Basic Energy Sciences Program Update

U.S. DEPARTMENT OF ENERGY | Office of Science

Basic Energy Sciences

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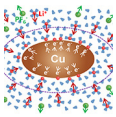

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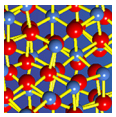

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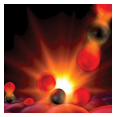

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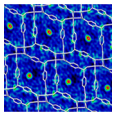

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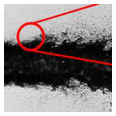

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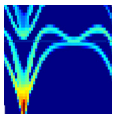

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About the cover: Self-assembled tunable network of polymer fibers (see p. 7).

Basic Energy Sciences Program Update

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. The research disciplines covered by BES—condensed matter and materials physics, chemistry, geosciences, and aspects of physical biosciences—are those that discover new materials and design new chemical processes. These disciplines touch virtually every aspect of energy resources, production, conversion, transmission, storage, efficiency, and waste mitigation.

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

Program Updates

National Synchrotron Light Source-II

In fiscal year (FY) 2015, BES completed construction of the National Synchrotron Light Source-II (NSLS-II) at Brookhaven National Laboratory (BNL). NSLS-II produces extremely bright beams of x-ray, ultraviolet, and infrared light used to examine a wide range of materials, including superconductors and catalysts, geological samples, and biological materials to accelerate advances in energy, environmental science, and medicine.

NSLS-II will enable scientists to continue building on the 32-year legacy of research at BNL's first light source, NSLS, which directly resulted in two Nobel Prizes and contributed to a third. The NSLS-II construction project was completed ahead of schedule and on budget to usher in the next chapter of light source capability. The planning, design, and construction of the NSLS-II facility (627,000 ft^2) spanned 10 years, and, when all beamlines are fully built out, NSLS-II will be able to support thousands of scientific users each year.

As a DOE Office of Science user facility, NSLS-II will offer researchers from academia, industry, and national laboratories new ways to study chemical and material properties and functions with nanoscale resolution and extreme sensitivity using the most advanced state-of-the-art x-ray techniques. NSLS-II is among the brightest synchrotron light sources in the world and has the capacity to operate 60 or more beamlines when fully developed.

The science programs to be undertaken at NSLS-II will play a crucial role in addressing grand challenges in basic energy sciences that face the nation and the world. NSLS-II capabilities will fuel major advances that enable new energy technologies—such as nanocatalyst-based fuel cells; widespread, economical use of solar energy; high-temperature superconductors to deliver electricity more efficiently to the nation's electric grid; advanced batteries for electric vehicles and grid-scale storage; and next-generation nuclear power systems.

National Synchrotron Light Source-II. NSLS-II at BNL will enable the study of chemical and material properties and functions with nanoscale resolution and exquisite sensitivity by providing world-leading capabilities for x-ray imaging and high energy-resolution x-ray scattering and spectroscopy. [Image courtesy BNL]

Computational Materials Sciences

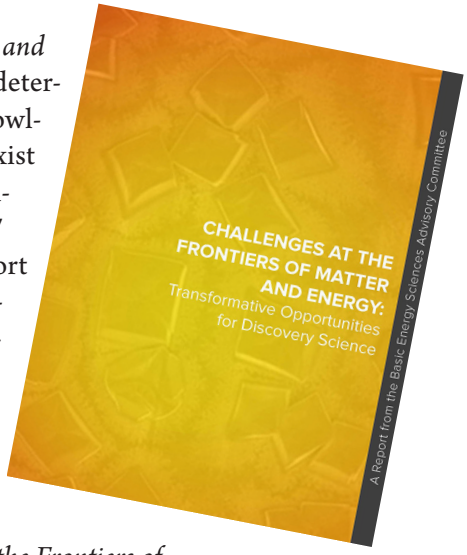
BES made three new awards in FY 2015 in computational materials sciences. The research under these awards will integrate theory and computation with experiments and provide the materials community with advanced tools and techniques in support of the national Materials Genome Initiative (MGI). MGI is a multiagency effort aiming to reduce by a factor of two the time from discovery to deployment of new advanced materials, with the goal to revitalize American manufacturing.

For these awards, BES sought integrated, multidisciplinary teams to perform research and develop validated community codes and databases for predictive design of functional materials. The awardees proposed new approaches to enhance the use of large datasets derived from advanced characterization of materials, materials synthesis, processing, properties assessments, and data generated by large-scale computational efforts that model materials phenomena. Each of these projects will perform research that utilizes and develops community software for leadership class computing as well as for general use by the scientific community. Awards total $8 million annually for 4 years starting in FY 2015.

These projects are expected to develop open-source, robust, validated, user-friendly software (and the associated experimental and computational databases) that captures the essential physics and chemistry of relevant systems and can be used by the broader research community and industry to accelerate the design of new functional materials. The goal of this research activity is to leap beyond simple extensions of current theory and models of materials toward a paradigm shift in which specialized computational codes and software, coupled with innovative use of experimental and theoretical data, enable the design, discovery, and development of new materials, and, in turn, create innovative, advanced technologies. Given the importance of materials to virtually all technologies, computational materials sciences occupy a critical area in which the United States needs to remain competitive in the 21st century through global leadership in innovation.

