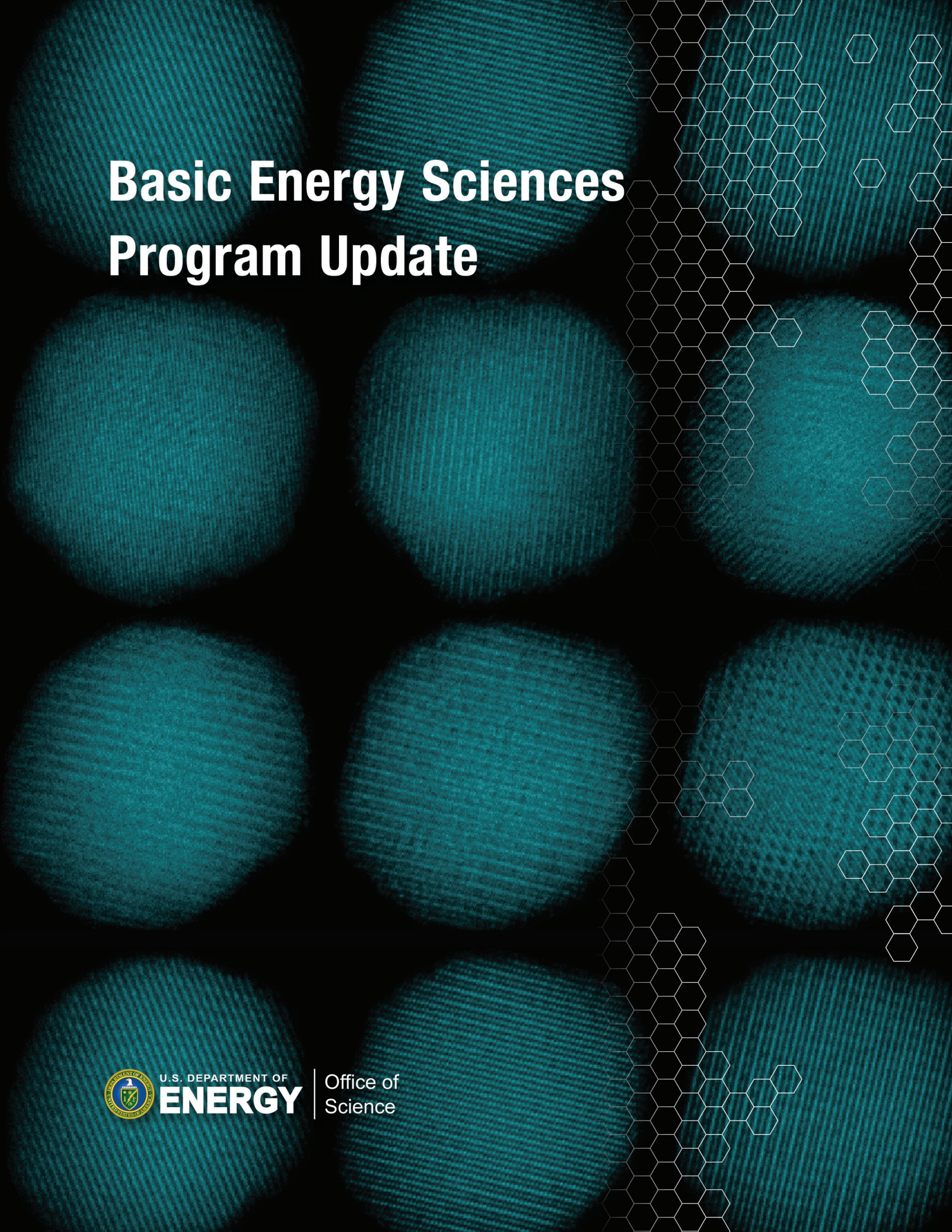
Basic Energy Sciences Program Update



U.S. DEPARTMENT OF ENERGY | Office of Science

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

~5,600 Ph.D. SCIENTISTS | **~1,800** STUDENTS

BES BY THE NUMBERS

FY 2017

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

36 ENERGY FRONTIER RESEARCH CENTERS

$724 MILLION RESEARCH BUDGET

NEARLY **16,000** USERS AT **12** BES FACILITIES

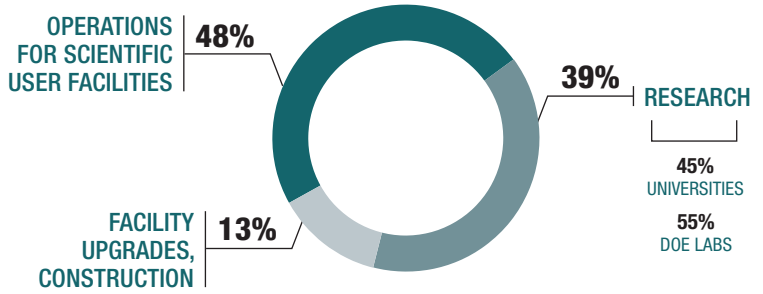
$915 MILLION SCIENTIFIC USER FACILITY OPERATING BUDGET

OVER **1,000** CORE RESEARCH PROJECTS

~15% AVERAGE NEW GRANT SUCCESS RATE

2 ENERGY INNOVATION HUBS

$233 MILLION FACILITY UPGRADES, CONSTRUCTION BUDGET



BES Mission

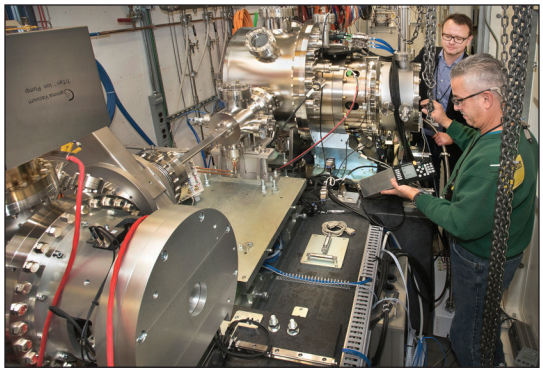
The U.S. Department of Energy's (DOE) Office of Basic Energy Sciences (BES) supports fundamental research to understand, predict, and ultimately control matter and energy at the electronic, atomic, and molecular levels to provide the foundations for new energy technologies and to support DOE missions in energy, environment, and national security. BES research disciplines—including condensed matter and materials physics, chemistry, geosciences, and aspects of biosciences—emphasize discovery of new materials 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 such as imaging and spectroscopy for the study of chemical transformations of matter and the characterization of a wide range of materials from hard metals to fragile biological samples. 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

National Synchrotron Light Source II Experimental Tools

In fiscal year (FY) 2017, BES completed the National Synchrotron Light Source II (NSLS-II) Experimental Tools (NEXT) major item of equipment construction project at Brookhaven National Laboratory. The NEXT project delivered five "best-in-class" beamlines at NSLS-II with unique advanced scientific capabilities. The NEXT beamlines cover a wide range of photon energies, from vacuum ultraviolet to hard x-ray, and techniques ranging from spectroscopy and scattering to microprobes and imaging. When fully commissioned,



Inner-Shell Spectroscopy (ISS) Beamline During Installation. [Courtesy Brookhaven National Laboratory]

the source-plus-beamline performance of the NEXT beamlines will be a world-class combination of flux, resolution, and spot size. Readiness for operation with beam (i.e., technical commissioning phase) in the already-operating NSLS-II facility was reviewed and approved for each beamline as soon as its construction was complete. First-light dates for the five NEXT beamlines ranged from April 2016 to February 2017. The NEXT beamlines also will significantly increase user capacity at NSLS-II and support a wide range of research programs. These beamlines will address urgent needs identified by the U.S. research community for responding to the DOE mission of achieving transformational energy solutions in the near term while simultaneously expanding knowledge of fundamental energy science.

