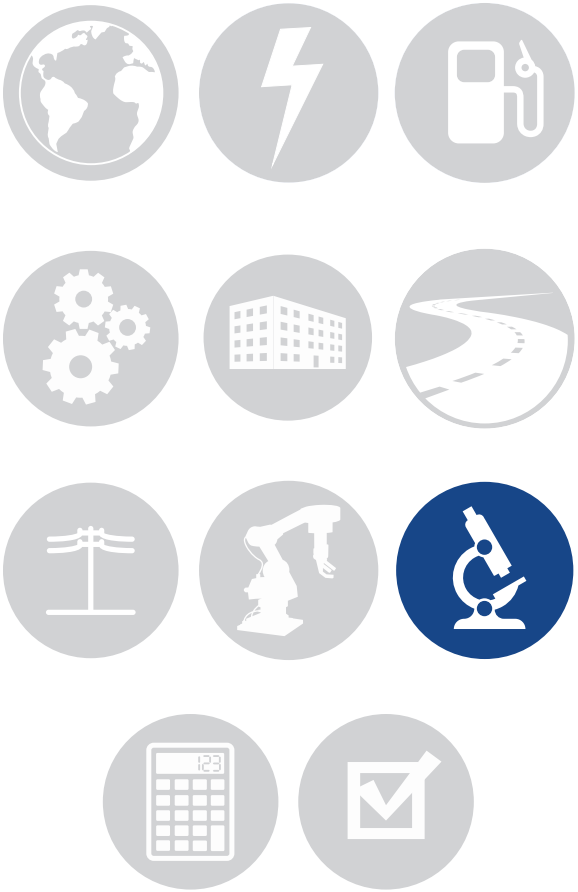
Quadrennial Technology Review 2015

Chapter 9: Enabling Capabilities for Science and Energy

Supplemental Information



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U.S. DEPARTMENT OF ENERGY

Quadrennial Technology Review 2015

Examples and Case Studies

Chapter 9: Enabling Capabilities for Science and Energy

Introduction

Basic science expands our understanding of the natural world and provides the foundational knowledge upon which the energy technologies of the future are based. In some instances, a scientific discovery can obviate technical hurdles to broader implementation of existing technologies; in others, it can be the catalyst for a completely new suite of technologies.

The scientific discoveries described in the following sections were supported by the Department of Energy's Office of Science and enabled by the unique tools and/or multidisciplinary research centers described in *Enabling Capabilities for Science and Energy*. Each discovery has relevance to one or more of the energy technology areas described in the 2015 Quadrennial Technology Review.

These discoveries represent a small fraction of the basic science supported by the Office of Science. For more scientific discoveries from Office of Science-supported researchers at universities, national laboratories, and in the private sector, see the News section of the Office of Science website (http://science.energy.gov/news/).

Understanding and Controlling Matter: From the Atomic-Scale to the Mesoscale

Preventing Laptop Fires and "Thermal Runaway"

In recent years, several computer manufacturers have recalled lithium ion (Li-ion) laptop batteries because of several incidents of spontaneous ignition. Researchers at the Center for Electrochemical Energy Storage (CEES), an Energy Frontier Research Center led by Argonne National Laboratory (ANL), have proposed a new approach to preventing such fires that draws on one of the trends in contemporary materials science—"self-healing" materials.

