 weight percent of energy-rich hydrogen, a long-standing DOE goal for hydrogen storage. Large water channels enhance hydrogen mobility in the structure, and the compound forms at about 4,000 times normal atmospheric pressure (400 MPa) and 44°F (280 K). Results could have implications for the mineralogy of icy planetary bodies and for energy storage technology.



BASIC ENERGY SCIENCES
Image Credits

FRONT COVER

Atomic-Resolution Topographic Rendering of a Borophene Surface. The borophene sheet, imaged with a scanning tunneling microscope, forms large buckled wrinkles (as seen in the center) in response to an underlying silver crystal. These atomic-scale wrinkles may steer the flow of electrons and could lead to other surprising properties. Courtesy Center for Nanoscale Materials at Argonne National Laboratory (ANL).

PAGE 6

New See-Through Material for Electronics. The junction of a layer of the transparent hole-conducting material (primarily yellow) with an electron-conducting layer (primarily green). Courtesy Scott Chambers and Steven Spurgeon, Pacific Northwest National Laboratory. Zhang, K., et al. 2015. "Perovskite Sr-Doped $LaCrO_3$ as a New p-Type Transparent Conducting Oxide,"*Advanced Materials* **27**(35), 5191–95. DOI:10.1002/adma.201501959.

Superacid Repair and Enhancement of Thin Films. Artistic rendering of a laser beam generating excitons (bound electron and hole) in an atomically thin molybdenum disulfide (MoS_2) semiconductor film. Courtesy Der-Hsien Lien, Lawrence Berkeley National Laboratory (LBNL). Amani, M., et al. 2015. "Near-Unity Photoluminescence Quantum Yield in MoS_2," *Science* **350**(6264), 1065–68. DOI:10.1126/science.aad2114. See also Amani, M., et al. 2016. "Recombination Kinetics and Effects of Superacid Treatment in Sulfur- and Selenium-Based Transition Metal Dichalcogenides," *Nano Letters* **16**, 2786–91. DOI:10.1021/acs.nanolett.6b00536.

Defects, Electrons, and an Old Controversy. Neutron diffraction shows aluminum impurities introduced in samarium hexaboride (SmB_6) single crystals. These inclusions explain different measurements reported for the material's low-temperature electrical properties. Courtesy T.M. McQueen and W.A. Phelan, Johns Hopkins University. Phelan, W.A., et al. 2016. "On the Chemistry and Physical Properties of Flux and Floating Zone Grown SmB_6 Single Crystals," *Scientific Reports* **6**, 20860. DOI:10.1038/srep20860. See also Phelan, W.A., et al. 2014. "Correlation Between Bulk Thermodynamic Measurements and the Low-Temperature-Resistance Plateau in SmB_6," *Physical Review X* **4**, 031012. DOI:10.1103/PhysRevX.4.031012.

PAGE 7

Fast and Furious Bucket Brigade. Confinement of water molecules (red and grey atoms) in a subnanometer carbon nanotube (orange) allows for rapid proton transport along the one-dimensional chain of water. Courtesy Y. Zhang and A. Noy, Lawrence Livermore National Laboratory. Tunuguntla, R. H., et al. 2016. "Ultrafast Proton Transport in sub-1-nm Diameter Carbon Nanotube Porins," *Nature Nanotechnology* **11**, 639–44. DOI:10.1038/NNANO.2016.43.

Tunable Ferroelectric Nanoparticles. Modeled multi-domain polarization structure in a 30-nm-diameter lead titanate ($PbTiO_3$) sphere embedded in a medium of strontium titanate ($SrTiO_3$). Courtesy Olle Heinonen, ANL. Mangeri, J., et al. 2017. "Topological Phase Transformations and Intrinsic Size Effects in Ferroelectric Nanoparticles," *Nanoscale* **9**, 1616–24. DOI:10.1039/c6nr09111c.

Energy Cascades in Artificial Quasicrystals. Bright-field transmission electron microscopy image of a patterned quasicrystalline artificial spin ice lattice. Courtesy Vuk Brajuskovic, Charudatta Phatak, and Amanda Petford-Long, ANL. Brajuskovic, V., et al. 2016. "Real-Space Observation of Magnetic Excitations and Avalanche Behavior in Artificial Quasicrystal Lattices," *Scientific Reports* **6**, 34384. DOI:10.1038/srep34384.

PAGE 8

Sunlight Powers Ammonia Production. Light-harvesting cadmium sulfide (CdS) nanocrystals photosensitize the nitrogenase molybdenum-iron (MoFe) protein to reduce nitrogen to ammonia. Courtesy Al Hicks, National Renewable Energy Laboratory. Brown, K.A., et al. 2016. "Light-Driven Dinitrogen Reduction Catalyzed by a CdS:Nitrogenase MoFe Protein Biohybrid," *Science* **352**(6284), 448–50. DOI:10.1126/science.aaf2091.

Bimetallic Materials Do More with Less. Scanning electron micrograph of nickel-gallium films after annealing showing the aggregation of microparticles into a catalytically active, polycrystalline thin film. Courtesy Daniel A. Torelli and Nathan S. Lewis, California Institute of Technology. Adapted with permission from Torelli, D. A., et al. 2016. "Nickel–Gallium-Catalyzed Electrochemical Reduction of CO_2 to Highly Reduced Products at Low Overpotentials," *ACS Catalysis* **6**(3), 2100–04. DOI:10.1021/acscatal.5b02888. Copyright 2016 American Chemical Society.

New View of Catalyst's Structural Dynamics. Electron microscope image taken during the catalytic conversion of ethylene to ethane. Courtesy Eric Stach and Anatoly Frenkel, Brookhaven National Laboratory (BNL). Li, Y., et al. 2015. "Complex Structural Dynamics of Nanocatalysts Revealed in Operando Conditions by Correlated Imaging and Spectroscopy Probes," *Nature Communications* **6**, 7583. DOI:10.1038/ncomms8583.