Computational Chemical Sciences

Computational Chemical Sciences is a new BES activity in FY 2017 to develop open-source modular software tools that can be reused as plug-and-compute tools for the basic energy sciences community. Computational Chemical Sciences joins a parallel program in Computational Materials Sciences, which started in FY 2015, to help both research communities prepare for the arrival of exascale computing facilities and optimize usage of existing petascale computers, leveraging U.S. leadership in the development of computational codes. Today's best chemical simulation codes are unable to efficiently use

more than one percent of the processors available on existing leadership-class supercomputers. Critically needed is a systematic effort to modify or replace existing computational chemistry codes with codes that are well adapted to anticipated exascale architectures.

The FY 2017 appropriation provided $14 million for new awards in computational chemical sciences. These awards focus on the creation of computational codes and associated experimental and computational databases for the design of chemical processes and assemblies. These research efforts combine the skills of experts in theoretical chemistry, modeling, computation, and applied mathematics. Researchers will develop new *ab initio* theory, mining data from both experimental and theoretical databases, and experimentally validate the codes. These computational codes will advance the predictive capability for chemical processes and assemblies, using DOE's scientific user facilities (including both advanced experimental and leadership-class computational capabilities). This research will result in publicly accessible databases of experimental and computational data and open-source, robust, validated, user-friendly software that captures the essential physics and chemistry of relevant chemical systems. The ultimate goal is use of these codes and data by the broader research community and by industry to dramatically accelerate chemical research in the United States.

2017 EFRC-Hub-CMS Principal Investigators' Meeting

On July 24–25, 2017, more than 600 energy researchers from the Energy Frontier Research Centers (EFRCs), BES Energy Innovation Hubs, Computational Materials Sciences (CMS) awards, and DOE staff participated in a combined principal investigators' meeting. Plenary talks were followed by scientific oral and poster presentations, panel discussions, and networking events. To highlight the accomplishments of early-career scientists and further the development of the future scientific energy workforce, BES sponsored the Student and Postdoc Team Science Contest. From the 16 finalists, BES selected the top teams based on how well their research exemplified the opportunities provided by the center funding modality, scientific excellence, integration of theory and experiment, and topical diversity, as well as the quality of their presentation. BES also challenged the community to share the excitement and mystery of science using sound via an optional Intersection of Sound and Science Podcast Contest.

Strategic Planning

In FY 2017, BES conducted four strategic planning workshops to identify basic research needed in the areas of energy and water, next-generation electrical energy storage, catalysis science, and future nuclear energy. Reports from these workshops summarize the current state of technology and define a set of priority research directions for basic research investment. These reports are available at science.energy.gov/bes/community-resources/reports/.

Basic Research Needs for Energy and Water

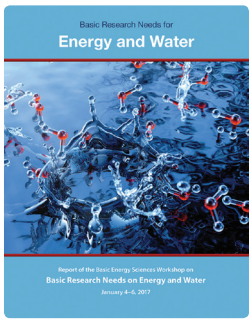
Water is precious and unique. This indispensable resource is essential not only for life, but also for practically all forms of economic activity. The food we eat, the clothes we wear, the goods we use, and the electricity we consume all require water. Cooling power plant components, refining petroleum, producing fuel, and extracting energy resources from the Earth make up a significant fraction of water use. Moreover, water treatment, distribution, and use are large consumers of energy.

The connection between water and energy means that issues in one area—for instance, too much or too little water—can profoundly affect the other. The looming challenge is to address the coupled needs of sufficient energy and clean water for a thriving economy and national security.

This challenge presents an enormous opportunity for fundamental energy science. Fertile basic research opportunities, ripe for exploration, span

disciplines—such as chemistry, geosciences, biosciences, and materials sciences—and scales, starting with molecular phenomena. Energy-water systems, whether manufactured or part of the natural world, exhibit extraordinary dynamics and complexities. The "water" is not simply water—it is typically a complex fluid with multiple chemical, particulate, and biological components. The molecular interactions of water with these components, with other fluids, and at material interfaces remain a mystery. Basic science is essential to solve this and other mysteries related to energy and water.

To lay out the scientific challenges and opportunities for energy-water systems, BES sponsored the Basic Research Needs Workshop on Energy and Water near Washington, D.C., on January 4–6, 2017. Approximately 140 national and international scientific experts attended the workshop. Four priority research directions were identified to understand the chemical processes and materials underlying the interdependence of energy and water and to harness the potential for technological impact:



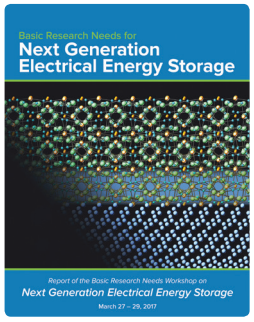
- Predict static and dynamic properties of multicomponent fluids
- Achieve mechanistic control of interfaces and transport in complex and extreme environments
- Exploit specific material-fluid interactions to design and discover innovative fluids and materials
- Advance science to harness the subsurface for a transformational impact on water

Basic Research Needs for Next Generation Electrical Energy Storage

Advances in how electricity is stored have the potential to transform nearly every aspect of society, from transportation to communication to electricity delivery and domestic security. New energy storage systems will support the energy requirements for advanced technologies and strengthen critical infrastructure. This vision for the future can be achieved only through next-generation, high-performance batteries and related energy storage media that are safe, reliable, and affordable.

Energy can be stored in many forms, such as electrical, mechanical, thermal, and chemical, and then converted into electricity when needed. Batteries and related devices rely on electrochemical energy conversion. Unlike digital electronics that work by moving electrons through circuits, batteries move electrons, atoms, ions, and molecules through demanding chemical environments. The process can dramatically change the chemistry and structure of battery materials, limiting their performance over time. Achieving greater efficiency, reliability, and resiliency in energy storage technologies requires a new level of understanding and control over the dynamics that govern electrochemical phenomena.

Science is poised to meet these challenges. Real-time nanoscale characterization of operating batteries will elucidate fundamental mechanisms of function and failure. Predictive computational simulations will move beyond the discovery of new materials and chemistries to unlock innovative system functionalities. Further, holistic approaches to the synthesis of materials, structures, and architectures will deliver new levels of electrochemical performance, enabling higher efficiency, extended lifetimes, and lower costs for energy storage devices. The integration of this knowledge promises a revolution in technologies and manufacturing processes for next-generation batteries.