Strategic Planning

In 2014, DOE's Office of Science charged the BES Advisory Committee (BESAC) with assessing the progress made on the five grand challenges identified in the 2007 BESAC report, *Directing Matter and Energy: Five Challenges for Science and the Imagination*, and determining what new knowledge opportunities exist to advance energy science. Just as the 2007 grand challenges report reflected the underlying concept of directing (controlling) matter and energy from the perspective of the BES research portfolio, the new report, *Challenges at the Frontiers of Matter and Energy: Transformative Opportunities for Discovery Science*, reflects the breakthrough potential of current and prospective BES research, based on advances achieved to date in answering the five original grand challenge questions. Five new transformative opportunities were identified that have the potential to transform many of today's energy-related technologies:



- Mastering Hierarchical Architectures and Beyond-Equilibrium Matter
- Beyond Ideal Materials and Systems: Understanding the Critical Roles of Heterogeneity, Interfaces, and Disorder
- Harnessing Coherence in Light and Matter
- Revolutionary Advances in Models, Mathematics, Algorithms, Data, and Computing
- Exploiting Transformative Advances in Imaging Capabilities Across Multiple Scales

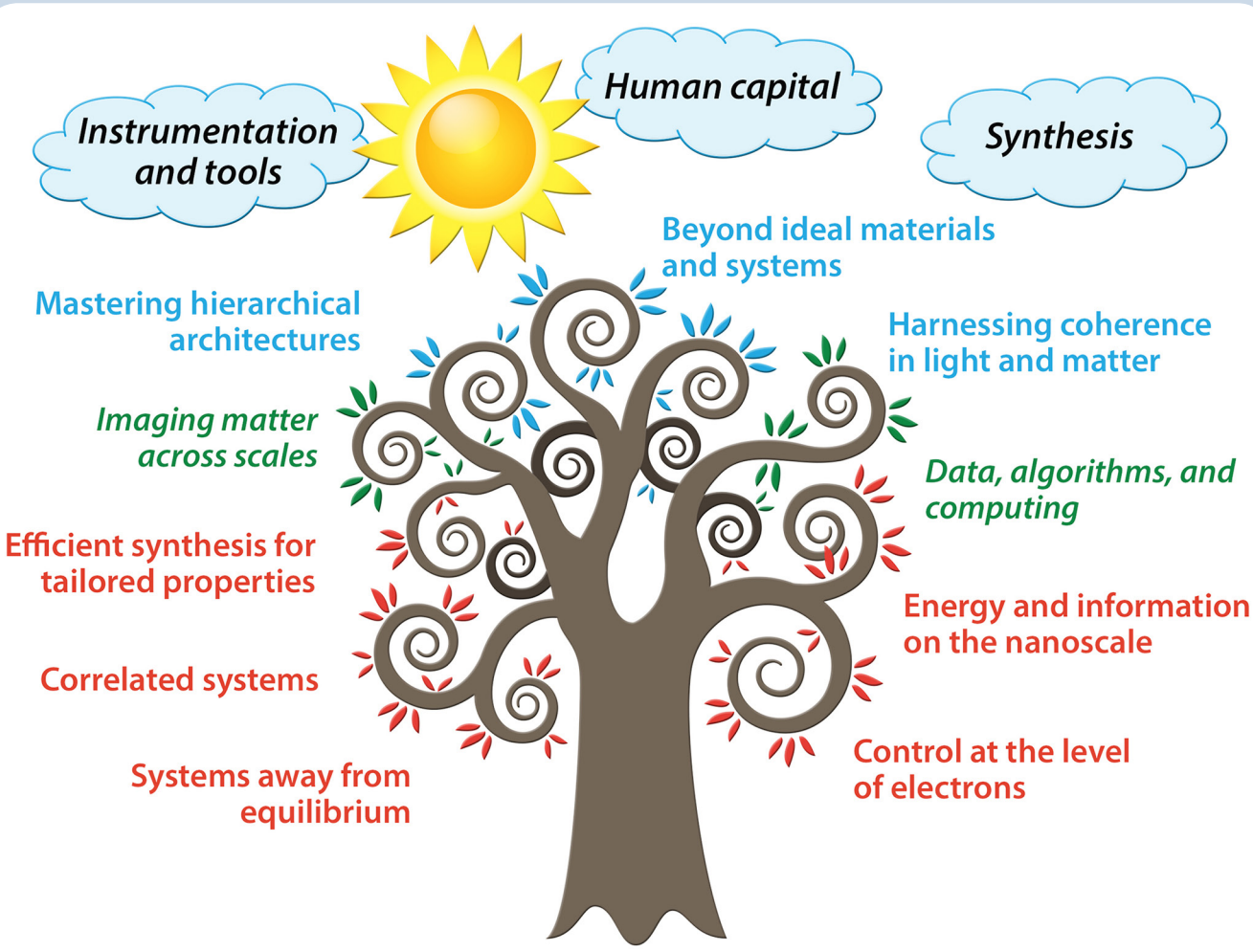
Seizing each of these five transformative opportunities, as well as accelerating further progress on grand challenge research, will require specific, targeted investments in the areas of synthesis, the ability to make molecules and materials in specific desired architectures; instrumentation and tools, a category that includes theory and computation; and human capital, the most important asset for advancing BES grand challenges and transformative opportunities.

