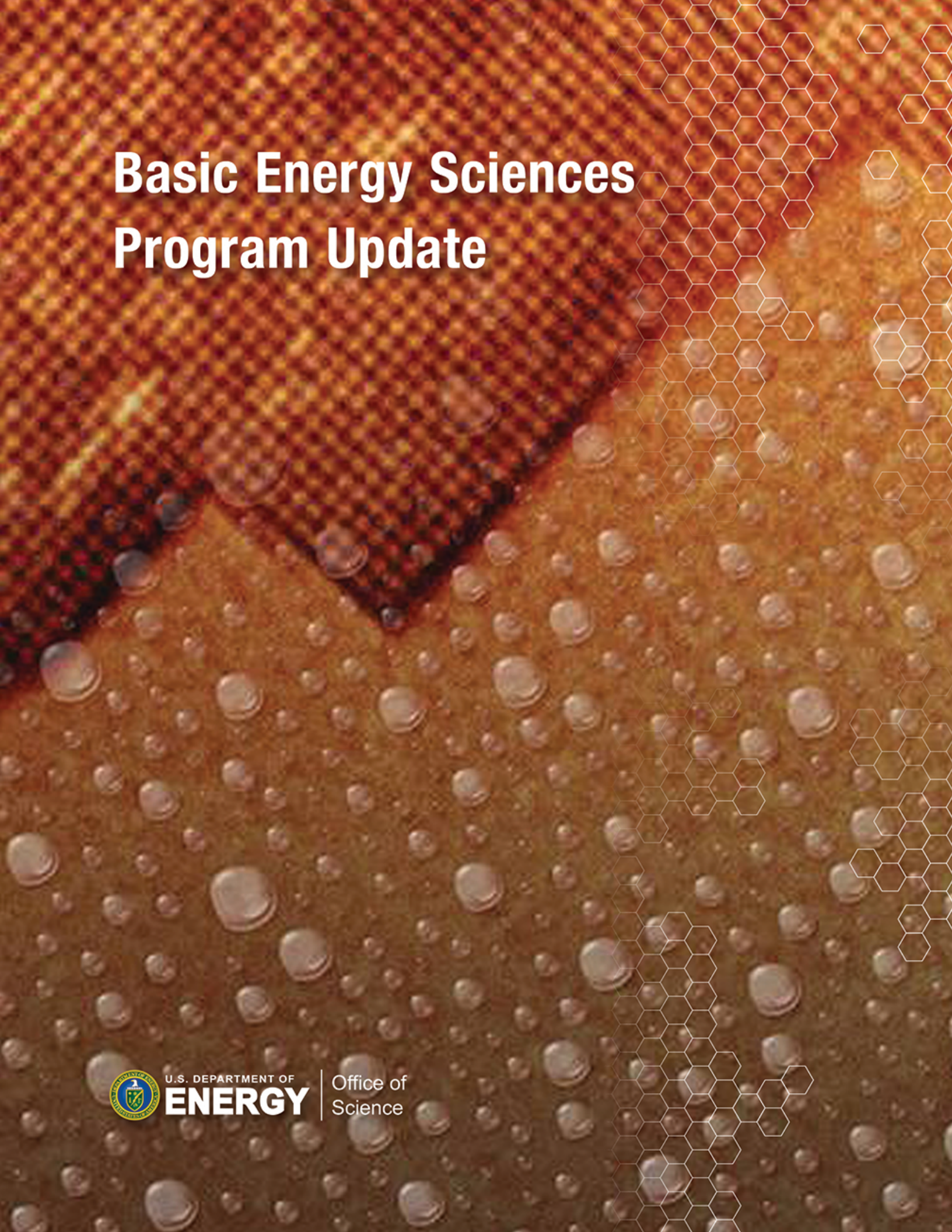
Basic Energy Sciences Program Update



U.S. DEPARTMENT OF ENERGY | Office of Science

BES RESEARCH SPANS

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

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

25 CORE RESEARCH AREAS

SUPPORTED RESEARCHERS

~6,100 Ph.D. SCIENTISTS | **~2,100** STUDENTS SUPPORTED

BES BY THE NUMBERS

FY 2019

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

46 ENERGY FRONTIER RESEARCH CENTERS

$784 MILLION RESEARCH BUDGET

MORE THAN **16,000** USERS AT **12** BES FACILITIES

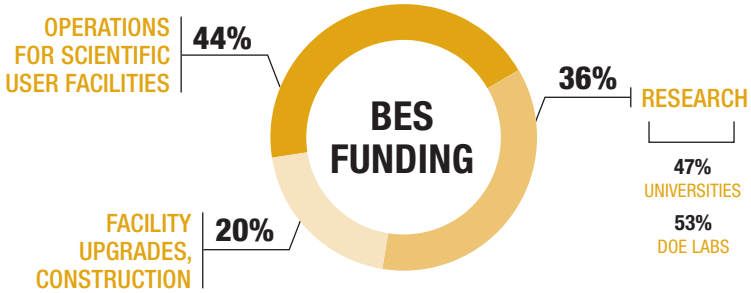
$955 MILLION SCIENTIFIC USER FACILITY OPERATING BUDGET

NEARLY **1,400** CORE RESEARCH PROJECTS

~21% AVERAGE NEW GRANT SUCCESS RATE

2 ENERGY INNOVATION HUBS

$427 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. This research provides the foundations for new energy technologies and supports 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 phenomena and the 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 materials of all kinds, ranging 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

Energy Frontier Research Centers

On July 29–30, 2019, about 650 researchers from the Energy Frontier Research Centers (EFRCs) and DOE staff participated in a principal investigators' meeting that marked the 10th anniversary of this landmark program and celebrated accomplishments of the 82 centers that have been supported since 2009. In its first decade, the program has involved more than 1,600 senior investigators and more than 5,400 students at some 170 institutions. Collectively, the EFRCs have generated more than 11,600 peer-reviewed publications and nearly 1,000 domestic and international patent applications. More than 100 companies have benefited directly from EFRC research.

The meeting included a plenary session with distinguished speakers and panel discussions on EFRC impact and science-to-technology transition. DOE Under Secretary for Science Paul Dabbar announced the winners of a DOE-sponsored Ten at Ten Contest to mark the ten-year anniversary of the program. These EFRC researchers or groups of researchers, past and present, best exemplified the extraordinary impact that the EFRCs have had on people, science, and technology. Recognized projects focused on energy storage, photovoltaics and solar energy, chemical analysis and gas separation, new materials development, and education and knowledge transfer (see page 8).

The plenary session was followed by scientific oral and poster presentations 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 14 finalists, BES selected six teams based on scientific excellence, topical diversity, presentation quality, and how well their research exemplified opportunities provided by the EFRC funding modality. BES also held an optional video contest to challenge the community to educate, inspire, and entertain an informed but not expert audience about the extraordinary science, innovation, and people in the EFRCs.

Data Science

BES supported 19 data science awards for knowledge discovery in chemical and materials research in FY 2019. These awards, totaling $27.6 million over 3 years, will advance the use of modern data science approaches (e.g., artificial intelligence, machine learning, graph theory, and uncertainty quantification) to accelerate discovery in chemical and materials sciences. Research targets complex chemical and materials processes,

defined as those whose macroscopic properties, reaction mechanisms, and dynamic behavior cannot be predicted from a known combination of the properties of individual components and are outside the scope of existing theoretical approaches. Data science approaches, in combination with experimental and theoretical methods, are expected to accelerate the discovery of fundamentally new chemical mechanisms and material systems with exceptional properties and dynamic behavior, as well as lead to new understanding of physical and chemical phenomena.