To usher in a new era of electrochemical energy storage with significantly higher performance,

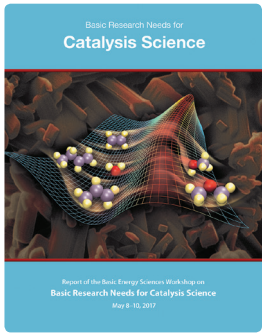
lower cost, greater reliability, and increased safety, BES sponsored the Basic Research Needs Workshop on Next Generation Electrical Energy Storage near Washington, D.C., on March 27–29, 2017. Around 140 national and international scientific experts attended the workshop. Five priority research directions were identified that will underpin future capabilities of electrical energy storage:

- Tune functionality of materials and chemistries to enable holistic design for energy storage
- Link complex electronic, electrochemical, and physical phenomena across time and space
- Control and exploit the complex interphase region formed at dynamic interfaces
- Revolutionize energy storage performance through innovative assemblies of matter
- Promote self-healing and eliminate detrimental chemistries to extend lifetime and improve safety

Basic Research Needs for Catalysis Science to Transform Energy Technologies

Catalysis is the core of modern chemical conversions—in fact, the production processes for the vast majority of fuels and chemicals use catalysts. Solid and molecular catalysts increase chemical transformation rates (i.e., reactivity) by lowering energy barriers for chemical reactions and can increase the yield of desired products (i.e., selectivity) by controlling the relative rates of competing reactions. High catalytic reactivity and selectivity reduce the required energy input, the number of process steps, and unwanted by-products in the overall catalytic conversion. New catalysts will enable more efficient chemical transformations of raw materials and interconversion of the energy stored in chemical bonds with thermal and electrical energy. Advancing the understanding of and ability to control catalyzed reactions is essential to ensure the long-term economic viability of the energy and chemical industries.

Over the past decade, advances in the characterization of working catalysts, theory and computation, and high-precision chemical and materials synthesis have enabled impressive progress in catalysis science. This progress has provided detailed insight into how reactions occur and has led to increased appreciation of the intrinsic complexity of catalytic processes. Understanding this complexity has further enabled advances in areas as diverse as high-temperature transformation of hydrocarbons, low-temperature conversion of highly functionalized bio-derived compounds, highly selective synthesis of complex molecules, and improved electrochemical processes. By integrating the knowledge gained from studies of homogeneous, heterogeneous, and biological catalysts, scientists are beginning to understand and take advantage of the remarkably diverse capabilities of catalysts based on multifunctional molecular complexes, functionalized porous materials, and stabilized nanostructures and single atoms.



To accelerate the progress of basic research on catalytic processes that underpin energy resource conversion or utilization, BES sponsored the Basic Research Needs Workshop on Catalysis Science near Washington, D.C., on May 8–10, 2017. More than 100 national and international scientific experts attended the workshop. Five priority research directions were identified that address complexity in catalysis science:

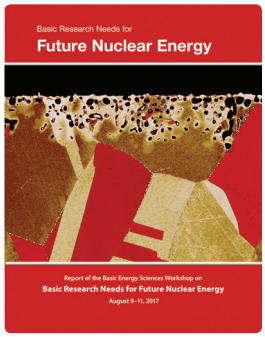
- Design catalysts beyond the binding site
- Understand and control the dynamic evolution of catalysts
- Manipulate reaction networks in complex environments to steer catalytic transformations selectively
- Design catalysts for efficient electron-driven chemical transformations
- Drive new catalyst discoveries by coupling data science, theory, and experiment

Basic Research Needs for Future Nuclear Energy

Concepts being developed for future, advanced nuclear reactors will go beyond producing an abundant, safe, and reliable supply of electricity to supporting lower-cost industrial production of materials and chemicals. However, realizing optimum future reactor concepts requires developing entirely different systems of coolants, fuels, and structural materials that can last through decades-to centuries-long reactor lifetimes and withstand some of the most extreme environments known—for example, operational temperatures that could exceed 1,000°C, intense radiation fields, and corrosive environments, among others.

These daunting requirements present an exciting and challenging opportunity for the chemical and materials sciences. They demand the discovery and design of revolutionary new materials and fuels, coupled with innovative approaches to materials synthesis and processing and optimization of the performance and certification of the new components. Combining modeling and simulation with *in situ* characterization methods will reveal and predict processes that dictate performance and degradation under extreme operational conditions. These coupled methods also will enable researchers to identify and understand the low-frequency events that can trigger cascading processes that may result in system failure. New computational tools and data analytics will expedite the identification of chemical compositions and structures of materials with tailored properties required to withstand the harshest reactor environments, followed by innovative synthesis and processing capabilities for materials production. Integration of the knowledge generated through this effort will accelerate the discovery-to-application process, providing the materials needed to realize the promise offered by advanced nuclear reactor concepts.

To identify high-priority basic research to enable future generations of nuclear energy systems, BES sponsored the Basic Research Needs Workshop on Future Nuclear Energy near Washington, D.C., on August 9–11, 2017. Approximately 110 national and international scientific experts attended the workshop. Five priority research directions were identified to understand the many physical and chemical processes underlying the performance of materials exposed to extremes of radiation, temperature, stress, and chemical reactivity:

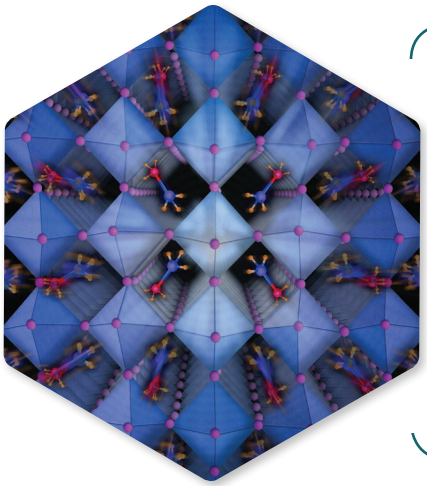


- Enable design of revolutionary molten salt coolants and liquid fuels
- Master the hierarchy of materials design and synthesis for complex reactor environments
- Tailor interfaces to control the impact of nuclear environments
- Reveal multiscale evolution of spatial and temporal processes for coupled extreme environments
- Identify and control unexpected behaviors from rare events and cascading processes

Research Highlights

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

- **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.
- **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.
- **Scientific User Facilities Division:** Supports research and development, planning, construction, and operation of scientific user facilities for development of novel nanomaterials and nanostructures and for materials characterization through x-ray, neutron, and electron beam scattering.



Hybrid Materials Increase Solar Cell Efficiency

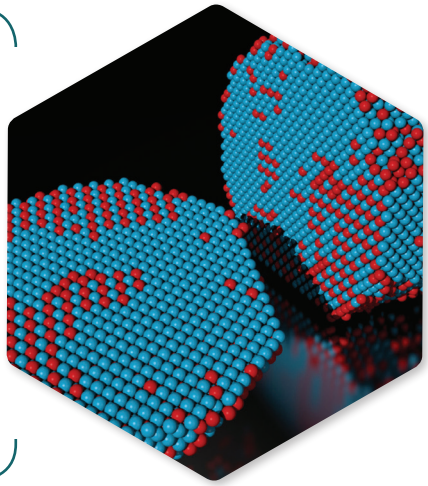
Breaking through the sunlight-to-electricity conversion limit

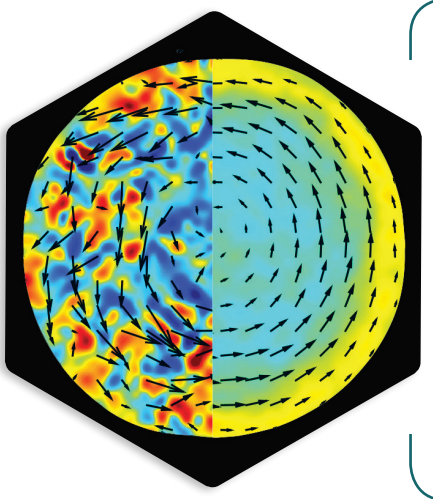
Solar-excited hot electrons cannot be used for electricity, so the associated energy is usually wasted as heat in conventional solar cells. In a new type of solar cell, known as a hybrid organic-inorganic perovskite cell, scientists found that lifetimes of such hot electrons are more than 1,000 times longer than those formed in silicon cells. The rotation of oppositely charged ions plays a key role in protecting them from adverse energy-depleting interactions. By slowing the cooling of excited hot electrons, scientists could produce more electricity, thus increasing the solar cell's efficiency beyond the conventional limit.