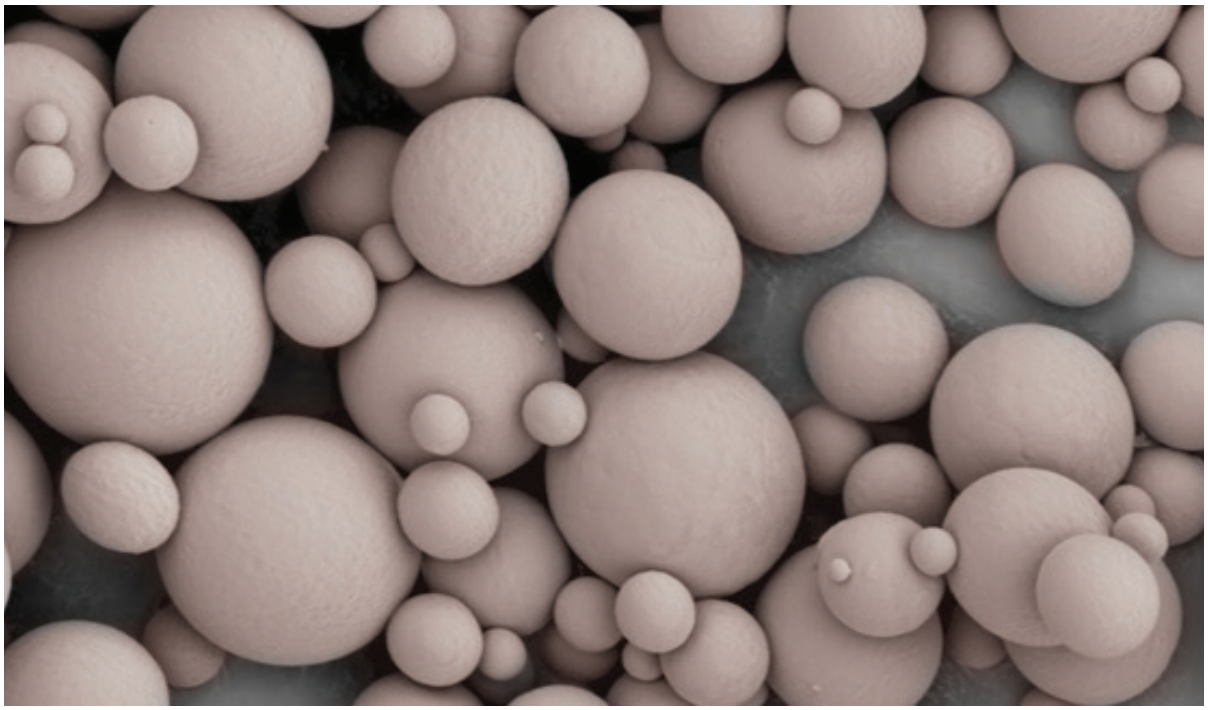
Each Li-ion cell has three layers—a positive electrode, a negative electrode, and a thin polymer layer between the two electrodes called the "separator." The separator performs two functions: it keeps the positive and negative electrodes apart, preventing a short circuit; and its tiny pores filled with an electrolyte permit lithium ions to flow between the two electrodes. If the separator is damaged, the electrodes can short-circuit and overheat, initiating a chemical reaction between the electrolyte and the electrode. Such a short circuit can trigger a "thermal runaway" whereby the increase in temperature of the cell accelerates the chemical reaction, adding more heat to the system and leading to the combustion of the battery materials.

To prevent thermal runaway, CEES researchers coated either the anode layer or the separator layer with tiny heat-sensitive solid polymer capsules, or "microspheres" (Figure 1). When the battery reaches a certain temperature, the microspheres melt, blocking the pores in the separator and shutting down battery operation. In both cases, the addition of the microcapsule coating did not negatively impact battery operation at room temperature, while at elevated temperatures, battery shutdown was achieved.

Further development of this system, with faster response times or alternative "triggers" such as cell voltage or current flow, may protect batteries in a variety of electronic devices from catching fire.

Figure 1 Microscopic image of heat-sensitive microspheres designed to melt at elevated temperatures, shutting down a lithium ion battery in the event of overheating.[1]

Credit: Scott R. White



Solar Shingles

The global market for photovoltaic (PV) devices that are integrated with the buildings they help power (known as building integrated PV, or BIPV) is expected to grow at a compound annual growth rate of 15% through 2019.[2] Part of their popularity stems from the smaller form factor; such devices are installed as part of the structure, rather than as an add-on. One such product developed by Dow Chemical Company is the Solar Shingle, an integrated PV device installed as part of a building's roof (Figure 2). The success of this product depended on developing an effective active material for this technology. In

Figure 2 With help from the Advanced Photon Source (APS), Dow Powerhouse™ Solar Shingles advanced from research to manufacturing to installation of new roofs for U.S. homes in less than 5 years.[4]

Credit: Dow Solar

bringing this product to market, Dow researchers leveraged the Advanced Photon Source (APS), an X-ray light source user facility located at ANL, to develop the active material for this technology.[3]

A central challenge in developing new energy systems is the ability to observe in real time how the active material behaves during synthesis processing and under functional conditions. By using in situ X-ray diffraction and scanning techniques available at the APS, Dow researchers mapped the process-structure-property relationships in copper indium gallium selenide, the four-component active material in Solar Shingles. This directly led to the development of a successful process to form a semiconductor phase having optimal solar photovoltaic properties.

The research has since been scaled up into a manufacturing process for the first commercial solar shingles, Powerhouse™ Solar Shingles. This product is currently available in 18 states nationwide including California, Texas, and New York, and also in Canada.