Quantum Information Science

In FY 2019, BES announced 20 new awards totaling $37.2 million for targeted research in materials and chemistry to advance the important emerging field of quantum information science (QIS). QIS seeks to exploit intricate quantum mechanical phenomena to create fundamentally new ways of obtaining and processing information. It is expected to play an increasingly important role in the information technology of the future, with the promise of potentially powerful new capabilities in computing, networking, and sensing. The research projects are aimed at synthesis and observation of material and chemical systems with exotic quantum properties as well as efforts to use quantum computing to better understand complex material and chemical systems. The goal of these awards is both to lay the groundwork for the development of new quantum information systems and to use current quantum information capabilities to advance research in chemical and materials sciences.

Computational Materials Sciences

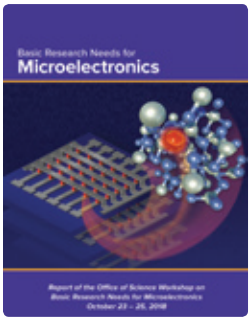
BES announced an investment of $32 million over four years beginning in FY 2019 that will accelerate the creation of computational codes and associated experimental and computational databases for the design of functional materials. Seven research projects were selected to develop open-source software that can take advantage of DOE's current leadership-class and future exascale computing facilities. The goal is to provide the software platforms and data needed to design new functional materials with a broad range of applications, including alternative and renewable energy, electronics, data storage, and materials for QIS. Research combines theory and software development with experimental validation, drawing on the resources of multiple DOE Office of Science (SC) user facilities. This research will result in publicly accessible databases of experimental and computational data, as well as open-source, robust, validated, and user-friendly software that captures the essential physics of relevant materials systems. Additional awards will be made under this program in FY 2020.

Strategic Planning

In FY 2019, BES conducted three strategic planning activities to identify basic research needed in the areas of microelectronics, chemical upcycling of polymers, and liquid solar fuels. Two roundtables and a Basic Research Needs workshop engaged the research community in solving problems for the nation's energy future. The resulting reports (available at science.osti.gov/bes/community-resources/reports) summarize the current state of technology and define a set of priority research directions or opportunities for basic research investment.

Basic Research Needs for Microelectronics

Since the invention of the integrated circuit in 1958, advances in microelectronics have followed Moore's law and other scaling laws. These improvements have led to over a billion-fold increase in the number of transistors on a chip.



DOE SC programs have always been at the cutting edge of microelectronics, making major contributions to the scientific understanding, materials, and advanced instrumentation that enabled

innovations to promote scaling. These contributions have driven transformative advances in microelectronics for the challenging demands of DOE's high-performance computing and science facilities. Now, strong evidence exists that scaling is approaching its physical and economic limits, and yet the growth of data-centric computing and sensor networks is redefining computing workloads and microelectronics needs. In addition, greatly improved microelectronics are needed for the nation's electricity grid if it is to be energy efficient, resilient to natural phenomena and intentional attack, and agile in adapting to fluctuations in demand and power generation. Sustained and rapid progress in microelectronics science and technology from millivolt to megavolt scales is thus essential if the nation is to continue pushing the boundaries of science within DOE and, more significantly, to lead the global information and power technology revolution.

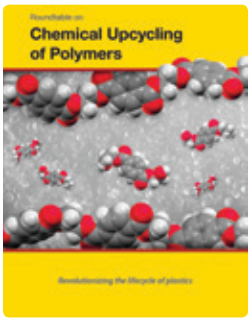
In October 2018, SC convened a workshop to address Basic Research Needs for Microelectronics by a "co-design" approach. Co-design involves multidisciplinary collaboration that considers the interdependencies among fundamentals of materials and chemistry, device physics, computing architectures, and software stacks for developing information processing systems of the future. Participants focused on scientific issues associated with advanced microelectronics technologies for applications relevant to DOE missions, including computing, power grid management, and science facility workloads. Five priority research directions were identified:

- Flip the current paradigm: Define innovative material, device, and architecture requirements driven by applications, algorithms, and software.
- Revolutionize memory and data storage.
- Reimagine information flow unconstrained by interconnects.
- Redefine computing by leveraging unexploited physical phenomena.
- Reinvent the electricity grid through new materials, devices, and architectures.

In the future, computing systems encompassing new materials, devices, architectures, algorithms, and software will be needed to maintain the continued upward trajectory in performance that Moore's law scaling has historically provided. Among the challenges is discovery science that can lead to microelectronics for exascale computers and beyond with a small footprint and low power utilization. Such high-performance computation will be necessary for analyzing and managing the vast amount of data that will be generated by future SC facilities to enable new discoveries. Furthermore, advances in new microelectronics materials, and their integration within a co-design framework, are required to transform power electronics and the electricity grid into a modern, agile, resilient, and energy-efficient system.

Roundtable on Chemical Upcycling of Polymers

Plastics are ubiquitous in modern life. They are made from synthetic carbon-based polymers—organic macromolecules made up of many repeating subunits called monomers—and are designed to be durable and resistant to degradation. Global plastics production has reached a rate of over 400 million metric tons per year, with over 8 billion metric tons produced in the past 50 years. Average annual production has increased by 36% in the past decade and is projected to grow to 700 million metric tons in 2030—about 80 kg of plastics produced for every human on earth. Globally, 20% of discarded plastics are recycled (<10% in the United States), primarily using mechanical processes, and about 25% are incinerated for energy recovery. More than half are deposited into landfills or released into the environment. Thus, plastic waste poses a long-term environmental challenge.



Plastics represent a resource for making chemicals, fuels, and materials. Although incineration

eliminates wastes and recovers some of the energy used to make the plastic, it uses up the potential resource and creates unwanted byproducts. Mechanical recycling—which involves shredding, heating, and remolding of the plastics—is more efficient than making them from petroleum products, using less than half as much energy to generate new plastics. However, mechanical recycling degrades, or downcycles, the polymers. Chemical recycling deconstructs polymers to produce molecular intermediates that can be used as building blocks to make new products, offering the opportunity to turn discarded plastics into higher-valued products. However, current chemical recycling approaches are energy-intensive and require further processing to make products. Polymer upcycling represents a new approach that couples deconstruction and reconstruction processes by first selectively deconstructing polymers into chemicals, fuels, or molecular intermediates that then are reconstructed into high-value products under mild conditions. Polymer upcycling holds the promise of changing the paradigm for discarded plastic from waste to valued resource by moving to a circular lifecycle for plastics.

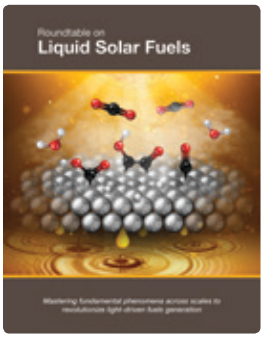
BES held a Roundtable on Chemical Upcycling of Polymers in April 2019 to identify the fundamental challenges and research opportunities that could transform discarded plastics to higher-value fuels, chemicals, and materials. Four priority research opportunities were identified to address the complex chemical transformations and physical processes underlying the upcycling of discarded plastics:

- Master the mechanisms of polymer deconstruction, reconstruction, and functionalization.
- Understand and discover integrated processes to upcycle mixed plastics.
- Design next-generation polymers for chemical circularity.
- Develop novel tools to discover and control chemical mechanisms for macromolecular transformations.

Through fundamental research into the chemical upcycling of polymers, a new paradigm will emerge in which discarded plastic is captured and becomes a resource, enabling efficient production of high-value chemicals, fuels, and new polymeric materials and reducing the accumulation of plastic wastes in the environment. In addition, chemical upcycling will shift the raw material for making polymers from fossil fuels—a process that is predicted to consume as much as 20% of the world's oil production in 2050—to discarded plastics.