Deciphering Material Properties Atom by Atom

Precise location and identity of 23,000 atoms revealed

Scientists determined the three-dimensional (3D) position of 6,569 iron and 16,627 platinum atoms in an iron-platinum nanoparticle with 22-picometer resolution. They correlated the observed chemical order/disorder and defects in the atomic structure with magnetic properties at the single-atom level. This work opens the door to determining 3D atomic arrangements and chemical order/disorder of a wide range of nanostructured materials with high precision. It also gives researchers the ability to study material properties on the single-atom level that could transform the understanding of structure-property relationships at the most fundamental level.





Blurring the Line Between Animate and Inanimate

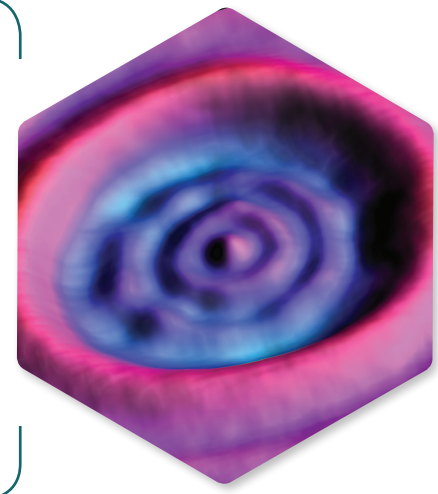
Self-organized, soft machines propel fluid for hours across meters

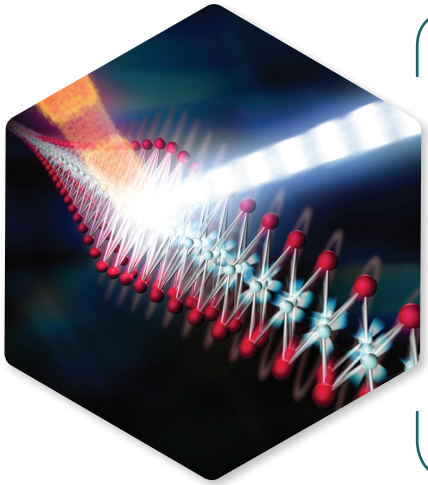
Scientists discovered a new mechanism that creates a self-propelling fluid via energy-harvesting machines composed of filaments and molecular motors. For the first time, an otherwise directionless fluid was constrained to autonomously flow unidirectionally through three-dimensional, meter-long channels until the machines' chemical energy was depleted. Notches in the pipe control the direction of the flow, and the structure of the machines regulates its strength and speed. Self-propelled fluids could save energy for a range of technologies that depend on controlled fluid transport, including tiny sensors, diagnostic devices, microfluidic fuel cells for phones, and cooling methods for supercomputers.

Directly Seeing a Relativistic Quantum Crater

Novel defect control enables direct imaging of trapped electrons

Imaging the charge density waves for electrons can further a fundamental understanding of exotic electronic states. Recently, scientists imaged the electron charge density of a quantum dot in graphene. Using scanning tunneling microscopy, they visualized for the first time the unusual tunneling behavior of relativistic electrons confined to circular boundaries. The charge carrier density was imaged in a circular junction constructed in a graphene layer on top of insulating boron nitride. This new understanding of electron physics can further the advancement of quantum transport through graphene, potentially helping to launch new graphene-based quantum electronic devices for future computers and sensors.





Ringing an Atomic Bell to Probe Electrons

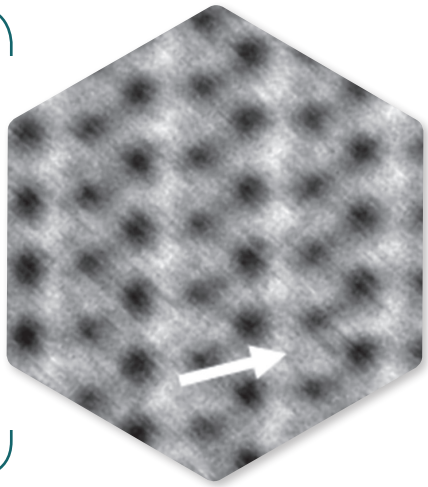
New approach measures coupling of atomic vibrations and electrons

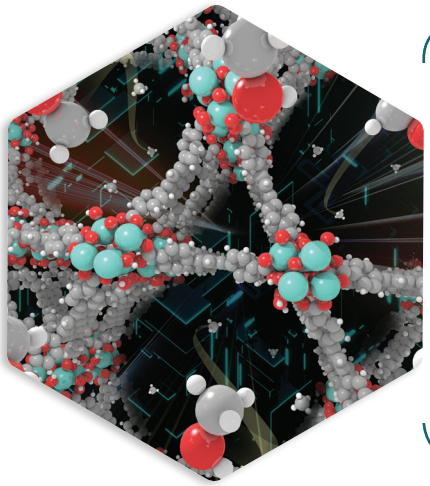
The electronic structure within a material quickly readjusts to changes in atomic positions. The coupling of the atomic positions and the electron orbitals controls how much readjustment, in terms of energy and momentum, is required. In this research, a laser pulse was used to excite atomic vibrations in a solid, like ringing a bell. In ultrafast time-sensitive recordings, this technique precisely clocked the atomic and electronic motions and quantified the coupling, which was ten times stronger than predicted. Understanding how the electron responds to atomic rearrangements is the basis for harnessing the electron effects that are at the foundation of new superconducting and magnetic materials.

Seeing How Next-Generation Batteries Charge-Up

Electron microscopy visualizes magnesium in a battery electrode

Multivalent batteries using doubly charged magnesium (Mg^{2+}) ions instead of singly charged lithium (Li^{+}) ions have the potential to significantly increase energy density and safety, while reducing cost compared to today's Li-ion batteries. A major challenge for Mg batteries is developing a cathode material that can accommodate migration of Mg during discharge. Using sophisticated electron microscopy, scientists could see where Mg inserts into the structure of a cathode material—even at low concentration. These insights are leading to improved design rules for superior cathode materials, bringing this technology several steps closer to fulfilling its promise.