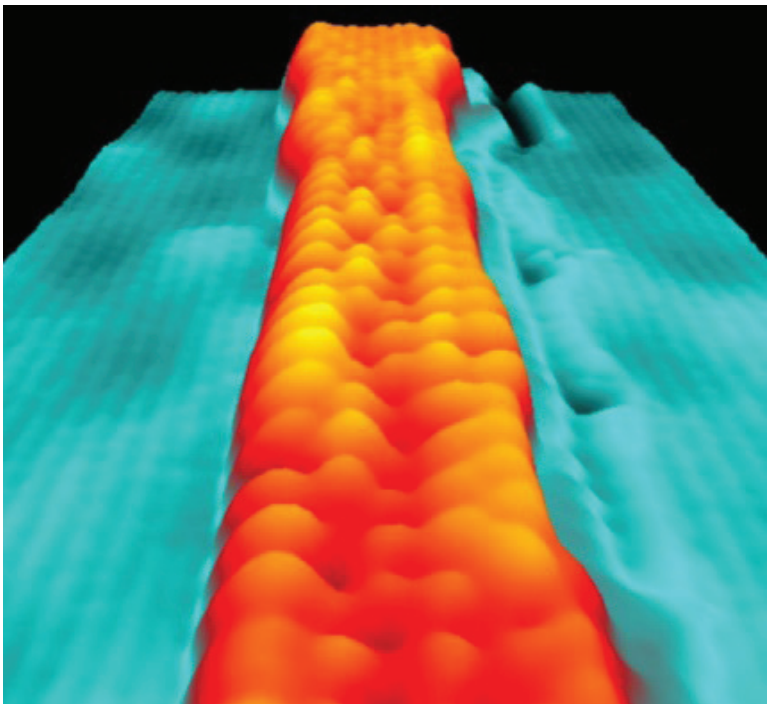
For 'Ribbons' of Graphene, Width Matters

Graphene, a one-atom thick layer of carbon atoms arranged in a honeycomb structure, is more than 100 times stronger than steel, stretchable, nearly transparent, and electronically tunable. Since its discovery in 2004, researchers have continued to study graphene's unique fundamental properties, which could enable its use in a wide array of technologies, from batteries to low-power nanoelectronics. Researchers at the University of Wisconsin-Milwaukee have recently developed a procedure to synthesize graphene 'ribbons' with electronic properties that are a function of their width.

Starting with epitaxial graphene on silicon carbide, researchers used a nanoparticle assisted etching technique to make very narrow ribbons of graphene that are only ten to a few tens of atoms across. Using scanning tunneling spectroscopy to measure the electronic properties of the ribbons, they found that new electronic and magnetic states are formed at the hydrogen-decorated edges of the ribbons, causing graphene to change from an efficient conductor to a semiconductor (Figure 3). The size of the semiconducting gap depends critically on the width of the ribbon. Above a threshold of 3 nanometers (nm) the gap has a constant value of 0.4 electron volts (eV) (compared to 1.1 eV for the semiconductor silicon). As the width of the graphene ribbons decreases, the semiconducting gap increases, up to 1.6 eV for a 1 nm ribbon. These results are in agreement with theoretical calculations.

Figure 3 A scanning tunneling microscopy image of a graphene nanoribbon (orange) supported on silicon carbide (blue). Atoms are visible as individual 'bumps'.[5]

Credit: Lian Li



The findings demonstrate the feasibility of tuning the

properties of graphene, opening the prospect of building energy-efficient nanoscale electronic devices from graphene ribbons. Future research will explore whether replacing hydrogen with oxygen on the edges of the ribbons will cause them to become metallic. If successful, this could open up the possibility of nanoscale electronic components made from a single material.

Understanding the Impact of Radiation on Materials

Future energy technologies will place increasing demands on materials that can withstand extremes in stress, temperature, pressure, chemical reactivity, radiation flux, and electric or magnetic fields. For nuclear energy, one of the prime challenges is the deleterious effect of radiation on the properties of materials used in the core of the reactors. Two recent studies have shown some of the multiple ways in which radiation can impact material properties over the lifetime of a reactor.

Figure 4 Comparison of (a) un-irradiated and (b) ion- irradiated copper pillars compressed by 10%. The irradiated pillars exhibit non-uniform deformation due to increased hardness following irradiation.