Roundtable on Liquid Solar Fuels

Sunlight is Earth's most abundant energy resource. Remarkable advances in photovoltaic technologies are allowing society to better capitalize on this resource for electricity generation. Harnessing the power of the sun to produce energy-rich chemicals directly from abundant feedstocks such as water, carbon dioxide, and nitrogen promises a plentiful supply of sustainable, transportable, and storable solar fuels to meet future U.S. energy needs. Furthermore, solar fuels can provide pathways for efficient chemical energy storage to complement existing electrical energy storage. Solar fuels can also produce diverse chemicals, products, and materials with low environmental impact.



Solar fuels generation—often termed artificial photosynthesis—involves the direct conversion of solar energy to chemical energy using man-made materials and chemical processes. Significant progress has been made to boost the efficiency of solar-driven hydrogen production. Much less progress has been made in the area of liquid solar fuels, an approach that requires chemically transforming carbon dioxide and other small molecules into promising fuel targets. Hydrocarbons and oxygenates produced from carbon dioxide conversion will be compatible with existing fuels infrastructure. They could also be valuable for production of commodity chemicals and materials. The generation of ammonia and other

nitrogen-containing species, which can be used as fuels, fertilizers, and other commodities, presents an opportunity to exploit an extremely abundant feedstock—atmospheric nitrogen.

BES held a Roundtable on Liquid Solar Fuels in August 2019 to examine fundamental challenges and research opportunities for generating energy-rich liquids from abundant feedstocks using sunlight as the only energy input. Four priority research opportunities were identified to address critical physical and chemical phenomena required for selective, stable, and efficient direct production of liquid solar fuels using an artificial photosynthesis approach:

- Understand the mechanisms that underpin constituent durability and performance.
- Control the catalyst microenvironment to promote selective and efficient fuel production.
- Bridge the time and length scales of light excitation and chemical transformations.
- Tailor interactions of complex phenomena to achieve integrated multicomponent systems.

Artificial photosynthesis approaches offer the promise of efficient and scalable generation of liquid fuels using sunlight. Past foundational progress has brought us to a point at which fundamental breakthroughs are needed to overcome significant scientific challenges that still exist and to facilitate a more complete mechanistic understanding of solar energy capture and conversion as well as integrated component and system performance. These research opportunities present new horizons for fundamental chemistry and materials research needed to develop technologies for liquid solar fuels generation.

Basic Research Initiative for Microelectronics RFI

To inform the launch of a multiprogram basic research initiative in support of microelectronics and semiconductor sectors, SC issued a request for information (RFI) on July 12, 2019. The RFI invited interested parties to provide input on the topical areas, innovation mechanisms, impact, and potential collaborations (including public-private partnerships) that could be implemented under this initiative. SC was particularly interested in ways in which unique DOE facilities, expertise, and capabilities can be leveraged to support continued U.S. innovation and global leadership in microelectronics. Approximately 50% of the 49 distinct responses came from universities, 25% from laboratories, and 25% from industry. Respondents generally agreed that broad multidisciplinary activities are needed to drive innovation. There was support for public-private partnerships involving industry, academia, and national laboratories, with a caution that intellectual property must be carefully considered up front. A general need for improved modeling and simulation capabilities in relevant fields was cited. Multiple respondents agreed that DOE is a logical agency to support this initiative, particularly if existing expertise and facilities at the national laboratories can be leveraged.

Quantum Information Science RFI

SC issued a notice of intent and RFI on May 20, 2019, to solicit community input on aspects of the planned Quantum Information Science Centers funding opportunity announcement (FOA). The RFI invited interested parties to provide input on the topical areas, organization, requirements, review criteria, and assessment process of prospective QIS Centers. SC received 38 distinct responses representing the views of 9 DOE national laboratories, 22 universities, and 11 companies. This input highlighted the need for the envisioned centers to achieve progress beyond what the component efforts could accomplish if supported individually. Also cited was the need for the centers to leverage existing DOE investments in research and facilities as well as existing industrial technology and capabilities. The feedback on topical areas and scope, collaboration and partnerships, management and organization, assessment and success criteria, and impact was integrated into the FOA released in FY 2020.

BES Researchers Recognized with Prestigious Awards

2019 Nobel Prize in Chemistry

John B. Goodenough

M. Stanley Whittingham

The 2019 Nobel Prize in Chemistry was awarded to Professors John B. Goodenough, M. Stanley Whittingham, and Akira Yoshino for the development of lithium-ion batteries. These batteries have enabled many advances, including mobile phones and plug-in electric vehicles. From transportation to grid resiliency, they are important for a sustainable future.

Goodenough and Whittingham are longtime BES-supported researchers. Goodenough, of the University of Texas at Austin, is Principal Investigator for the BES grant, "Materials and Interfacial Chemistry for Next-Generation Electrical Energy Storage," first awarded in 2010 and most recently renewed in 2019. His current work represents an expansion of his original research on the development of advanced electrode materials for rechargeable batteries that is the basis of his Nobel Prize recognition.

Whittingham, of Binghamton University, directs the NorthEast Center for Chemical Energy Storage (NECCES), a BES Energy Frontier Research Center launched in 2009. His current research is an extension of his Nobel Prize–winning work into electrical energy storage using intercalation of lithium ions into electrode materials.

Goodenough and Whittingham have played integral roles over the years in federal advisory committee–related activities, helping the Office of Science and DOE chart an effective path forward in transformative research on energy storage. BES continues to support an array of battery-related research that builds on their work.

Inaugural Class of Distinguished Scientist Fellows

DOE named five national laboratory scientists as the first cohort of Distinguished Scientist Fellows in 2019. The newly established award, authorized by the America COMPETES Act and bestowed on national laboratory scientists with outstanding records of achievement, provides each Fellow with $1 million over three years to be devoted to one or more projects of the Fellow's choosing.

José Rodriguez

José Rodriguez, of Brookhaven National Laboratory (BNL), received the award for discoveries of the atomic basis of surface catalysis for the synthesis of sustainable fuels and for significantly advancing *in situ* methods of investigation using synchrotron light sources. Rodriguez's BES-supported research has focused on catalysts used to produce clean, efficient, and renewable fuels and to control environmental pollution.

Rodriguez will devote his award funding to the development and construction of new tools for performing extremely rapid, time-resolved measurements to uncover the reaction mechanisms of catalytic processes as they occur under variable conditions—such as those encountered during real-world reactions important to energy applications. These studies will include processes on metal-oxide catalysts, which are frequently used in the production of clean fuels and other chemicals through hydrogenation of carbon monoxide and carbon dioxide, or the conversion of methane to hydrogen.

The 2019 Fellows also include: Sally Dawson, BNL; Ian Foster, Argonne National Laboratory; Joshua Frieman, Fermi National Accelerator Laboratory; and Barbara Jacak, Lawrence Berkeley National Laboratory.

BES Early Career Scientists

Established in 2010, the DOE Office of Science Early Career Research Program supports the individual research projects of outstanding scientists early in their careers and stimulates research careers in the disciplines supported by the Office of Science. The researchers highlighted here were funded by BES in the 2010 inaugural cohort and are examples of how this program has enabled promising scientists to establish independent research careers.

Feng Wang

University of California at Berkeley and Lawrence Berkeley National Laboratory

Graphene, a one-atom-thick sheet of carbon, exhibits incredible structural flexibility, electrical transport, and optical responses. Professor Wang's research focused on understanding and controlling the electronic structure in graphene and other two-dimensional materials by combining advanced device fabrication, electrical control, and laser spectroscopy. Wang built on the research directions established in his early career award and now leads a BES-funded research project on electrical and optical properties in two-dimensional van der Waals heterostructures.