Designed Catalyst Produces Fuels from Natural Gas

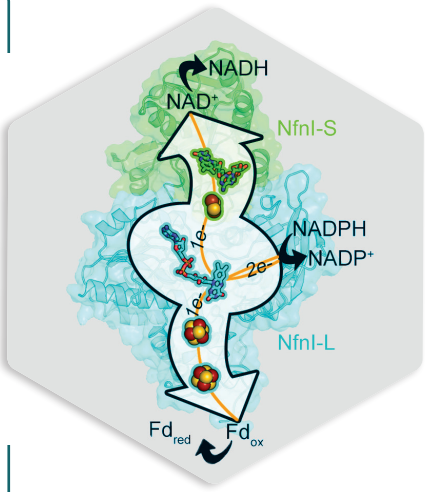
Framework converts methane to methanol under mild conditions

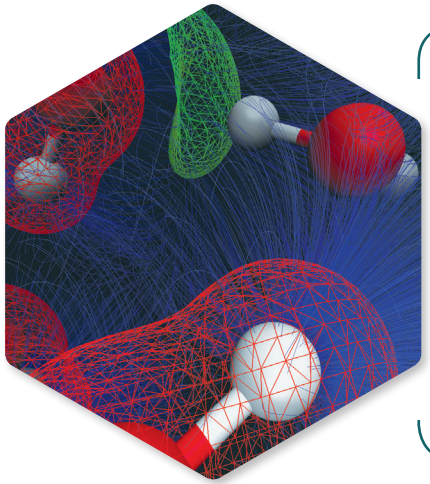
Copper oxide (Cu-oxo) clusters synthesized on the nodes of the zirconium-based NU-1000 metal–organic framework (MOF) oxidized methane to methanol with high selectivity at only 150°C. Scientists used theory and *in situ* x-ray analysis to determine the reaction pathway and confirmed the role of Cu in the conversion process. The MOF was shown to retain porosity, important for exposing the catalytic Cu-oxo site to methane. Further catalyst improvements will achieve better stability and higher activity for long-term catalytic conversion of methane to liquid fuels.

Flavins Perform Electron Magic

Study explains how organisms extract energy from their environment

Electron bifurcation is a clever means that living things use to better extract energy from their metabolic processes. Bifurcation takes two intermediate electrons and creates one high- and one low-energy electron. How bifurcation works was a mystery—until now. Scientists studied what happens after the flavin cofactor, a compound containing nitrogen and several six-membered rings that is closely related to the vitamin riboflavin, accepts two intermediate-energy electrons. The study found a highly energetic, short-lived flavin intermediate that is created after the first electron is sent away. The flavin rapidly channels its energy to the remaining electron, bumping up its energy. The kinetic, thermodynamic, and structural principles revealed in this study provide a foundation for understanding how bifurcating enzymes merge unique cofactors with catalytic sites to accomplish a diverse array of biochemical reactions.





Solving Mysteries of How Water Works

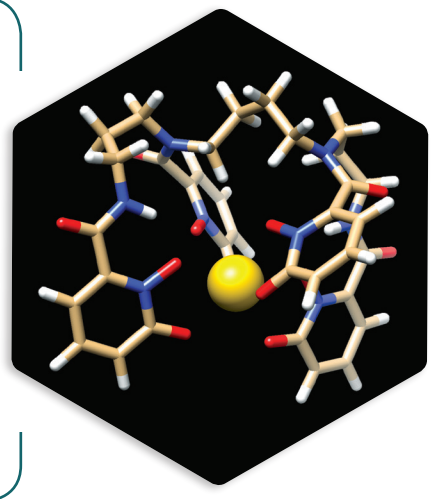
Theoretical tools to predict water's behavior in different systems

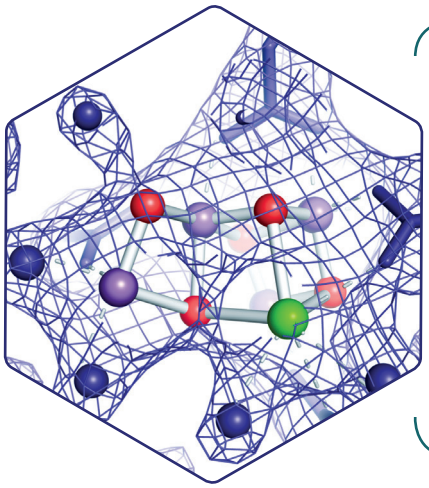
Scientists have strived to understand how a network of hydrogen bonds controls water's behavior. Researchers pioneered an approach that identifies how this network is structured using a model cluster composed of six water molecules around a positively charged cesium ion. They isolated the response of each water molecule in the network to accurately compute the way water is deformed according to its local electric field from the surrounding environment. These insights could lead to breakthroughs in detecting vibrational signatures of crystallization or water under extreme conditions.

Stabilizing the Heaviest 4+ Ion of the Periodic Table

Berkelium complex formed under mild aqueous conditions

Berkelium (Bk) chemistry is largely unexplored due to its short half-life and highly radioactive nature. It preferentially exists in aqueous solutions as Bk^{3+}, but oxidation to Bk^{4+} under very drastic conditions has been reported. In this research, the stabilization of Bk^{4+} was achieved under mild aqueous conditions, using a chelating siderophore derivative. The resulting neutral complex exhibits sensitized luminescence, providing information on the electronic structure of the metal ion. This behavior contrasts with formation of negatively charged complexes of neighboring trivalent actinides. The charge differences impact macromolecular recognition by the siderocalin protein and may lead to innovative Bk separation and purification processes.





Detailed Snapshots of Water Splitting Reaction

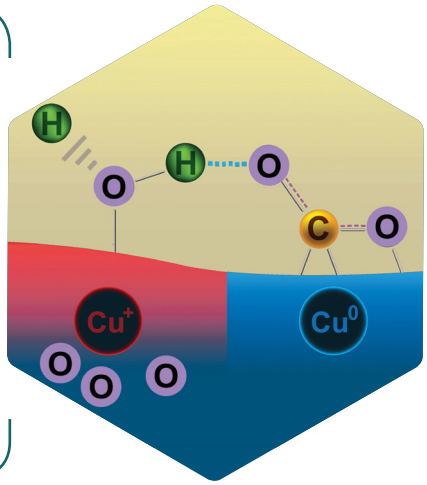
X-ray laser reveals mechanism of water oxidation in Photosystem II

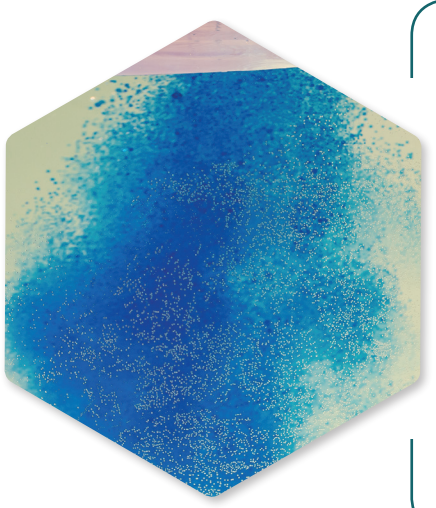
Most of the oxygen in the atmosphere has been generated by the light-induced oxidation of water by photosystem II (PS II) in plants, algae, and cyanobacteria. Femtosecond x-ray pulses from the Linac Coherent Light Source were used to obtain damage-free, room-temperature, high-resolution structures of PS II in two intermediate states that occur before O-O bond formation and evolution of O_2. These results reveal details about the mechanism of water oxidation during photosynthesis and help discriminate proposed O-O bond formation mechanisms.