Credit: Sharon, J.A.; Hattar, K.; Boyce, B.L.; Brewer, L.N. "Compressive Properties of <110> Cu Micro-Pillars after High-Dose Self-Ion Irradiation." Materials Research Letters (2:2), 2014; pp. 57-62.

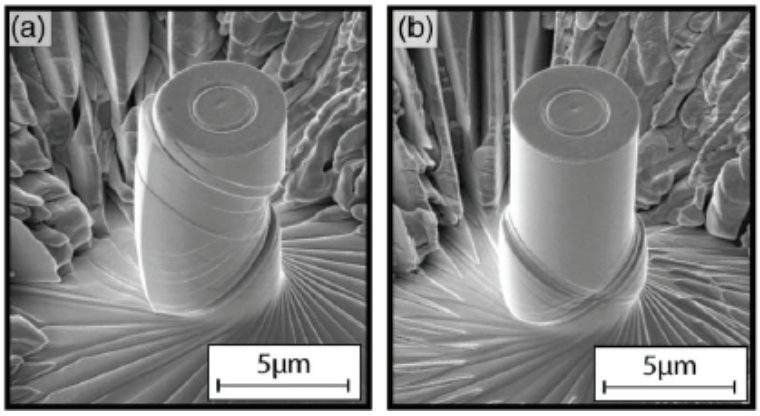
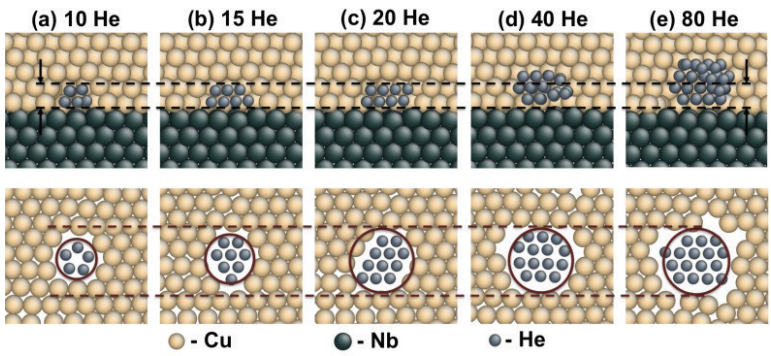


Figure 5 Computer simulations of helium atom clustering at copper-niobium interfaces (top) and in pure copper (bottom) as the amount of helium atoms is increased from 10 to 80. At up to 20 helium atoms, the helium packing is more compact at the interface than the bulk.

Credit: Kashinath, A., A. Misra, and M. J. Demkowicz. "Stable Storage of Helium in Nanoscale Platelets at Semicoherent Interfaces." Physical Review Letters 110.8 (2013). © 2013 American Physical Society



To predict the lifetime of materials and safe operational conditions for a reactor, it is important to understand how changes in strength and the underlying atomic structure and composition of materials evolve with exposure to radiation. To simulate the impact of the radiation exposure expected at the end-of-life for nuclear reactors, copper pillars were exposed to high dose ion irradiation. Using nanoscale testing and characterization techniques at the Center for Integrated Nanotechnologies, an Office of Science nanoscale science research center, the researchers showed that the strength, or hardness, of the material increased as the radiation damage increased to end-of-life levels (Figure 4).[6] Harder materials can lose their ductility and potentially fail in unexpected ways–an important condition to understand for reactor lifetime extension.

Another effect associated with irradiation of materials in a nuclear reactor is the creation of gas bubbles. Helium atoms are produced when neutrons interact with many metals. These helium atoms can

coalesce to form bubbles within the metal, causing it to swell and eventually fracture. A recent computational modeling study has shown that the structure of interfaces within the metal can alter the rate of helium absorption. The researchers found that tailored metallic interfaces containing specific periodic structures absorb helium with nearly three times the efficiency of the bulk metal, and do so in a more favorable configuration. Compared to a similar number of helium atoms in the bulk, the helium at the tailored interfaces forms bubbles with greater stability and higher packing, reducing the detrimental swelling effects observed during reactor service (Figure 5).[7]

The research results in these two studies provide greater understanding of the mechanical behavior of materials over the life of a nuclear reactor component and could be used to design improved materials for reactor applications. Beyond nuclear energy generation, such damage-resistant materials could have applications in sectors that require materials to perform under harsh operating conditions, for example in national security, non-nuclear energy production, and manufacturing.