Marivi Fernández-Serra

Stony Brook University

Fundamental understanding of the interactions and processes occurring at the liquid-metal interface is needed to improve future energy production and delivery systems such as fuel cells and batteries. Professor Fernández-Serra's research used quantum-mechanical computational methods to understand how the rates of chemical reaction occurring at the liquid-electrode interface can be modified to optimize a system's power. She now leads a project on the development and application of computational methods for understanding interfacial charge transfer in photocatalytic water-splitting materials.

Ivan Bazarov

Cornell University

Powerful particle accelerators are only as good as the quality of the beams that they accelerate. A fundamental beam quality, beam brightness, is one measure of its usefulness. Professor Bazarov investigated the fundamental limits to beam brightness available from photoinjectors and shed a new light on the mechanisms of photoemission as they relate to fundamental beam properties. Since his early career award, Bazarov has expanded his research to topics relevant to the Offices of High Energy Physics and Nuclear Physics.

ENERGY FRONTIER RESEARCH CENTERS

10@10 AWARDS

To mark the ten-year anniversary of the Energy Frontier Research Center (EFRC) program, BES selected ten awardees that embody the extraordinary impact that the EFRCs have had on people, science, and technology. More about the EFRC program: science.osti.gov/bes/efrc

Workforce Development Awards

Erin L. Ratcliff

Center for Interface Science: Solar Electric Materials (CISSEM)

For embracing multidisciplinary team science to characterize and control the chemical and physical interactions between electrical contacts and active layers in emerging solar energy technologies.

Michael Naguib

Fluid Interface Reactions, Structures and Transport Center (FIRST)

For developing a new family of two-dimensional materials based on transition metal carbides and nitrides that have proven to be transformative battery and supercapacitor electrode materials.

Katlyn M. Turner

Materials Science of Actinides (MSA)

For her dedication to EFRC research from undergraduate through graduate studies, transferring research knowledge and techniques between institutions, and maintaining strong ties between collaborating groups.

Scientific Ideas Awards

Mercouri Kanatzidis, Robert P. H. Chang

Argonne Northwestern Solar Energy Research (ANSER)
Center for Light Energy Activated Redox Processes (LEAP)

For the first demonstration of all-solid-state solar cells using halide perovskite materials.

Jeffrey R. Long, Thomas M. McDonald, Douglas A. Reed, Rebecca L. Siegelman, C. Michael McGuirk

Center for Gas Separations (CGS)

For the discovery of cooperative adsorption in metal-organic frameworks.

Candace Haigler, James Kubicki, B. Tracy Nixon, Hugh O'Neill, Alison Roberts, Ming Tien, Yaroslava Yingling, Jochen Zimmer

Center for Lignocellulose Structure and Formation (CLSF)

For elucidating the structure and function of plant cellulose synthase and cellulose synthesis complex.

Carrie Siu, Yuhchieh Lin, Ieuan Seymour, Jatin Rana

NorthEast Center for Chemical Energy Storage (NECCES)

For developing a fully rechargeable multi-electron 2-lithium battery cathode.

Technologies and Tools Awards

Paul Dauenhauer

Catalysis Center for Energy Innovation (CCEI)

For developing the quantitative carbon detector 3D-printed metal catalytic microreactor.

Harold Kung, Cary Hayner, Mark Hersam

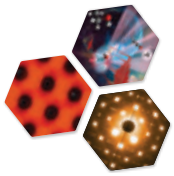
Center for Electrochemical Energy Science (CEES)

For developing graphene encapsulation of lithium-ion battery anodes and cathodes.

David Bierman

Solid-State Solar Thermal Energy Conversion Center (S^3TEC)

For developing an ultra-high efficiency thermophotovoltaic power conversion device.



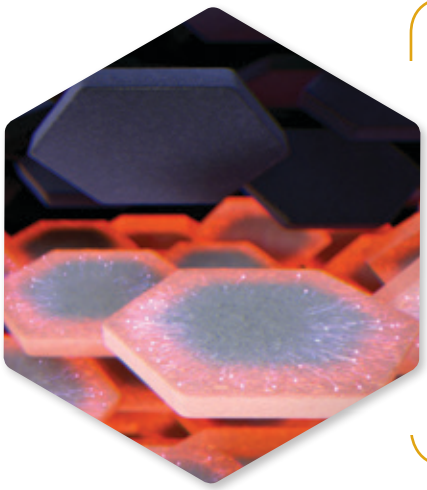
Research Highlights

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.



Battery End-Run Spreads Lithium in Electrodes

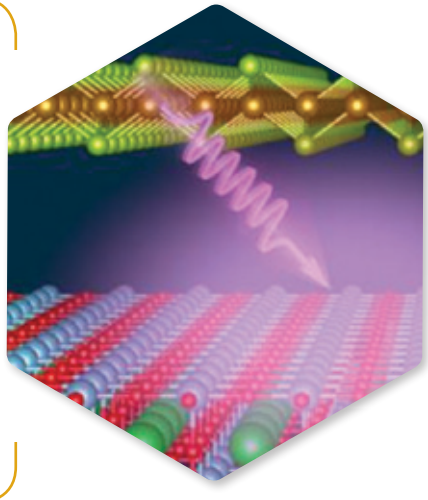
Controlling lithium ion flow could lead to better batteries

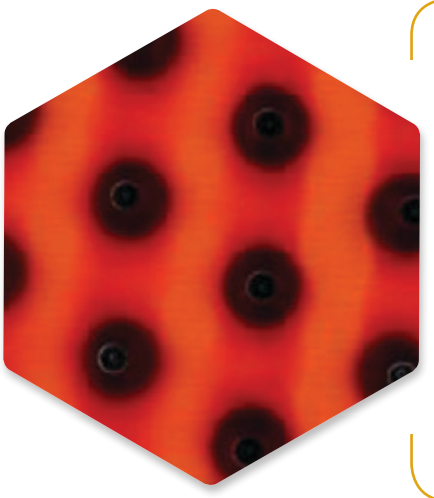
Scientists used chemically sensitive x-ray microscopy to map lithium transport during battery operation and discovered an unexpected surface diffusion of lithium that affects how quickly lithium moves through an electrode particle. The surface path determines whether the particle forms local regions of extreme lithium concentration, resulting in mechanical instability and degradation of the electrode structure. As lithium batteries charge and discharge, mechanical stresses occur in the electrodes, leading to reduced battery lifetimes. These new insights into how lithium migrates can guide the engineering of safer, longer-lasting, and higher-performance lithium batteries.

This Superconductor Does Not Take Light Lightly

Low-energy optical control offers way to manipulate superconductivity

Scientists have discovered a new superconducting material that responds to light, namely a thin film of iron and selenium on a thin layer of an insulating material. The combination transmits electricity without loss when cooled to 24 Kelvin (–416°F). When exposed to low-energy ultraviolet light, the material acts as a superconductor at higher temperatures. The critical temperature increases by 25%, and the new superconducting state remains stable even after the light is turned off. This state will persist for days unless a series of high-voltage pulses is applied to the back of the substrate or the sample is warmed to room temperature and recooled. This effect may improve next-generation quantum computers and sensors.