This report breaks new ground in its assessment of the scientific landscape today versus just a few years ago. The 2007 report noted that if the five identified grand challenges were met, the ability to direct matter and energy would be measured only by the limits of human imagination. This new report shows that, prodded by those challenges, the scientific community now is positioned to seize

new opportunities whose impacts promise to be transformative for science and society, as well as dramatically accelerate progress in pursuit of the original grand challenges. The full report is available at http://science.energy.gov/bes/community-resources/reports/.

Research Highlights

The remaining pages describe select research highlights from across the BES portfolio. Understanding and Controlling Matter (pp. 4–5) includes advances in which materials were designed for a specific functionality resulting in improved energy technologies. Harnessing Material and Chemical Processes to Create Matter (pp. 6–7) highlights improvements to understanding chemical and material synthesis, from small molecules to nanoscale materials. Modeling and Simulation of Complex Phenomena (pp. 8–9) features highlights that describe the role of new theories and methodologies in advancing understanding of chemical processes and materials.



BES Grand Challenges and Transformative Opportunities. A graphical representation of the blossoming scientific opportunities spanned by the 2007 grand challenges (red) and transformative opportunities (blue and green) in the 2015 BESAC report, *Challenges at the Frontiers of Matter and Energy: Transformative Opportunities for Discovery Science*. The clouds represent three areas for focused efforts to accelerate progress on the grand challenges and transformative opportunities.

Understanding and Controlling Matter

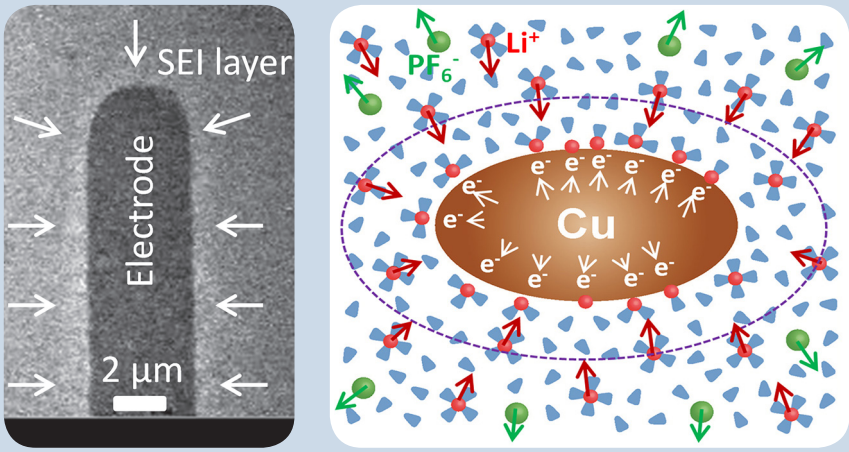
Real-Time, *In Situ* Measurements Improve Understanding of Battery Interfaces

Lithium (Li)-ion batteries operate by shuttling ions between two electrodes separated by an electrolyte. A factor influencing battery capacity and life is the electrode-electrolyte interaction layer, also called the solid electrolyte interphase (SEI) layer. However, structural and chemical changes occurring at this layer have been a mystery because of challenges in directly probing the solid-liquid interface under operating reaction conditions.

For the first time, scientists at the Joint Center for Energy Storage Research, a BES Energy Innovation Hub, have created a new approach for directly observing molecular-level changes in the SEI layer and at the electrode surface under dynamic operating conditions. This new technique, *in situ* liquid-cell secondary ion mass spectrometry (SIMS), showed that when Li metal deposits on a copper electrode, solvent molecules condense around the electrode. Chemically, this solvent layer tends to be depleted of salt anions found in the rest of the electrolyte and it has a reduced concentration of Li^+ ions. This process leads to the formation of a lean electrolyte layer adjacent to the electrode, thereby contributing to cell overpotential—the additional energy needed to drive battery operation.

The new capability provides unprecedented molecular-level dynamic information on the SEI layer's initial formation and also could be used to probe other chemical processes involving solid-liquid interfaces, such as electrocatalysis, biofuel conversion, and biomineralization.

Zhu, Z., et al. 2015. "Mass Spectrometric Determination of Molecular Structural Evolution at the Solid Electrolyte Interphase in Lithium-Ion Batteries," *Nano Letters* **15**(9), 6170–76. DOI: 10.1021/acs.nanolett.5b02479.