Low-Cost, High Performance Photovoltaics

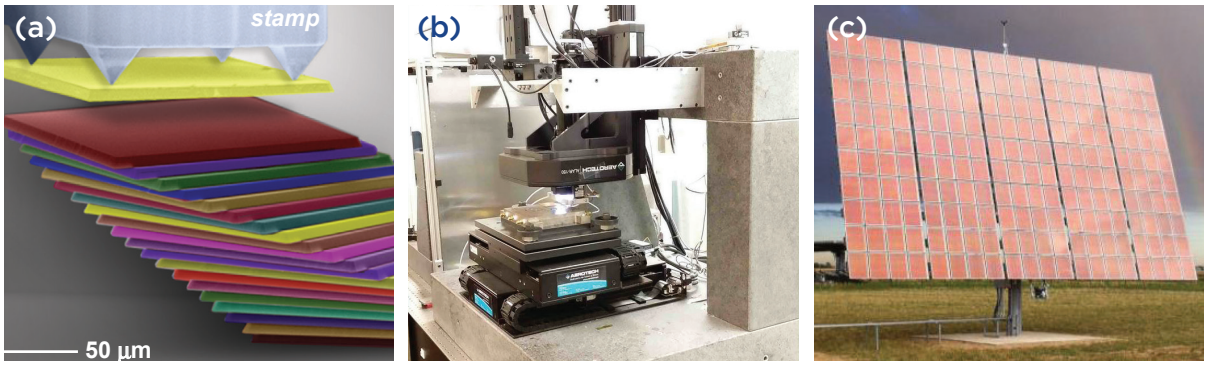
The biggest single barrier to widespread adoption of solar power continues to be the cost of solar cells. Researchers at the University of Illinois-Urbana Champaign (UIUC) have developed an extensive intellectual property (IP) portfolio related to printable, high performance, flexible, and stretchable electronics and photovoltaics that could help transform the economics of solar power.

The researchers developed new methods for growing III-V compound semiconductor solar cells that allow them to be printed on a variety of surfaces, including flexible sheets of plastic (Figure 6a and 6b). This micro-transfer printing process also enables integration of preformed circuit elements with optical over-layers for directing and focusing the light, and fabrication of cells with controllable transparency, opening up new solar energy conversion applications.

The materials science advances resulting from this work have led to new materials strategies for solar cells and new printing-based manufacturing tools that enable production of thousands of stacked multijunction microcells with high solar energy conversion efficiencies. Solar photovoltaic cells made with compound semiconductors have measured efficiencies of up to 43.9%, nearly twice as efficient as the best silicon-based cells in converting sunlight to electricity. The new growth and manufacturing methods help reduce the cost of deploying these high efficiency cells for utility-scale power generation.

Figure 6 (a) Micro-transfer printing method for rapid, deterministic assembly of micro/nanomaterials into stacked microcells; (b) Semiconductor 'printer' as a large-area, high-volume manufacturing tool for low-cost high performance photovoltaics; (c) Concentrator PV modules with world record efficiencies of 37.1% at the module level are made up of high performance microcells that exhibit 43.9% efficiency.[8]

Credit: (a) Kim, S.; Wu, J.; Carlson, A.; Jin, S.H.; Kovalsky, A.; Glass, P.; Lui, Z.; Ahmed, N.; Elgan, S.L.; Chen, W.; Ferreira, P.M.; Sitti, M.; Huang, Y.; Rogers, J.A.; "Microstructured Elastomeric Surfaces with Reversible Adhesion and Examples of Their Use in Deterministic Assembly by Transfer Printing." Proceedings of the National Academy of Sciences (107:40), 2010; pp. 17095-17100. Credit: John Rogers (University of Illinois Urbana-Champaign) (c) Semprius, Inc.