Flowing for Function

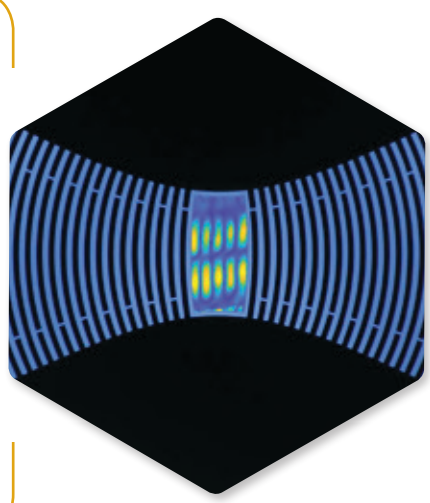
Magnetically responsive liquid regulates solid shapes, properties

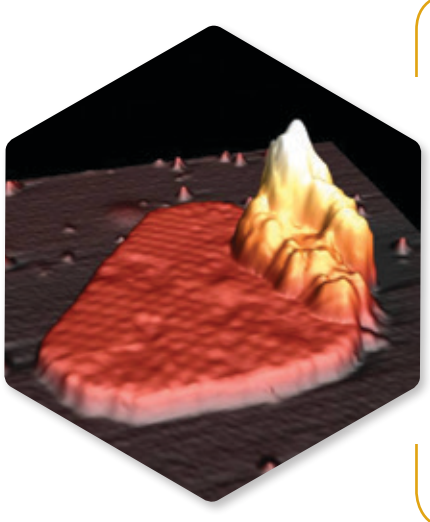
Researchers have combined an active liquid with a solid textured surface to create dynamic surface coatings. They can seamlessly resculpt both nano- and macroscale surface features of these hybrid materials into an endless variety of complex topographies. Triggered by a simple magnetic field, topographies form and reconfigure as the liquid flows above and within the textured surface. Resulting surface responses display intriguing spatial and time-based fluid dynamics and energy conversion properties and introduce a wide range of novel functions when interfaced with other solids and liquids. Applications could lead to breakthroughs in energy-efficient buildings, microelectronics, self-cleaning surfaces, and more.

Sound Waves Carry Quantum System Information

Novel communication method brings quantum technology closer

Scientists are eyeing quantum systems as key to next-generation, atomic-scale electronics for computation and communication. A persistent challenge, however, has been transferring information between different types of technologies such as quantum memories and quantum processors. One possibility to realize such hybrid systems is to manipulate and connect quantum states of matter with sound waves by coupling the sound waves with the spins of electrons in the material. Researchers demonstrated spin transitions driven by sound waves on long-lived spin ensembles in silicon carbide through different quantum systems. The results provide new ways to control these systems and open venues of research and technological applications such as quantum sensing with microelectromechanical systems (MEMS).





Getting Metal Under Graphite's Skin

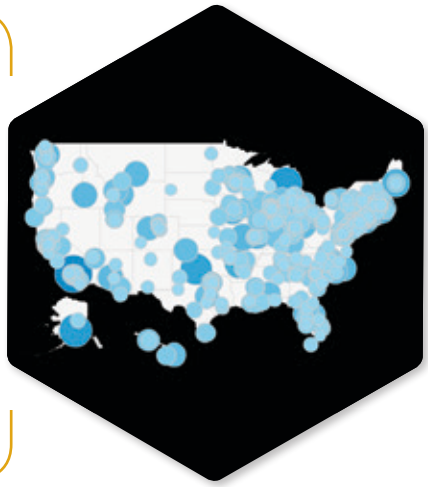
Below-surface islands protect metals, enable novel properties

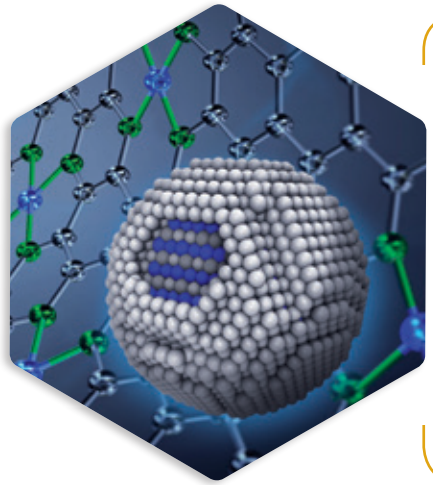
Graphene is a carbon material that allows electrons to move rapidly along its surface, making it ideal for electronic or magnetic applications. One way to protect metals from degradation and have them interact with graphene is to encapsulate them in graphite. Scientists developed a process for inserting metals under a graphite surface using high-speed ions to make holes in the surface, creating entry portals. High-temperature deposition of the metals through these portals allowed the deposited atoms to move below the surface forming crystalline islands, protecting the metal and creating a possible way to tailor rare earth metals to have valuable transport, catalysis, magnetism, or friction properties. These complex structures could be used to form 2D quantum materials with new applications in solar cells and quantum computing.

Materials Project Reaches 100,000 User Milestone

Marks 75% year-over-year average increase in users

Harnessing the power of supercomputing and state-of-the-art electronic structure methods, the Materials Project provides open, web-based access to computed information on known and predicted materials as well as powerful analysis tools to inspire and design novel materials. As a result, the process of discovering and developing advanced materials has been made faster, less expensive, and more predictable. In 2019, the project reached the milestone of 100,000 global users, including participants in every U.S. state, a 75% year-over-year average increase. Statistics show roughly 95 new registrants and 2,100 user sessions every day, with 35,000 new users added last year alone.





Improved Fuel Cell Catalysts with Less Platinum

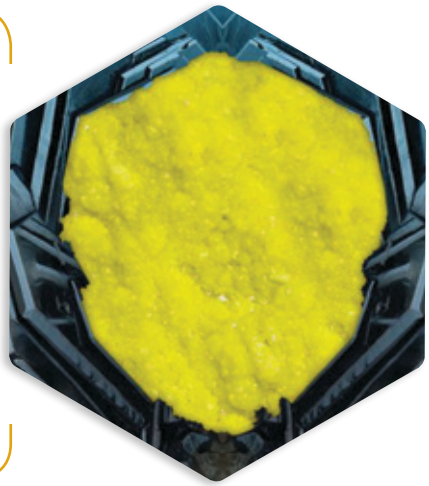
New catalyst design meets cost, activity, and durability goals

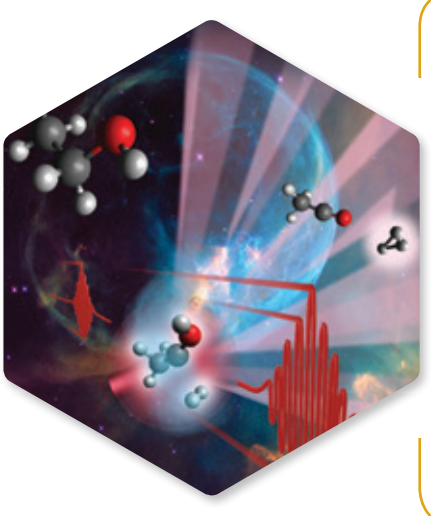
Scientists identified highly active yet stable catalysts for use in fuel cells that contain only a quarter of the platinum currently used. Innovative approaches for reducing the amount of platinum in catalysts, while maintaining the high activity and stability that platinum provides, are of intense interest. The costly metal plays a crucial role in catalyzing multiple reactions in proton-exchange membrane fuel cells (PEMFCs). Interactions between platinum-cobalt particles and a precious metal-free support contribute to the improved fuel cell performance. PEMFCs are highly efficient and represent a future powertrain for light- and heavy-duty vehicles.

Surprising Structure of Uranium Bound in Hematite

Atomic view shows how toxic uranium binds to iron minerals

While studying the binding of uranium to iron-bearing materials, researchers made two unexpected discoveries: (1) uranium binding is quite versatile and (2) vacancies created in the atomic structure of hematite during its formation can accommodate uranium. This binding process had never before been identified, but the methods used to make this finding could explain a number of mysteries previously reported in the scientific literature. The work opens the door to new studies on how other radioactive contaminants bind to soil minerals and will lead to more accurate predictions of how these contaminants behave in the environment.