Subsurface Oxide Critical for Catalysis

Essential first step for activating CO_2 on a Cu surface revealed

The best catalyst for converting carbon dioxide (CO_2) into liquid fuels and feedstock chemicals is currently copper (Cu), yet considerable uncertainty remains on the role of the Cu surface and chemistry during catalysis. Experiments combined with theory showed that CO_2 binds to Cu surfaces in a bent configuration when water vapor is present. A partial subsurface layer of oxygen was essential for this binding configuration, playing a critical role in initial steps for activating CO_2 and subsequent electrochemical reduction to fuels and other target products. These results provide a foundation for the rational development of new electrocatalysts.





Reusable Sponge for Mitigating Oil Spills

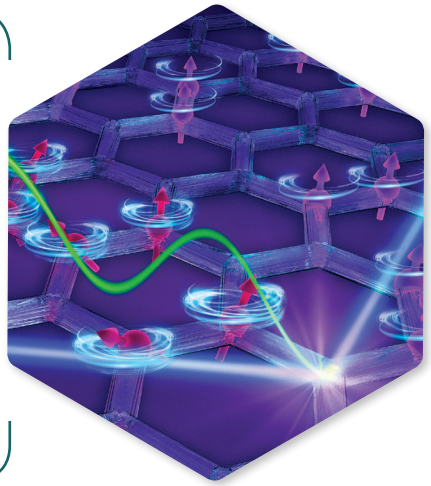
Oleo Sponge could make oil spill cleanup more efficient

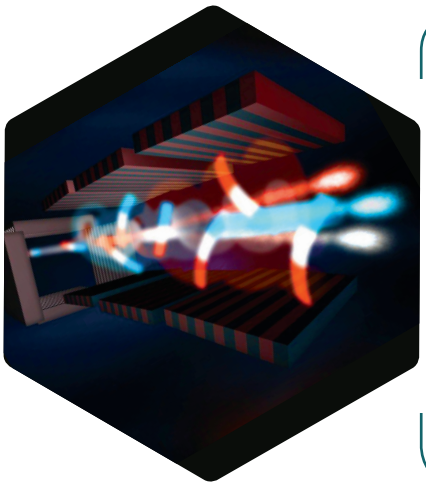
A new foam called the Oleo Sponge was invented by scientists at the Center for Nanoscale Materials. Oleo Sponge not only easily adsorbs oil from water but also is reusable and can pull dispersed oil from an entire water column, not just from the surface. Many materials can grab oil, but there has been no way, until now, to permanently bind them into a useful structure. The technique developed by the scientists creates a thin layer of metal oxide "primer" within the interior surfaces of a polyurethane foam and then binds oil-loving molecules to the primer. The resulting block of foam can be wrung out for reuse (usually hundreds of times), also recovering the oil. The technique itself is quite flexible and can be adapted to other types of cleanup by attaching different molecules to target specific substances.

Explaining a New State of Matter

First comprehensive quantum spin liquid mapped

In quantum spin liquids, the spins of the constituent electrons become entangled and fail to form a static ordered state, such as in a conventional magnet. The elusive nature of these materials makes confirming their existence difficult. Using the Spallation Neutron Source, researchers completed a comprehensive inelastic neutron scattering study of single crystals of the paramagnetic insulator ruthenium chloride (α-$RuCl_3$), a predicted host to a type of quantum spin liquid called a Kitaev spin liquid. The results were consistent with the Kitaev model, encouraging further study of the use of quantum spin liquids as components in future quantum computers.





Making More Colorful and Powerful X-Rays

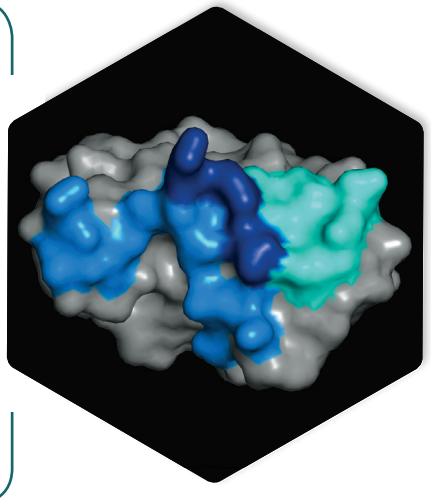
New scheme provides customizable x-ray pulses

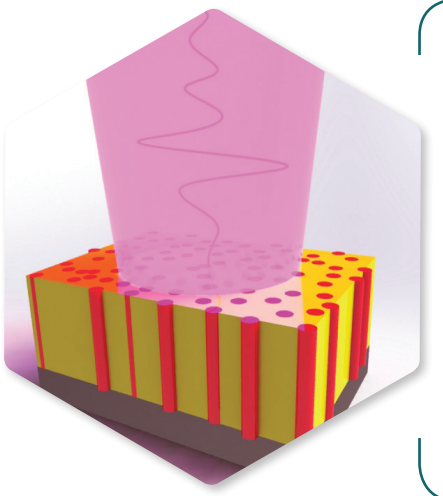
X-ray free-electron lasers provide femtosecond x-ray pulses with a narrow energy bandwidth and unprecedented brightness. Some experiments require multiple pulses, initiating a physical or chemical process with one pulse and then probing it with the next. A new scheme at the Linac Coherent Light Source takes one pulse and produces up to three intense multicolor pulses. The "fresh-slice" scheme produces highly customizable x-ray pulses with unprecedented performance, offering new insights into ultrafast physical and chemical changes. This research paves the way for creating completely new scientific instrument concepts and improving performance of existing instruments.

On Track to Design a Zika Virus Vaccine

Molecular structure reveals how antibody recognizes the virus

The Zika virus causes mild symptoms in most who contract it, but in newborn babies the virus can cause devastating neurodevelopmental abnormalities. Researchers extracted antibodies from blood samples taken from subjects in Mexico and Brazil that were exposed to Zika. They then used the Stanford Synchrotron Radiation Lightsource to solve the structure of one promising antibody in complex with the Zika virus binding domain. Revealed on the virus structure was a ridge where the antibody binds and blocks the virus from initiating an infection. This new information potentially can lead to design of a Zika vaccine. A ridge-triggered response vaccine could also be effective against similar flaviviruses like the dengue virus.





Toward Terahertz-Speed Magnetic Memory

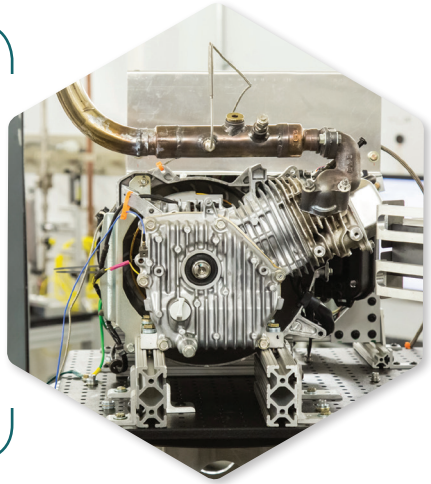
Advance could revolutionize the design of future memory devices

Personal electronics could operate at much higher speeds if memory devices could read and write data in terahertz (THz) frequency. Room-temperature colossal magnetoresistance (CMR), which involves a huge change in materials' resistance under magnetic fields, could simplify device development. A team including researchers from the Center for Integrated Nanotechnologies demonstrated room-temperature CMR at THz frequencies and intermediate magnetic fields for the first time in high-quality vertically aligned nanocomposite thin films. Although CMR usually is driven by a magnetic field, in this case the researchers added THz optical pulses to stimulate and enhance the CMR effect. This approach could enable the design of novel memory devices.