PAGE 9

Ultrafast Snapshots of Molecular Motion. Scientists aligned nitrogen molecules with laser light (red), then probed their subsequent rotation by taking ultrafast snapshots with an electron beam (blue). Courtesy SLAC National Accelerator Laboratory. Yang, J., et al. 2016. "Diffractive Imaging of a Rotational Wavepacket in Nitrogen Molecules with Femtosecond Megaelectronvolt Electron Pulses," *Nature Communications* **7**, 11232. DOI:10.1038/ncomms11232.

Exquisite Control of X-Ray Light. Counter-rotating circularly polarized laser beams (red) are crossed in a gas target to generate angularly separated extreme ultraviolet harmonics with right- and left-circular polarization (blue, purple, and magenta). Courtesy Steve Burrows and the Kapteyn-Murnane Group, University of Colorado, Boulder. Hickstein, D.D., et al. 2015. "Non-Collinear Generation of Angularly Isolated Circularly Polarized High Harmonics," *Nature Photonics* **9**, 743–50. DOI:10.1038/nphoton.2015.181.

Molecules Extract Ions from Nuclear Waste. Tailored molecules capture specific ions from solution. Courtesy Bruce Moyer, Oak Ridge National Laboratory (ORNL). Jia, C., et al. 2015. "Chelate Effects in Sulfate Binding by Amide/Urea-Based Ligands," *Organic & Biomolecular Chemistry* **13**, 6953–57. DOI:10.1039/c5ob00618j.

PAGE 10

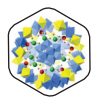
New Strategy for Nanoparticle Self-Assembly. Formation of large-scale, three-dimensional binary crystals with predictable lattice symmetry, as determined by the cubic geometry and DNA-encoded interactions between cubes and spheres. Courtesy Oleg Gang, BNL. Lu, F., et al. 2015. "Superlattices Assembled Through Shape-Induced Directional Binding," *Nature Communications* **6**, 6912. DOI:10.1038/ncomms7912.

Giving Friction the Slip with New Carbon Films. Molecular dynamics simulations unravel the catalytic creation mechanism of anti-wear carbon films from oils. Computer simulation of the diamond-like carbon lubricant between copper surfaces shows self-healing lubrication (green = copper; grey = carbon; purple = hydrogen). Courtesy Badri Narayanan, Joseph Insley, and Subramanian Sankaranarayanan, ANL. Erdemir, A., et al. 2016. "Carbon-Based Tribofilms from Lubricating Oils," *Nature* **536**, 67–71. DOI:10.1038/nature18948

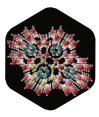
Advanced Metrology for High-End Tools. Researchers designed and fabricated pseudo-random test samples to characterize metrology systems at the nanoscale. The minimum feature size was 1.5 nm, providing the highest resolution of the artificial calibration samples ever achieved. Courtesy Sergey Babin (aBeam Technologies, Inc.), Raymond Conley (ANL), and Valeriy Yashchuk (LBNL). Reproduced from Babin, S., et al. 2015. "1.5 nm Fabrication of Test Patterns for Characterization of Metrological Systems," *Journal of Vacuum Science & Technology B, Nanotechnology and Microelectronics: Materials, Processing, Measurement, and Phenomena* **33**(6), 06FL01/1–5. DOI:10.1116/1.4935253, with the permission of the American Vacuum Society.

PAGE 11

Membrane Dynamics in Live Cyanobacteria. Schematic thylakoid membrane morphology. Photosynthetic Antenna Research Center (PARC) EFRC. Courtesy Laura-Roxana Stingaciu, ORNL. Stingaciu, L., et al. 2016. "Revealing the Dynamics of Thylakoid Membranes in Living Cyanobacterial Cells," *Scientific Reports*, **6**, 19627. DOI:10.1038/srep19627.



Formation of Metal-Oxide Nanoclusters. Schematic of the reaction mechanism leading to the formation of a giant polyoxometalate. The core component, a complex silicon-molybdenum oxide, reacts with molybdenum oxide and iron ion in acidic solution. Over the course of 24 hours or more, a shell forms around the core, and the core-shell structure eventually crystallizes. Courtesy Panchao Yin, ORNL. Reprinted with permission from Yin, P., et al. 2016. "X-ray and Neutron Scattering Study of the Formation of Core–Shell-Type Polyoxometalates," *Journal of the American Chemical Society* **138**(8), 2638–43. DOI:10.1021/jacs.5b11465. Copyright 2016, American Chemical Society.



Structure of Hydrogen-Stuffed, Quartz-Like Ice. The recently discovered C_0 phase structure in the hydrogen and water system. Large red and small pink spheres indicate oxygen and hydrogen atoms of water, respectively, while blue and green spheres indicate disordered hydrogen molecules, which are 50 percent occupied. Energy Frontier Research in Extreme Environments EFRC. Courtesy Timothy Strobel, Carnegie Institution for Science. Strobel, T.A., et al. 2016. "Hydrogen-Stuffed, Quartz-like Water Ice," *Journal of the American Chemical Society* **138**(42), 13786–89. DOI:10.1021/jacs.6b06986.

DISCLAIMER: This report was prepared as an account of work sponsored by an agency of the United States government. Neither the United States government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States government.

Printed with soy ink on recycled paper

Contact

Basic Energy Sciences
U.S. Department of Energy
SC-22/Germantown Building
1000 Independence Ave., SW
Washington, DC 20585
sc.bes@science.doe.gov
Phone: 301.903.3081
Fax: 301.903.6594
science.energy.gov/bes/

May 2017