Forming the Ion that Made the Universe

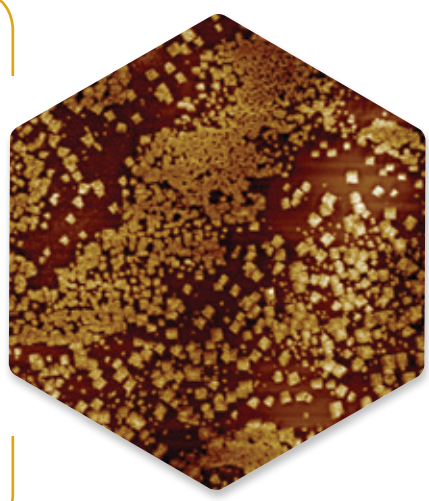
Research offers details on the chemistry of the trihydrogen ion

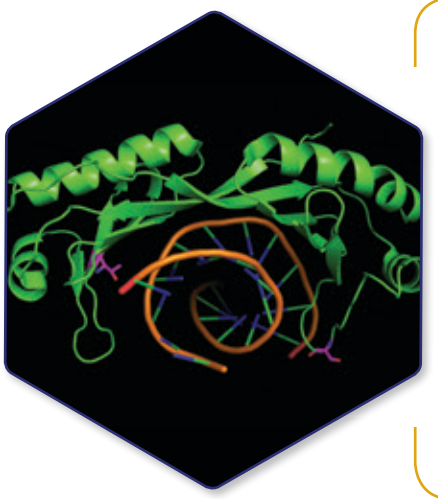
The trihydrogen cation, H_3^+, is the most abundant ion in the universe and the starting point for almost all molecules, but its chemistry at the molecular level is relatively unknown. Researchers discovered how the cation forms by using intense femtosecond laser pulses and instrumentation to hit organic molecules and detect the resulting ions from experimental measurements. They measured the timescales, yield, and how chemical bonds were broken and formed, revealing key details about each step of the reaction, which occurs on ultrashort (faster than one millionth of a millionth of a second) timescales. These findings are important for astrochemistry and for understanding how organic molecules form and behave in the universe. They are also relevant when intense lasers are used for surgical procedures.

Driving Product Selectivity Through Addition

Increasing reduction reaction selectivity leads to desired products

Scientists are working to find ways to efficiently convert carbon dioxide (CO_2) into specific multicarbon chemicals such as fuels. Researchers developed a method that takes advantage of the interaction between organic additives and metal electrodes to drive the electrocatalytic reduction of CO_2 to form multicarbon products. They combined an organic salt additive with a copper electrode for the CO_2 reduction reaction and found that the additive enhanced production of ethylene. Studies showed the additive led to the formation of nanostructures at the copper surface, generated a protective layer that stabilized the nanostructures during electrocatalysis, and promoted carbon-carbon coupling to generate multicarbon products. This finding can lead to new strategies for efficient production of specific chemicals via CO_2 conversion.





How Plant Cells Decide When to Make Oil

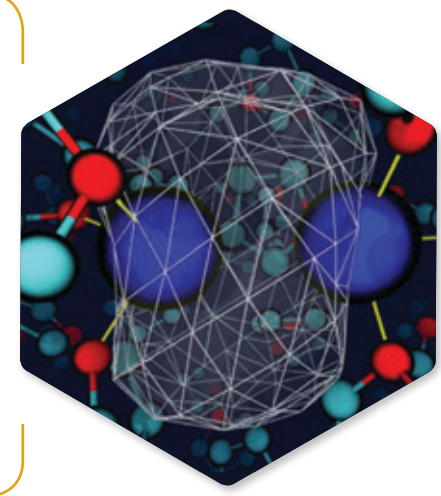
Newly discovered signaling details could enable higher production

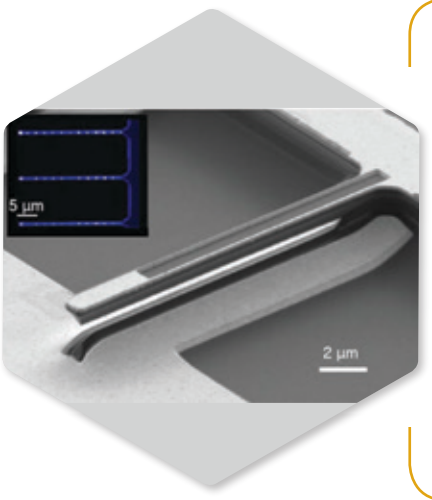
When crops have high sugar levels, they produce energy-dense oil stored in the seeds. Oil production slows when sugar levels are low. Previous research established clear links between a protein complex that senses sugar levels in plant cells and another protein that serves as the “on switch” for oil production. Using this knowledge, researchers demonstrated that using combinations of genetic variants that increase sugar accumulation in plant leaves drives up oil production. The new work provides a more detailed understanding of the link between sugar signaling and oil production, identifying precisely which molecules regulate the balance and how. This understanding could lead to plants that produce substantial amounts of oil for use as biofuels and other bioproducts.

Solvents Change Chemical Identity of Solutes

In many chemical reactions, solvents are not mere spectators

Numerous chemical reactions happen in solution. New research shows that in many such reactions, the solvent is not just a medium where reactants encounter each other. Researchers studying a sodium dimer in the weakly polar solvent tetrahydrofuran found that when the solvent and solute interact (energetically on the same order as a hydrogen bond), the solvent can control the bond dynamics and chemical identity of simple solutes. Bonding interactions between the solvent and sodium atoms led to unique coordination states where each coordination state had its own dynamics and spectroscopic signatures. This research highlights the value of carefully selecting the solvent to create a specific environment in certain condensed-phase chemical systems.





Increasing Spin Time of Quantum Bits

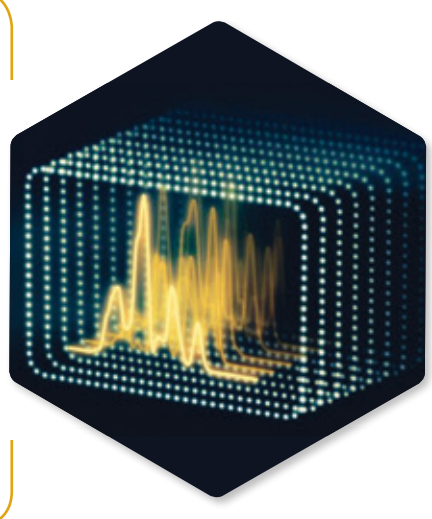
Technique advances path to scalable quantum networks

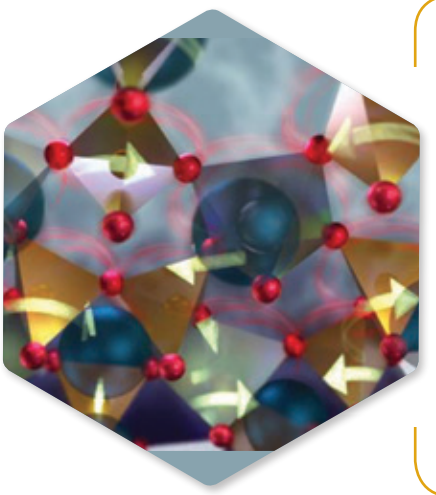
By implanting silicon ions in diamond with extreme precision and then controlling the strain on the crystal structure, scientists have significantly increased the spin lifetimes of solid-state quantum bits, or qubits, the basic information storage component of quantum computers. Researchers at the Center for Integrated Nanotechnologies implanted the ions as part of a multi-institutional effort that developed a new approach to increase crystal strain. This approach, using a nano-electro-mechanical device, opens the door to achieving a long-time goal of producing single phonons required for developing scalable quantum networks that have the potential to change how data is generated and sent.