Understanding Battery Interfaces. The combination of *in situ* transmission electron microscopy (left) and *in situ* liquid-cell SIMS (right) can yield chemical, structural, and morphological information on a battery's solid-liquid interface where the electrode and electrolyte meet. [Images adapted with permission from Zhu et al. 2015. Copyright 2015 American Chemical Society]

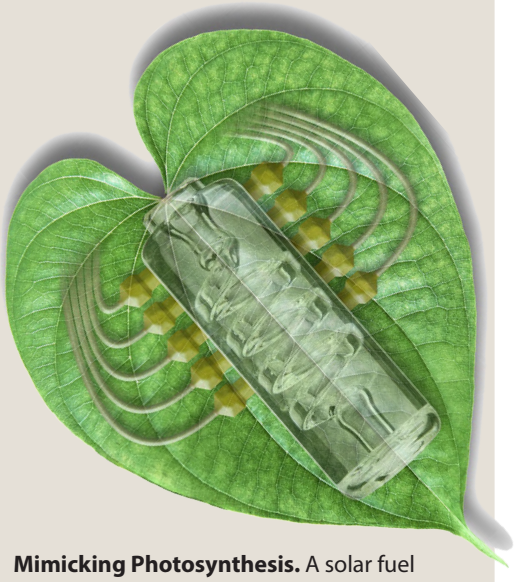
Protective Semiconductor Coatings that Enable Solar Fuel Production

A solar device that could convert light directly into energy-rich fuels instead of electricity would revolutionize the ability to store energy from sunlight. Given previous investments in developing light-absorbing semiconductors for photovoltaics, adapting common photovoltaic materials like silicon and gallium arsenide for use in such a solar fuels generator would be advantageous. Unfortunately, these materials degrade rapidly when submerged in the aqueous solutions required to produce fuels.

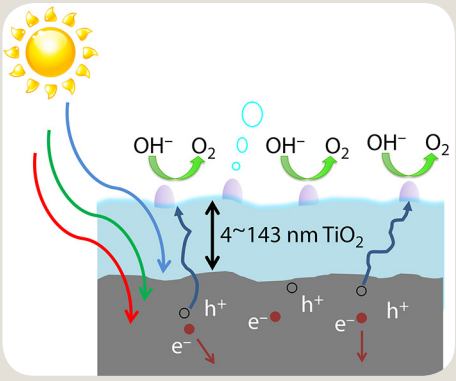
Scientists at the Joint Center for Artificial Photosynthesis (JCAP), a BES Energy Innovation Hub, recently discovered a method to protect common semiconductors from corrosion in water, while still allowing them to absorb light and generate charge for fuel production. Protective coatings that are sufficiently thick to prevent corrosion typically block incidental light or prevent electrical charges produced by the semiconductor from reaching the reactive surface. JCAP researchers used a process called atomic layer deposition to produce a transparent, but electrically conductive coating of titanium dioxide on light-absorbing semiconductors. Imperfections in the coating enable charge conduction. By positioning a chemical catalyst on the water-exposed surface of the protective coating, light absorption by the semiconductor and subsequent charge transfer to the catalyst can drive reactions needed for fuel formation.

This strategy of exploiting imperfections in the protective coating is an important new tool that could significantly expand the list of candidate materials suitable for use in sustainable and efficient solar-driven fuel production.

Hu, S., et al. 2014. "Amorphous TiO_2 Coatings Stabilize Si, GaAs, and GaP Photoanodes for Efficient Water Oxidation," *Science* **344,** 1005–09. DOI: 10.1126/science.1251428.



Mimicking Photosynthesis. A solar fuel generating device would mimic the natural photosynthesis carried out in a leaf, capturing solar energy and converting it into chemical energy or liquid fuel.



Protective Semiconductor Coating. The titanium dioxide (TiO_2) protective layer stabilizes the silicon photoanode against corrosion so that hydroxide ions (OH^-) in the electrolyte can be continuously oxidized to oxygen gas (O_2). [Image from Hu et al. 2014. Reprinted with permission from AAAS]

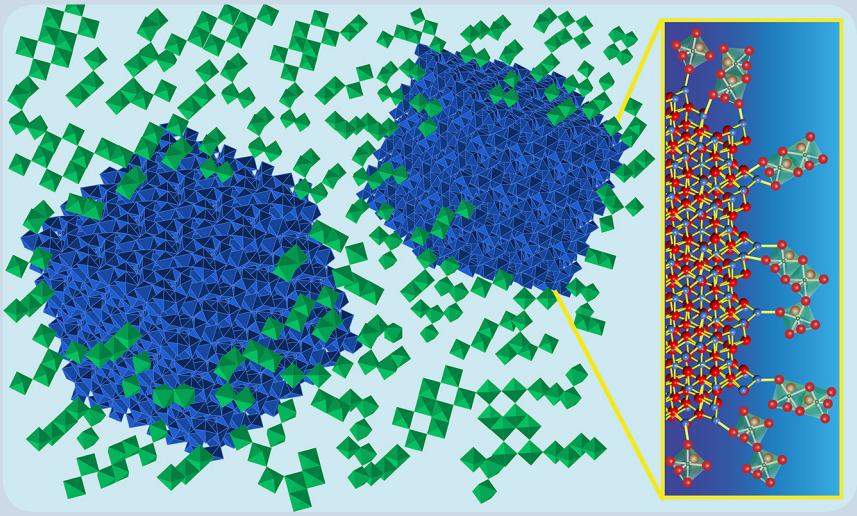
Smarter "Smart" Windows Enabled by Nanoscience

In the past few decades, nanoscience has been an engine of innovation leading to significant improvements in modern energy technologies. At the root of opportunities enabled by nanoscience is the fact that all the elementary steps of energy conversion (e.g., charge transfer, molecular rearrangement, and chemical reactions) take place on the nanoscale. Thus, the development of new nanoscale materials, as well as methods to characterize, manipulate, and assemble them, creates an entirely new paradigm for developing revolutionary energy technologies.