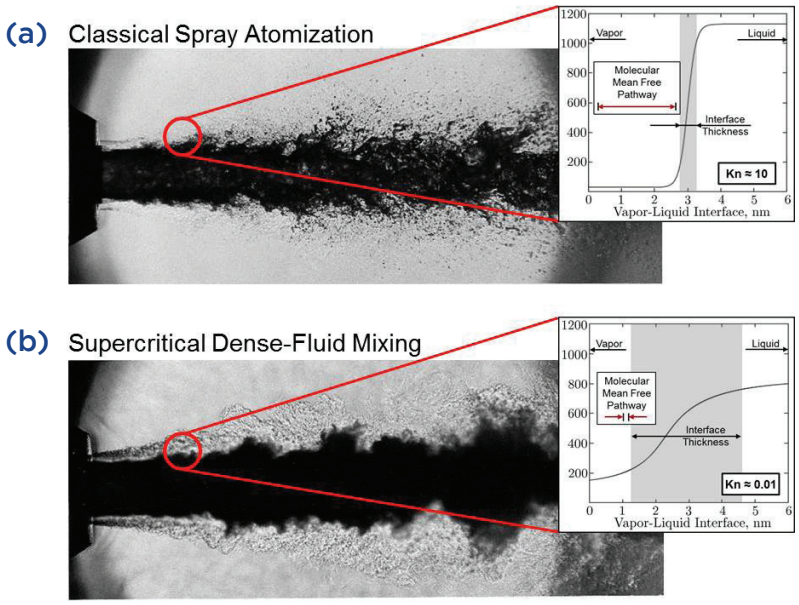
To commercialize this IP portfolio, UIUC researchers John Rogers and Ralph Nuzzo cofounded Semprius. Their current commercial implementation of this technology holds the world record for module-level efficiency of 37.1% (Figure 6c).

New Conceptual Model for High-Pressure Fuel Injection Processes

Understanding and predicting fuel injection processes in advanced transportation and power systems is widely recognized as a critical research area 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 toward the design of optimized, high-efficiency, low-emissions systems.

Figure 7 The high-speed images above show how gas-liquid interfacial structure changes as a function of pressure for a given set of injection conditions. (a) At lower pressure, the gas-liquid interface is molecular and dominated by surface tension where droplets form. (b) At higher pressure, 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 have a profound effect on combustion performance and emissions.[9]

Credit: American Institute of Aeronautics and Astronautics (AIAA)



Researchers at the 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 (Figure 7a) is replaced by diffusion dominated mixing without drop formation at supercritical conditions (Figure 7b). 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. Liquid fuel diffuses into the ambient gas in a manner that is markedly different from the classical picture typically assumed. This work has led to the development of a novel model of liquid injection processes that can be applied to a variety of combustion systems.

The development and application of this new theory will be invaluable for the design of advanced combustion systems.

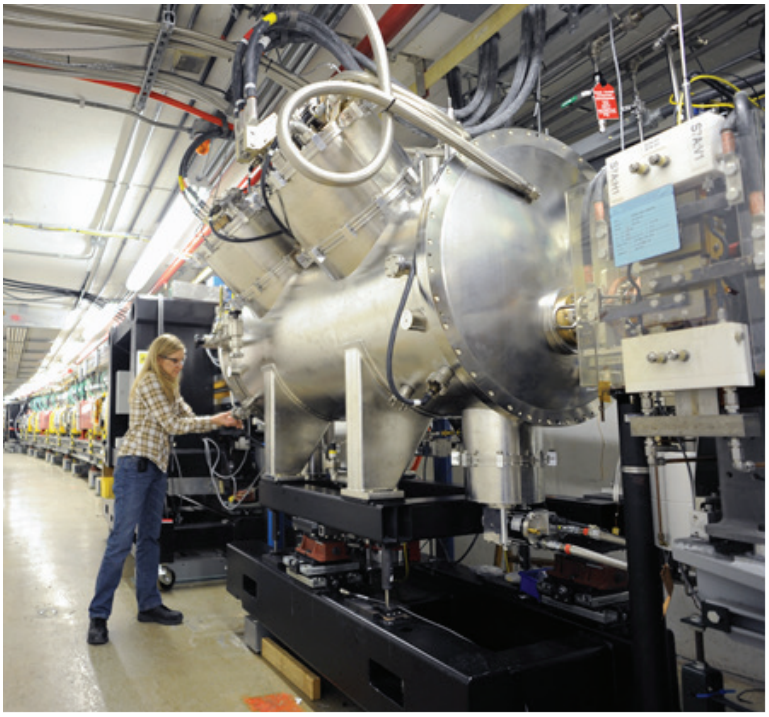
New Technology Advancement Will Improve the Performance of High-Energy Light Sources

The U.S. leadership in X-ray light sources has enabled far-reaching advances in diverse fields of science and technology. The facilities have benefited from continued investments in accelerator science and detectors,

pushing the frontier of light source technologies. A recent example from the APS at ANL harnesses superconducting magnet technology for a new device that has significantly boosted the brightness of high-energy X-ray beams.