Ghost Imaging Speeds Study of Molecular Motions

Simplified method embraces randomness of x-ray pulses

X-ray free-electron lasers produce powerful beams of light enabling studies of ultrafast atomic motions. To interpret data taken with these light sources, researchers must understand how the x-ray pulses interact with matter and how those interactions affect measurements. Computer simulations by scientists at SLAC National Accelerator Laboratory suggest that such analyses could be simplified using a new technique called pump-probe ghost imaging. This method takes advantage of the randomness inherent in x-ray pulses as they interact with matter and reconstructs what objects look like without directly recording their images. By eliminating the conventional, time-consuming need to prepare paired, well-defined, short pulses and to control the time delay between them, ghost imaging could accelerate studies of fundamental interactions.





Particles Move Heat Faster than Speed of Sound

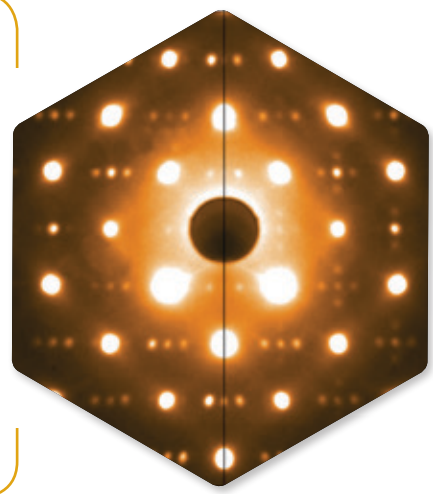
Neutron scattering reveals phasons that may boost electronics

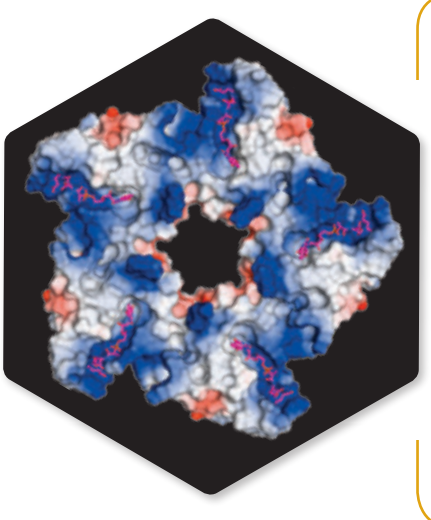
To create materials that handle heat well, scientists are exploring how vibrations within atomic structures carry and remove heat. These vibrations usually are limited by the speed of sound, but researchers at the Spallation Neutron Source and High Flux Isotope Reactor have observed particles that may have shattered this limit. Using neutron scattering, the team discovered ultrasonic particles called phasons that carry heat. These particles use a pattern of motion in which atoms rearrange themselves, allowing heat to move faster. Phasons enhance the thermal conductivity in insulators by 20% at room temperature, opening new paradigms for the design of electronics and sensors and potentially enabling a new type of thermal circuit breaker.

Using Light to Generate Order in an Exotic Material

Ultrafast laser pulses produce a previously unseen phase matter

When matter is excited by light, the material normally is quickly heated and results in a less orderly state. When the layered material lanthanum tritelluride was hit with a fast laser pulse, however, the hot electrons altered the atomic bonding constraints, and a new highly ordered state was shown to briefly come into existence. Such nonthermal states are only created via fast laser pulses that alter the standard phase. The extremely brief structural transitions were measured in time using ultrafast electron diffraction at SLAC National Accelerator Laboratory. This result provides a path forward to discovering transitory states of matter that may be useful for quantum applications, as well as the manipulation and control of ordered phases with light.





X-Ray Studies Provide Insights on New TB Drug

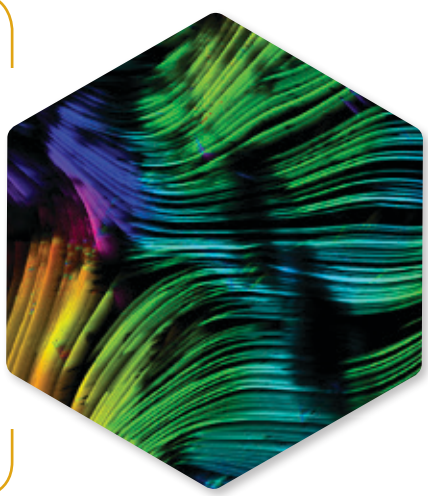
Experiments detail molecular structure of bacterial enzyme

An antibiotic, Pretomanid, recently approved by the U.S. Food and Drug Administration helps tackle deadly, treatment-resistant forms of *Mycobacterium tuberculosis*, which causes tuberculosis. X-ray experiments at the Advanced Light Source revealed the molecular structure of Ddn, a tuberculosis bacterium enzyme, in the presence and absence of a coenzyme. This structural information, along with earlier structure studies on a related enzyme, FGD1, at the Stanford Synchrotron Radiation Lightsource, benefited Pretomanid's development. This antibiotic works with two existing drugs to trigger the bacteria to release nitric oxide, poisoning the microorganisms. In a Phase III clinical trial, the three-drug regimen cleared tuberculosis within six months in 95 of 109 patients unresponsive to previous treatments.

Microscopes Spotlight Materials' Performance

4D-STEM maps out best or problematic atomic "hangouts"

Scientists are pushing the boundaries of electron microscopy with 4D-STEM, or four-dimensional scanning transmission electron microscopy. Using capabilities at the Molecular Foundry, researchers showed how 4D-STEM, when deployed with high-speed electron detectors and customizable algorithms, can provide direct insight into the performance of any material—from strong metallic glass, to flexible semiconducting films, and even beam-sensitive soft materials. Together, these technologies can advance materials research by pinpointing specific atomic or molecular "neighborhoods" that can compromise a material's performance or potentially improve it. Previously, electron microscopes were most useful for imaging hard materials able to withstand the energy of electron beams.



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FRONT COVER

Atomic Origins of Water-Vapor-Promoted Alloy Oxidation. High-resolution transmission electron microscopy image to reveal the atomic-level workings of water vapor on a nickel-chromium alloy oxidation, providing new insights that could help prevent metal corrosion. Courtesy Nathan Johnson, Pacific Northwest National Laboratory. *Nature Materials* **17**, 514–18 (2018). DOI: 10.1038/s41563-018-0078-5.

PAGE 6

John B. Goodenough. © Nobel Media. Photo: Alexander Mahmoud.

M. Stanley Whittingham. © Nobel Media. Photo: Alexander Mahmoud.

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Feng Wang. Courtesy Feng Wang.

Marivi Fernández-Serra. Courtesy Marivi Fernández-Serra.

Ivan Bazarov. Courtesy Ivan Bazarov.

PAGE 10

Battery End-Run Spreads Lithium in Electrodes. Artistic representation of how surface diffusion of lithium ions across battery nanoparticles changes an electrode. The red represents lithium-rich regions; the gray represents lithium-poor regions. Courtesy 3D Cube Graphics, SLAC National Accelerator Laboratory. *Nature Materials* **17**, 915–22 (2018). DOI: 10.1038/s41563-018-0168-4.

This Superconductor Does Not Take Light Lightly. The electrical conductivity of a single atomic layer of iron selenium (FeSe) deposited on an electrically insulating crystal [strontium titanate ($SrTiO_3$)] can be strongly modified when exposed to light. Researchers discovered that the light-induced changes in the substrate could substantially improve the superconducting properties of the FeSe film. Courtesy Cheng Cen, West Virginia University. *Nature Communications* **10**, 85 (2019). DOI: 10.1038/s41467-018-08024-w.