By capitalizing on advances in nanoscale synthesis, researchers from the Molecular Foundry at Lawrence Berkeley National Laboratory have developed a smart glass that can switch between blocking light, heat, or both, depending on how much voltage is applied. Central to the technology is a new designer electrochromic material, made from nanocrystals of indium tin oxide embedded in a glassy matrix of niobium oxide. Electrochromism is a reversible process that allows the glass to change its transmittance of light or heat in response to electrochemical charging and discharging. The researchers found a synergistic interaction at the interface between the glassy matrix and nanocrystal, leading to enhancement of the electrochromic effect. As a result, thinner coatings can be used without compromising performance.

This development addresses a critical need for rapid, inexpensive fabrication of stable nanoscale materials with tunable electrical and optical characteristics that can be scaled-up for large-area applications. Heliotrope Technologies, an early stage company, is developing these new materials and manufacturing processes for electrochromic devices with an emphasis on energy-saving smart windows.

Llordés, A., et al. 2013. "Tunable Near-Infrared and Visible Light Transmittance in Nanocrystal-in-Glass Composites," *Nature* **500**, 323–26. DOI: 10.1038/nature12398.



Smart Glass Material. Nanocrystals of indium tin oxide (blue) embedded in a glassy matrix of niobium oxide (green) form a composite material that can switch between transmitting or blocking light or heat with a small jolt of electricity. A synergistic interaction in the region where glassy matrix meets nanocrystal increases the potency of the electrochromic effect. [Image from Llordés et al. 2013]

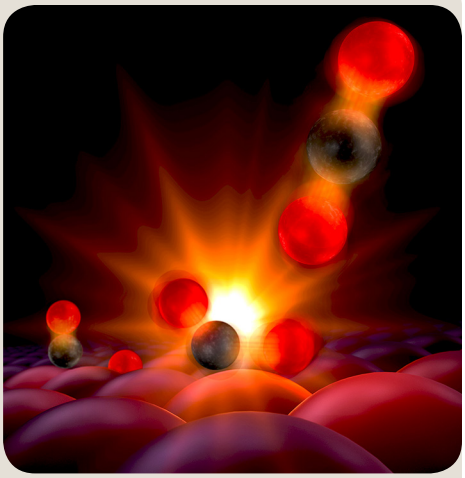
Harnessing Material and Chemical Processes to Create Matter

Traversing a Catalytic Reaction Pathway in Femtosecond Timesteps

Catalysts are species that alter the pathway of a chemical reaction and lower the energy required to form desired products (e.g., catalytic conversion of nitrogen in air into nitrogen species that can be used as fertilizers helps secure worldwide food production). For over a century, scientists have developed and used theories to predict how chemical elements and compounds react. Recently, accurate predictions of the rates at which catalytic reactions occur have become accessible, but only for the most elementary reactions and using idealized catalysts. In experiments, scientists have observed bond rupture and creation on catalytic surfaces before and after the event, not while they occur. By combining theory and experiment, researchers at SLAC National Accelerator Laboratory (SLAC) have now revealed the details of such events by means of ultrafast optical laser pulses. They detected the minute subatomic motions of species bound to a ruthenium surface as they overcome an energy barrier to form a new chemical bond, in this case adding an oxygen atom to carbon monoxide (CO) to form carbon dioxide (CO_2). That entire sequence lasts about a picosecond (10^{-12} s) and must be captured in femtosecond (10^{-15} s) steps. This discovery was made possible by combining the ultrafast capabilities of SLAC's Linac Coherent Light Source (LCLS) with the most advanced theories of chemical bonding and reaction.

This important reaction is relevant in the conversion of fossil fuels and biofuels to hydrogen gas for use as chemical feedstocks or in fuel cells. Only a detailed understanding of such processes will enable new catalysts that improve the efficiency of chemical reactions and lower energy consumption.

Öström, H., et al. 2015. "Probing the Transition State Region in Catalytic CO Oxidation on Ru," *Science* **347**(6225), 978–82. DOI: 10.1126/science.1261747.



Catalytic Reaction in Real Time. A carbon monoxide (CO) molecule (left), made of a carbon atom (black) and an oxygen (O) atom (red), reacts with atomic O (to the right of CO). The CO and O reactants, which are attached to the surface of a ruthenium catalyst, vibrate and bump into each other when hit with an optical laser pulse, and the carbon atom forms a transitional bond with the lone O atom (center). LCLS probes the reaction (upper right) as it proceeds in a time-resolved manner. [Image courtesy SLAC]

Designer Materials for Carbon Capture, Gas Separations, and Catalysis

The ability to efficiently and controllably separate and store different molecules is critically important to a broad range of energy-relevant technologies, including carbon capture, hydrogen storage, chemical sensors, hydrocarbon separations, and chemical production. Though possible today with traditional approaches, these processes are still energy intensive and therefore costly.

In the last decade, much scientific and technological attention has been paid to a class of materials known as metal-organic frameworks (MOFs). These highly porous materials typically consist of an array of metallic ion complexes (nodes) surrounded by organic molecules (linkers). MOFs can have extremely large internal surface areas, providing numerous sites for interactions and transport of guest molecules within the pores.