Figure 8 The superconducting undulator installed at the straight section of Sector 6 of the APS at Argonne National Laboratory.[10]

Credit: Argonne National Laboratory



Superconducting technology in magnetic devices for synchrotron light sources offers superior performance in higher peak field over the same distance compared to conventional permanent magnetic devices. Superconducting technology has been successfully utilized at synchrotron radiation facilities to build more powerful wigglers or bending magnets, devices that produce synchrotron X-rays. However, making small-period, strong-magnetic-field undulators that meet stringent field quality requirements has been a long-standing objective for accelerator science.

After more than 8 years of effort by physicists, engineers, and technicians, the first X-rays were produced from a novel superconducting undulator at the APS (Figure 8). This is the first such superconducting undulator operated at a third-generation synchrotron X-ray facility. At only 0.35 meter (m) long, this prototype device shows superior performance relative to the standard 2.4-m-long permanent magnetic devices used at the APS for producing high-energy X-rays.

The successful development of a superconducting undulator at the APS will provide current and future light sources with superior undulators, advancing the performance of those facilities and benefiting the science and technology communities that rely on them.

New Detector Sheds Light on Photosynthesis

A new type of X-ray detector capable of recording data from the incredibly short and intense X-ray laser pulses produced by the Linac Coherent Light Source (LCLS) at SLAC National Accelerator Laboratory (SLAC) has proven to be an essential and highly successful tool, enabling breakthrough scientific accomplishments. The Cornell-SLAC Pixel Array Detector (CS-PAD) is the result of collaborative efforts between Cornell University and SLAC. No other X-ray detector currently operating is capable of continuously capturing wide-dynamic range (>1000 X-rays/pixel), large format (>2 million pixels), femtosecond X-ray images at the required 120 Hz pulse rate of the LCLS.

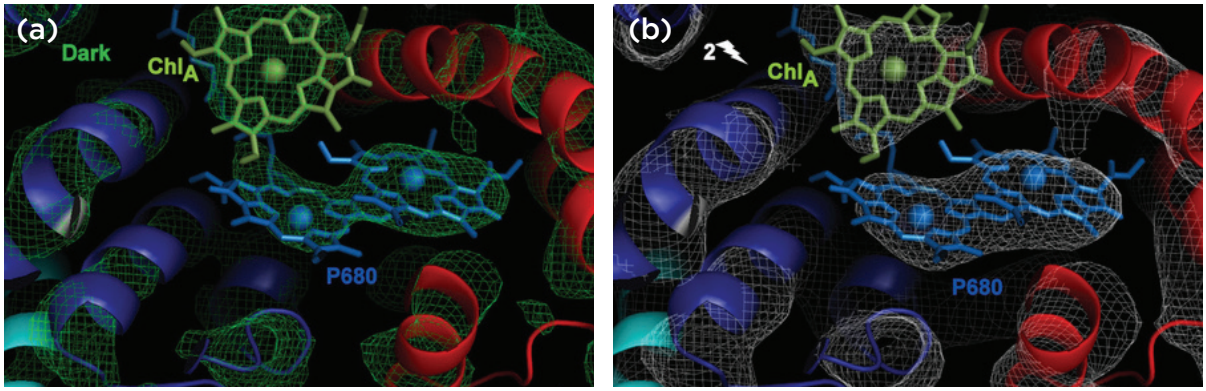
The CS-PAD detector was recently used by an international team of investigators to better understand photosynthesis, the fundamental process that plants use to convert energy from sunlight into chemical energy. Their experiment involved passing a stream of photo-excited microcrystals of the photosynthetic protein

complex into the LCLS pulse X-ray beam. Each pulse resulted in a complex X-ray diffraction image that lasted only tens of femtoseconds. The CS-PAD detector quantitatively captured each X-ray image for later analysis. The resulting massive data sets were subsequently analyzed to determine the time-dependent sequence of structural changes that occurred in the photosynthetic protein complex upon light activation. By observing these changes the researchers revealed novel mechanistic details of the photosynthetic process (Figure 9).

This example shows how the power and promise of the CS-PAD detector for time-resolved serial femtosecond crystallography can provide critical insights into catalytic processes in biomolecules.