Flowing for Function. Snapshots of multiscale topographical response to a hexagonal pattern of magnets. Courtesy Joanna Aizenberg and Wendong Wang, Harvard University. Reprinted by permission from Springer Nature from Wang, W., et al. 2018. "Multifunctional Ferrofluid-Infused Surfaces with Reconfigurable Multiscale Topography." *Nature* **559**, 77–82. DOI: 10.1038/s41586-018-0250-8. Copyright 2018.

PAGE 11

Sound Waves Carry Quantum System Information. An x-ray image of sound waves (center). *Nature Physics* **15**(5), 490–95 (2019). DOI: 10.1038/s41567-019-0420-0.

Getting Metal Under Graphite's Skin. A faceted metal island of the rare earth element dysprosium formed under a layer of graphite. The team deposited the metal at 577°C after they bombarded graphite with argon ions. The purple surface in the colorized scanning probe image is the graphite, the honeycomb pink feature is the dysprosium metal draped by a thin layer of graphite, and the yellow object is a dysprosium cluster above the graphite surface (scale: nanometers). Reprinted by permission from Elsevier from Zhou, Y., et al. 2018. "Defect-Mediated, Thermally-Activated Encapsulation of Metals at the Surface of Graphite." *Carbon* **127**, 305–11. DOI: 10.1016/j.carbon.2017.10.103.

Materials Project Reaches 100,000 User Milestone. Map shows Materials Project users across the United States, as evidenced by the average session duration. Courtesy Materials Project, www.materialsproject.org.

PAGE 12

Improved Fuel Cell Catalysts with Less Platinum. An artistic rendition of the synergistic catalyst showing core-shell active sites (blue) in platinum-cobalt nanoparticles (spheres) on a platinum group metal-free catalytic support. Courtesy Chris Galvin, Argonne National Laboratory. *Science* **362**(6420), 1276–81 (2018). DOI: 10.1126/science.aau0630.

Surprising Structure of Uranium Bound in Hematite. New geochemical research shows how a toxic material like uranium binds with iron-bearing minerals like hematite in the soil, allowing scientists to predict long-term behavior. Courtesy Environmental Molecular Sciences Laboratory. *Environmental Science and Technology* **52**(11), 6282–90 (2018). DOI: 10.1021/acs.est.8b00297.

Forming the Ion that Made the Universe. The trihydrogen cation, H_3^+, plays a major role in interstellar chemistry where it facilitates the formation of water and organic molecules. Researchers have discovered how the cation forms when organic molecules (particularly alcohols) are excited by an intense laser pulse (artist rendition). Knowing how the cation forms improves understanding of the chemistry that led to current life forms. Courtesy Patrick Pawlacyk and Marcos Dantus, Michigan State University. *Nature Communications* **9**(1), 5186 (2018). DOI: 10.1038/s41467-018-07577-0.

PAGE 13

Driving Product Selectivity Through Addition. *Ex situ* atomic force microscopy image of a copper electrode after 65 minutes of electrocatalysis at –1.07 V in 0.1 M potassium bicarbonate with 10 mM of phenanthrolinium dibromide. Reproduced with permission from Thevenon, A., et al. 2019. "*In situ* Nanostructuring and Stabilization of Polycrystalline Copper by an Organic Salt Additive Promotes Electrocatalytic CO_2 Reduction to Ethylene." *Angewandte Chemie International Edition* **58**(47), 16952–58. DOI: 10.1002/anie.201907935. Copyright Wiley-VCH Verlag GmbH & Co. KGaA.

How Plant Cells Decide When to Make Oil. The portion of WRINKLED1 (green "ribbon") that binds to DNA (orange, green, and blue "twisted ladder") to turn on the genes for oil production in plants. The magenta, red, and blue stick-figure portions of the molecule get phosphorylated by KIN10 to mark WRINKLED1, initiating a process that leads to its destruction. Interfering with these phosphorylation sites could be one way to stabilize WRINKLED1 to increase plant oil production. Courtesy John Shanklin, Brookhaven National Laboratory. *The Plant Cell* **30**, 2616–27 (2018). DOI: 10.1105/tpc.18.00521.

Solvents Change Chemical Identity of Solutes. A "snapshot" reveals that the surrounding tetrahydrofuran solvent deforms the bonding electron density around a sodium solute. The sodium cores are blue spheres; the valence electrons' density is represented as a transparent white surface with a white wire mesh enclosing most of the charge density. The bonds between the sodium and nearby solvent's oxygen sites are thin yellow lines. Courtesy Devon Widmer and Benjamin Schwartz, University of California, Los Angeles. *Nature Chemistry* **10**(9), 910–16 (2018). DOI: 10.1038/s41557-018-0066-z.

PAGE 14

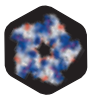
Increasing Spin Time of Quantum Bits. A scanning electron microscopy image of a single-crystal diamond cantilever. This tiny device allows scientists to exert control over a quantum system (µm = micrometers). Reprinted with permission from Sohn, Y. I., et al. 2018. "Controlling the Coherence of a Diamond Spin Qubit Through Its Strain Environment." *Nature Communications* **9**, 2012. DOI: 10.1038/s41467-018-04340-3.

Ghost Imaging Speeds Study of Molecular Motions. Computer simulations may provide insights into a simplified method of understanding how x-ray pulses interact with matter and how those interactions affect measurements. The method is called pump-probe ghost imaging. Courtesy Greg Stewart, SLAC National Accelerator Laboratory. *Physical Review X* **9**(1), 011045 (2019). DOI: 10.1103/PhysRevX.9.011045.

Particles Move Heat Faster than Speed of Sound. Heat usually moves by atomic vibrations that are limited by the speed of sound. Heat also can move by particles (phasons) related to atomic rearrangements that change with the movement of waves in the crystal structure. Using neutron scattering, scientists discovered supersonic phasons that could remove harmful heat in electronics and send signals faster. Phasons were observed in a mineral containing titanium (gray) and silicate (orange) polyhedrons linked at their corners. (Oxygen is red, while barium is the large blue spheres.) Below a critical temperature, the polyhedrons began to twist and slide (arrows). Courtesy Oak Ridge National Laboratory. *Nature Communications* **9**, 1823 (2018). DOI: 10.1038/s41467-018-04229-1.

PAGE 15

Using Light to Generate Order in an Exotic Material. Electron diffraction patterns before (left) and 1.8 ps after (right) photoexcitation with a near-infrared laser pulse, taken at 3.1 MeV electron kinetic energy. Reprinted by permission from Springer Nature from Kogar, A., et al. 2020. "Light-Induced Charge Density Wave in $LaTe_3$." *Nature Physics* **16**, 159–63. DOI: 10.1038/s41567-019-0705-3. Copyright 2020.



X-Ray Studies Provide Insights on New TB Drug. Surface rendering of the pentameric structure from Holo-1 shows a complementary groove with positive (blue) charges near the negatively charged tail of F_{420}. Available by a Creative Commons license, CC BY 3.0. Cellitti, S. E., et al. 2012. "Structure of Ddn, the Deazaflavin-Dependent Nitroreductase from *Mycobacterium tuberculosis* Involved in Bioreductive Activation of PA-824." *Structure* **20**(1), 101–12. DOI: 10.1016/j.str.2011.11.001.

Microscopes Spotlight Materials' Performance. 4D-scanning transmission electron microscopy (STEM) map traces the molecular structure of a small-molecule thin film. Courtesy Colin Ophus, Lawrence Berkeley National Laboratory. *Nature Materials* **18**, 860–65 (2019). DOI: 10.1038/s41563-019-0387-3. See also: *Nature Communications* **10**, 2445 (2019). DOI: 10.1038/s41467-019-10416-5.

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