DOE's Office of Science is supporting fundamental scientific research to design, synthesize, functionalize, and characterize MOFs, including work at the Center for Gas Separation Relevant to Clean Energy Technology, a BES Energy Frontier Research Center at the University of California, Berkeley, and the Nanoporous Materials Genome Center at the University of Minnesota. Research to date has resulted in the discovery of new MOFs for CO_2 capture, hydrogen separation and storage, hydrocarbon separation based on shape, and chemical synthesis such as the conversion of ethane to ethanol. Researchers are also designing MOFs to withstand the harsh environmental conditions that exist in many potential applications.

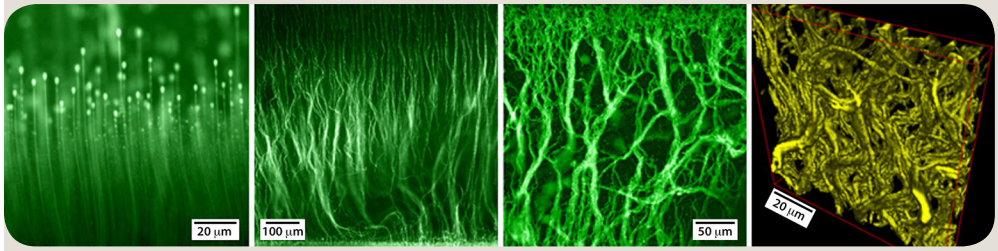
Given the large number of known and possible MOFs, exploring them all experimentally is inefficient. In recent years, significant research has focused on predictive modeling as a means to identify promising candidates for a particular functionality. Those efforts can then guide the targeted synthesis and characterization of a more limited number of materials. The diversity of MOFs is a challenge and an opportunity, both scientifically and technologically. Today's research on MOFs promises tailored multifunctionality designed *in silico* (on computers), which then can be synthesized for use in a diverse array of energy technologies.

Growing Nano "Hair" for Electrodes

Humankind's ability to create and manipulate the properties of materials has taken much inspiration from the natural world. Biology uses dynamic, out-of-equilibrium processes to assemble cellular components in response to specific signals. Mimicking this assembly approach to organize simple building blocks into complex architectures presents a unique opportunity to learn from nature and go beyond. In practice, however, using this "bottom-up" approach to form complex structures over multiple length scales has proven difficult, since the assembled structures fall apart once the applied stimulus used to direct their formation has been removed.

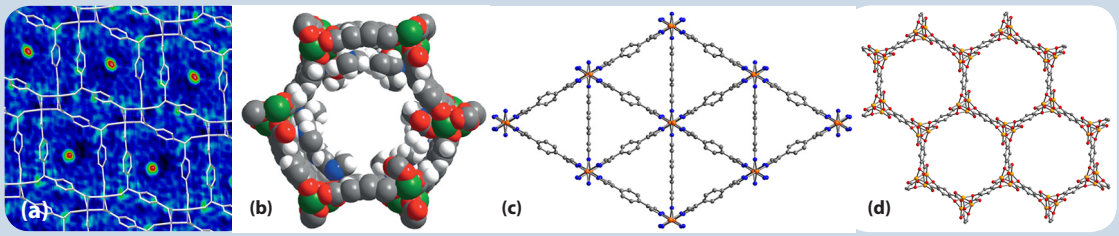
A new self-assembly process, also inspired by nature, has been discovered for fabricating stable, three-dimensional (3D) structures in response to an applied stimulus. Scientists at Argonne National Laboratory developed self-assembled tunable networks of polymer fibers similar to the "hairy" surfaces that exist in human bodies to protect blood capillaries from wear and infection. Using tiny, sticky epoxy droplets as building blocks, 3D structures ranging from wavy colloidal "fur" to highly interconnected networks were formed on an electrode surface in an electric field. The features of the resulting architectures were tuned by controlling the electric field and droplet surface properties to form arrays of tiny mushroom-shaped pillars, permanent wavy hair, or dense gel-like networks, which then were further coated with an atomically thin layer of conductive material.

This development addresses a critical need for rapid, inexpensive fabrication of stable nano- and mesoscale fibrous (or hairy) materials that can be assembled dynamically and reversibly in response to an applied electric field. Using this approach, tunable 3D architectures can be formed directly on electrode surfaces and further functionalized with conductive materials, a capability that makes this a promising candidate approach for forming low-cost, large–surface area electrodes in batteries and organic photovoltaic cells.



Self-Assembled 3D Architectures. Controlled synthesis results in a diversity of self-assembled structures formed by sticky epoxy droplets: (from left) array of "mushrooms," wavy colloidal hair, dense fiber network, and 3D reconstruction of the network. [Images from Demortière et al. 2014]

Demortière, A., et al. 2014. "Self-Assembled Tunable Networks of Sticky Colloidal Particles," *Nature Communications* **5**(3117). DOI: 10.1038/ncomms4117.



Representative MOFs. These images demonstrate the large diversity within this class of materials. These MOFs capture CO_2 **(a, b)**, separate hydrocarbons **(c, d)**, and convert ethane to ethanol **(d)**. [(a) Image from Plonka et al. 2013. (b) Image from McDonald et al. 2015. (c) and (d) Images courtesy University of California, Berkeley]

(a) Plonka, A. M., et al. 2013. "Mechanism of Carbon Dioxide Adsorption in a Highly Selective Coordination Network Supported by Direct Structural Evidence," *Angewandte Chemie International Edition* **52**, 1692–95. DOI: 10.1002/anie.201207808.