Neutrons Peer into a Running Engine

Performance of new aluminum alloy investigated

In a first-of-a-kind experiment, researchers at the Spallation Neutron Source used neutrons to investigate the performance of a new aluminum alloy in a gasoline-powered engine—while the engine was running. The automotive industry is interested in alloys that hold up to the high-heat demands of new, energy-efficient technologies. The new aluminum-cerium alloy showed exceptional stability at temperatures above 500°C, which is unheard of for aluminum alloys. With an aluminum alloy stable at high temperatures, engines could run hotter, and components could be made lighter, boosting efficiency and fuel economy.



FRONT COVER

Representative STEM Images of an Iron-Platinum (FePt) Nanoparticle at Different Orientations. A tilt series of 68 such images reveals the three-dimensional (3D) coordinates of 6,569 Fe and 16,627 Pt atoms in the nanoparticle with 22-picometer resolution. These measurements are used as direct input to density functional theory calculations to correlate crystal defects and chemical order/disorder with material properties at the single-atom level. Courtesy Yongsoo Yang and Jianwei (John) Miao, University of California, Los Angeles, and the Molecular Foundry, Lawrence Berkeley National Laboratory (LBNL). *Nature* **542**, 75–79, 2017. DOI:10.1038/542035a.

PAGE 6

Hybrid Materials Increase Solar Cell Efficiency. A "hot" electron in the center of this perovskite structure is surrounded by positive molecules (red and blue "dumbbells"). The distortion of the crystal structure and the liquid-like environment of the positive molecules (blurred dumbbells at edge) shield the hot electron, protecting and enabling it to survive 1,000 times longer than it would in conventional silicon solar cells. Courtesy Xiaoyang Zhu and Nicoletta Barolini, Columbia University. Reprinted with permission from Niesner, D., et al. 2016. "Persistent Energetic Electrons in Methylammonium Lead Iodide Perovskite Thin Films," *Journal of the American Chemical Society* **138**(48), 15717–726. © 2016 American Chemical Society.

Deciphering Material Properties Atom by Atom. The 3D coordinates of iron (red spheres) and platinum (blue) atoms are precisely identified in a nanoparticle. Courtesy Colin Ophus and Florian Niekiel, LBNL. *Nature* **542**, 75–79, 2017. DOI:10.1038/nature21042.

Blurring the Line Between Animate and Inanimate. Upon confinement and powered by tiny molecular motors, an "active" fluid transitions from locally chaotic to long-range unidirectional flow. The image portrays the instantaneous (left) and time-averaged (right) motion, along with localized counterclockwise (blue) and clockwise (red) whirlpools. The organization of the colored areas is a measure of the extent to which the fluid is flowing in one direction. From Wu, K., et al. 2017. "Transition from Turbulent to Coherent Flows in Confined Three-Dimensional Active Fluids," *Science* **355**(6331),1284. DOI:10.1126/science.aal1979. Reprinted with permission from AAAS.

PAGE 7

Directly Seeing a Relativistic Quantum Crater. Quantum waves of electronic charge density are confined to a small quantum dot in a graphene sheet. Scientists are using electron confinement to alter the physical properties of graphene and other quantum materials to better understand their behavior and meet specific application needs. Courtesy Michael F. Crommie and Alex Zettl, LBNL. *Nature Physics* **12**, 1032–36. 2016. DOI:10.1038/NPHYS3805.

Ringing an Atomic Bell to Probe Electrons. An infrared laser beam (orange) triggers atomic vibrations in a thin layer of iron selenide (FeSe) that has unconventional superconductivity. Ultrafast x-ray laser pulses (white) measure the atomic distance as the atoms oscillate in time like a clock. The motion of the Se atoms (red) and Fe atoms (blue) changes the energy of the electron orbitals around the atomic nuclei. These electron energies are recorded with angle-resolved photoemission spectroscopy (not shown). Courtesy Zhi-Xun Shen, Shuolong Yang, Patrick Kirchmann, and Greg Stewart, SLAC National Accelerator Laboratory.

Seeing How Next-Generation Batteries Charge-Up. Atomic-resolution image of an electrochemically cycled orthorhombic magnesium–vanadium pentoxide (Mg-V_2O_5) cathode. White arrow indicates where Mg occupancy is clear. Reprinted with permission from Mukherjee, A., et al. 2017. "Direct Investigation of Mg Intercalation into the Orthorhombic V_2O_5 Cathode Using Atomic-Resolution Transmission Electron Microscopy," *Chemistry of Materials* **29**, 2218–26. © 2017 American Chemical Society.

PAGE 8

Designed Catalyst Produces Fuels from Natural Gas. A copper-oxide cluster forms between zirconium nodes in the small pore of the metal–organic framework called NU-1000. Courtesy Kiley Schmidt and Manuel A. Ortuño. *Journal of the American Chemical Society* **139**(30), 10294–301, 2017. DOI:10.1021/jacs.7b02936.

Flavins Perform Electron Magic. Electron bifurcation catalyzes two simultaneous reactions. The bifurcating flavin cofactor (center) accepts two electrons and divides their energy into two energetically distinct one-electron pathways. Departure of the low-energy electron (top) creates a high-energy electron (bottom) capable of reducing ferredoxin, which has higher energy than the other reduced compound (NADH) and can be used for more difficult chemical reactions. Reprinted by permission from Macmillan Publishers Ltd: Nature Chemcal Biology. Lubner, C. E., et al. 2017. "Mechanistic Insights into Energy Conservation by Flavin-Based Electron Bifurcation," *Nature Chemical Biology* **13**(6), 655–59. © 2017. DOI:10.1038/nchembio.2348.

Solving Mysteries of How Water Works. A pioneering approach to "see" how intense local electric fields (blue curves) distort water's hydroxide (OH) vibrations shows that water's lone electron pairs (green) give rise to negative voltages relative to positive ones (red) due to the screened nuclei of water molecules and from the cesium ion. The coupling between these intense electric fields and the OH vibrations can be analyzed via these vibrational fields. *The Journal of Chemical Physics* **144**, 074305, 2016.

PAGE 9

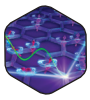
Stabilizing of the Heaviest 4+ Ion of the Periodic Table. Computed structure of Berkelium(IV) chelated by the multidentate hydroxypyridinonate ligand 3,4,3-LI(1,2-HOPO). Courtesy Gauthier Deblonde, LBNL, 2017. *Nature Chemistry* **9**, 843–49, 2017. DOI:10.1038/nchem.2759.