(b) McDonald, T. M., et al. 2015. "Cooperative Insertion of CO_2 in Diamine-Appended Metal-Organic Frameworks," *Nature* **519**, 303–08. DOI: 10.1038/nature14327.

(c) Herm, Z. R., et al. 2013. "Separation of Hexane Isomers in a Metal-Organic Framework with Triangular Channels," *Science* **340**(6135), 960–64. DOI: 10.1126/science.1234071.

(d) Xiao, D. J., et al. 2014. "Oxidation of Ethane to Ethanol by N_2O in a Metal-Organic Framework with Coordinatively Unsaturated Iron(II) Sites," *Nature Chemistry* **6**, 590–95. DOI: 10.1038/nchem.1956.

Modeling and Simulation of Complex Phenomena

The Materials Project: Powerful Computing and Analysis to Discover Novel Materials

Materials discovery and development is a key innovation driver for new energy technologies, yet 20 or more years can be required following initial discovery to move a material to market. By systematically computing properties of known (and currently unknown) materials, the DOE Materials Project aims to remove the guesswork from materials design and target experimental research to the most promising compounds.

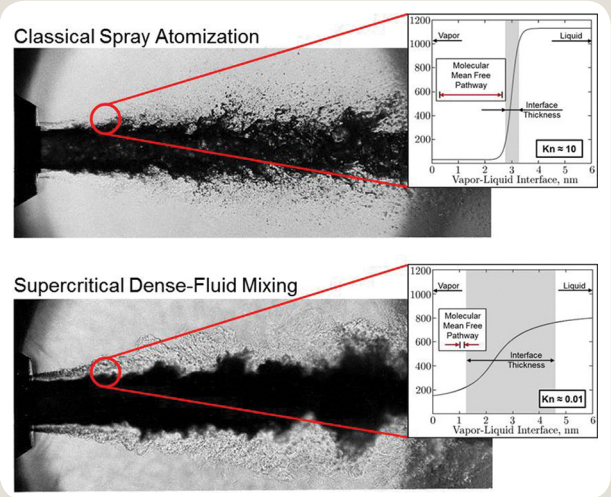
Researchers developed a methodology, including new, user-friendly software, for materials property calculations from first-principles with a particular focus on energy production and storage. The methodologies are scaled to "high-throughput," where tens of thousands of calculations are completed for very different chemical and structural systems. A screening funnel methodology is then applied to determine the order in which to calculate and screen properties. This process is based on the speed and robustness of the calculation, as well as the importance of the property for the application. For example, materials expected to operate in a corrosive environment can be screened first for stability in that environment and next for other appropriate properties. The methodology and data are housed at the National Energy Research Scientific Computing Center at Lawrence Berkeley National Laboratory (LBNL) and made publicly available through the Materials Project website (https://www.materialsproject.org). Data for more than 65,000 inorganic compounds can be searched and down-selected for various properties such as phase stability, aqueous corrosion, band structure, lithium battery properties, and reaction energies. As of December 2015, the Materials Project has more than 16,000 registered users, including over 2,000 from industry.

New Conceptual Model for High-Pressure Fuel Injection Processes

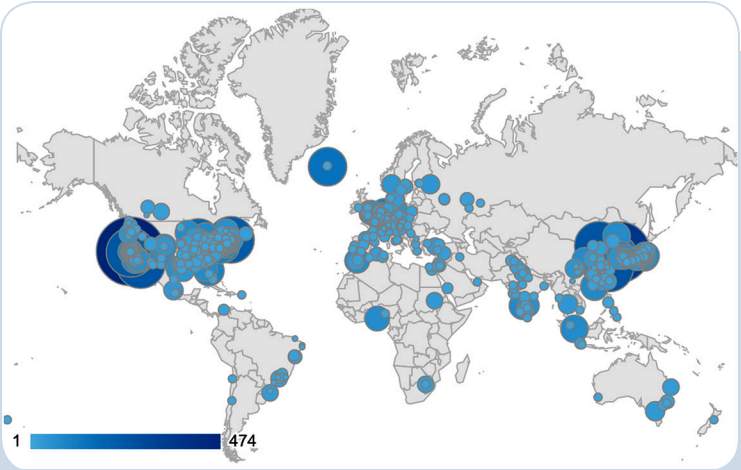
Understanding and predicting fuel injection processes in advanced transportation and power systems are widely recognized as critical research areas for modern combustion system design. Liquid injection largely determines mixture formation, which ultimately governs the detailed evolution of combustion. The lack of accurate, multiphase models presents a major barrier in designing optimized, high-efficiency, low-emission systems.