Detailed Snapshots of Water-Splitting Reaction. Structure of the oxygen-evolving manganese-calcium (Mn_4Ca) complex in photosystem II, with water molecules (blue spheres), Mn atoms (purple), Ca (green), and the bridging oxygen atoms (red). Blue mesh is the experimental electron density, and blue solid lines are the protein side chains that provide a scaffold for the catalytic complex, shown here in a light-activated state. Courtesy Junko Yano and Vittal Yachandra, LBNL. *Nature Chemistry* **9**, 843–49, 2017. DOI:10.1038/nchem.2759.

Subsurface Oxide Critical for Catalysis. Illustration of ambient pressure x-ray photoelectron spectroscopy of a copper (Cu^+ and Cu^0) surface in the presence of carbon dioxide (CO_2: C and O) and oxygen indicates the importance of a suboxide layer (bottom) in activating CO_2. Courtesy California Institute of Technology, LBNL, and the Joint Center for Artificial Photosynthesis. *Proceedings of the National Academy of Sciences of the USA* **114**, 6706–11, 2017. DOI:10.1073/pnas.1701405114.

PAGE 10

Reusable Sponge for Mitigating Oil Spills. The Oleo Sponge can pick up oil dispersed within a water column, a property held by no commercially available product. Courtesy Mark Lopez, Argonne National Laboratory. *Journal of Materials Chemistry A* **5**, 2929–35, 2017. DOI:10.1039/C6TA09014A.



Explaining a New State of Matter. As neutrons (blue line) scatter off the graphene-like honeycomb material, they produce a magnetic Majorana fermion (green wave) that moves through the material, disrupting or breaking magnetic interactions between "spinning" electrons. Courtesy Oak Ridge National Laboratory (ORNL). *Science* **56**(6342), 1055–59, 2017. DOI:10.1126/science.aah6015.

Making More Colorful and Powerful X-Rays. The head, core, and tail (blue, white, and red slices) of a single bunch of electrons (left) travel on different trajectories close to a corrugated metal wall. Each slice is controlled to travel straight only in a single undulator section, producing powerful x-ray pulses that can be finely and independently controlled. Courtesy Greg Stewart and Alberto Lutman, SLAC National Accelerator Laboratory. *Nature Photonics* **10**, 745–50, 2016. DOI:10.1038/nphoton.2016.201.

PAGE 11

On Track to Design a Zika Virus Vaccine. The "ridge" binding domain of the Zika virus surface protein that binds a potent human antibody. Antibodies isolated from infected patients bind to the virus protein by contacting the blue and cyan regions with their heavy and light chains, respectively, and to the dark blue region with both chains. Reprinted from Robbiani, D. F., et al. 2017. "Recurrent Potent Human Neutralizing Antibodies to Zika Virus in Brazil and Mexico," *Cell* **169**, 597–609. © 2017, with permission from Elsevier.

Toward Terahertz-Speed Magnetic Memory. Interactions of terahertz pulses (pink) with a vertically aligned nanocomposite film including zinc oxide nanopillars (red) embedded in the epitaxial $La_{0.7}Sr_{0.3}MnO_3$ film matrix (yellow), a perovskite manganite oxide semiconductor. Courtesy Chris Sheehan and Aiping Chen, Los Alamos National Laboratory. Lloyd-Hughes, J., et al. 2017. *Nano Letters* **17**(4), 2506–11. DOI:10.1021/acs.nanolett.7b00231.

Neutrons Peer into a Running Engine. A running gasoline engine, whose cylinder head was made from a new aluminum-cerium alloy, is tested *in situ* using the Spallation Neutron Source's VULCAN spectrometer. Courtesy ORNL.

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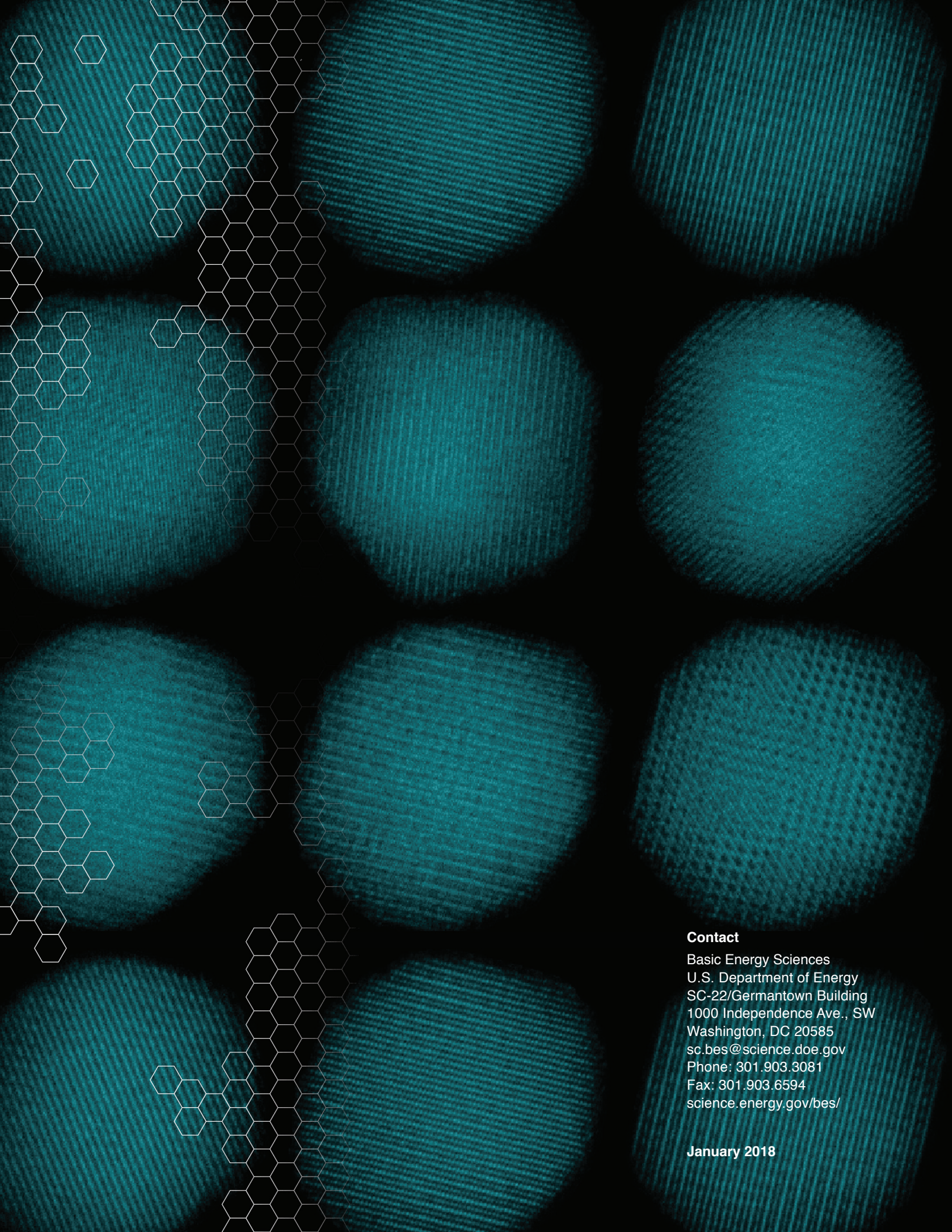

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January 2018