Researchers at Sandia National Laboratories' Combustion Research Facility have developed the first fundamental theory of gas-liquid interface dynamics with the goal of understanding the thermodynamics of fuel injection processes at actual device operating pressures. Advanced theory was used to explain and quantify experimental observations that show spray atomization is replaced by diffusion-dominated mixing without drop formation at supercritical conditions. At high pressures, the molecular gas-liquid interface broadens and surface tension diminishes. At a certain point, now quantified by the theory, the gas-liquid interfacial structure can no longer support atomization and formation of drops. At this point, liquid fuel diffuses into the ambient gas in a manner markedly different from the classical picture typically assumed. This result led to the development of a novel model of liquid injection processes that can be applied to a variety of combustion systems and will be invaluable in designing advanced combustion systems.

Dahms, R. N., and J. C. Oefelein. 2013. "On the Transition Between Two-Phase and Single-Phase Interface Dynamics in Multicomponent Fluids at Supercritical Pressures," *Physics of Fluids* **25**, 092103. DOI: 10.1063/1.4820346.



Understanding Fuel Injection Processes. Both images show how gas-liquid interfacial structure changes as a function of pressure for a given set of injection conditions. At lower pressure (top), the gas-liquid interface is molecular and dominated by surface tension where droplets form. At higher pressure (bottom), the gas-liquid interface broadens, and, eventually, the interface breaks down and there is no distinction between the liquid and vapor phases. This transition has a significant impact on mixing between a given fuel and oxidizer, which, in turn, can profoundly affect combustion performance and emissions. [Images reprinted with permission from Dahms and Oefelein 2013. Copyright 2013, AIP Publishing LLC. Modified from Mayer et al. 1998. "Atomization and Breakup of Cryogenic Propellants Under High-Pressure Subcritical and Supercritical Conditions," *Journal of Propulsion and Power*; reprinted by permission of the American Institute of Aeronautics and Astronautics, Inc.]



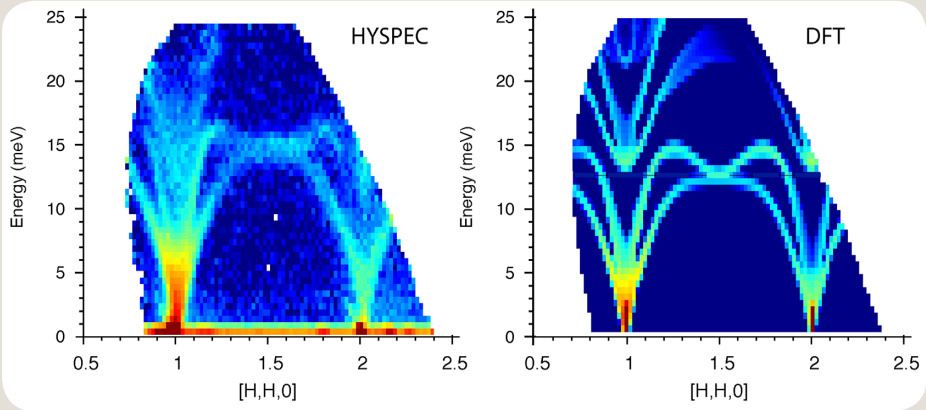
Geographical Representation of Materials Project Users (July 2015). Scientists and engineers worldwide use data from the DOE Materials Project to identify new electrolytes and electrode materials for batteries, thermoelectric materials, and photocatalysts for chemical conversions. [Image courtesy LBNL]

This work provides unprecedented data and materials design tools as well as comprehensive capabilities for scientists to share their processes and results. By offering materials researchers the information they need to design better materials, the Materials Project aims to facilitate innovation in materials research. Accelerating the pace of discovery and deployment of advanced material systems will be crucial to achieving global competitiveness in the 21st century.

Real-Time Simulations Help Tune Experiments

The ultimate goal of truly integrating modeling and experimentation is giving researchers the ability to interact with complex simulations "live" before and during an experiment. In a recent experiment on strontium titanate oxide ($SrTiO_3$) using the hybrid spectrometer (HYSPEC) instrument at the Spallation Neutron Source (SNS) at Oak Ridge National Laboratory, scientists concurrently ran *ab initio* molecular dynamics (AIMD) simulations on the Oak Ridge Leadership Computing Facility (OLCF) Eos cluster. The neutron scattering intensity was computed and simultaneously measured on the HYSPEC instrument. The AIMD simulations used 23,000 virtual cores on Eos and were executed at the same time as the neutrons scattered by the sample were accumulated by the HYSPEC detector system, thanks to an OLCF mechanism for scheduling jobs synchronized with SNS experiments. The calculations ran for 5 hours in order to compute 100,000 configurations of ions in the simulation box, from which anharmonic interatomic force-constants were extracted to compute the four-dimensional (4D) phonon dynamical structure factor. Concurrently, the experimental 4D phonon structure factor was mapped on HYSPEC using a high-quality single crystal.

The ability to run simulations during the experiment allowed the researchers to adjust their simulation and experiment path in real time and helped them refine the range of crystal orientations collected on HYSPEC. The goal is to make this approach routine for relevant experiments in the future.



"Live" Simulations of Anharmonic Phonons in $SrTiO_3$. (Left) Graph shows experimental data from HYSPEC of the ferroelectric instabilities in $SrTiO_3$. **(Right)** Graph shows calculated intensities. [Images courtesy O. Delaire, J. Hong, B. Winn, H. Cao, A. Savici, and L. Boatner, Oak Ridge National Laboratory]

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January 2016