Figure 9 Light absorption-induced changes in the electron density of components of the photosynthetic protein complex, Photosystem II. (a) The green mesh reflects the electron density before the reaction begins. (b) The white mesh shows the electron density after laser excitation initiates the reaction. The data used to generate the images were acquired with the CS-PAD detector.[11]

Credit: Reprinted by permission from Macmillan Publishers Ltd: Nature, 2014



Systems-Based Biological and Environmental Research for Energy

Sea Spray Particles Coated with Anthropogenic Organics Lead to Organic Salts and an Unexpected Geomorphology

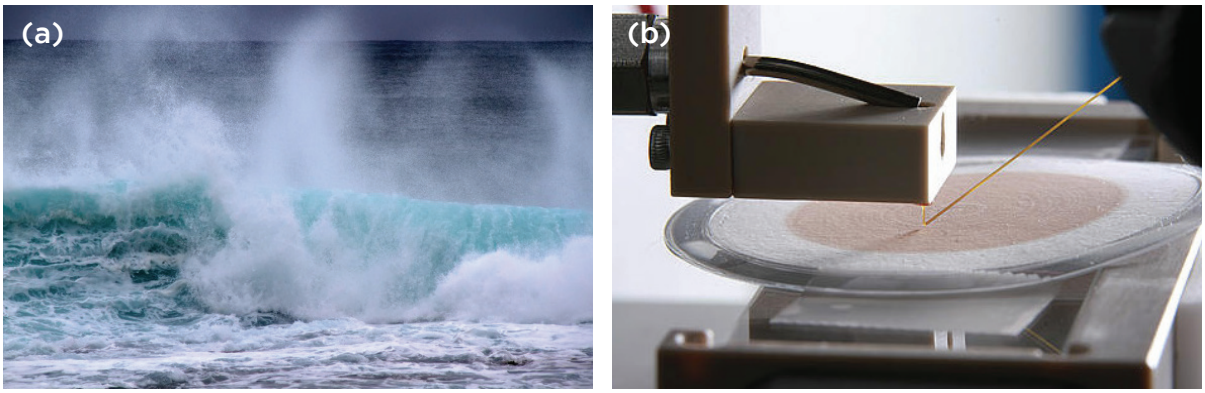
In addition to serving as a source of salt to coastal communities, sea spray particles are a significant source of atmospheric particles that serve as cloud condensation nuclei (CCN), which can grow to become cloud droplets and/or ice particles, and eventually clouds (Figure 10a). Clouds in turn represent a dominant radiative transfer control over Earth's climate. It has been known for more than a decade that sea spray particles can be coated with anthropogenic chemicals, but the significance of these coatings was poorly understood.

To explore the role organic chemical compounds play as coatings on sea spray particles, a team of researchers from the Pacific Northwest National Laboratory, Lawrence Berkeley National Laboratory (LBNL), and University of the Pacific, collected field samples of sea salt particles in the eastern Pacific Ocean. Using X-ray micro-spectroscopy and nanospray desorption electrospray ionization mass spectrometry (Figure 10b) techniques available at the DOE Environmental Molecular Sciences Laboratory (EMSL), the research team obtained composition and geomorphology information with nanoscale resolution on individual and groups of sea spray particles. The team of researchers discovered that when temperature and humidity is elevated, chemical reactions within the carbon-coated sea salt particles can lead to formation of organic salts. When cooled, the particles become glass-like lumps. The team also confirmed an anthropogenic origin for the organic chemical compounds that coated sea spray particles, demonstrating that human activity alters the efficiency and geomorphological distribution of sea spray particles that eventually become CCN.

Because organic-laden CCN derived from sea spray may have different geomorphological distributions than CCN derived from a pollution-free environment, it is likely that the optical properties associated with the evolution of clouds may be much more complex than existing models can evaluate. The authors concluded that a better understanding of the chemical kinetics involved in organic-laden sea spray particles is an important yet missing process in both atmospheric and climate models. Further analysis will be required to understand the evolution of clouds and reduce uncertainty in climate prediction models.

Figure 10 (a) Cloud droplets are initially formed as the result of water vapor condensation onto a seed particle; as the droplets grow, they become clouds. Over the oceans, sea spray is the dominant source of seed particles. Until recently, it was assumed that sea spray particles exhibited the same efficiency for cloud formation as other sources of CCN. This assumption was identified as a basis for major uncertainty in cloud and climate models. (b) Using sophisticated micro-spectroscopy and the nanospray desorption electrospray ionization mass spectrometry capabilities at EMSL, a team of researchers discovered that when sea spray particles are coated with organics, the geomorphology can radically change and organic salts can form. This new information is critical to advancing cloud climate models and energy balance codes over the world's oceans.[12]

Credit: (b) Pacific Northwest National Laboratory



Engineered Poplar Lignin Improves Wood Degradability

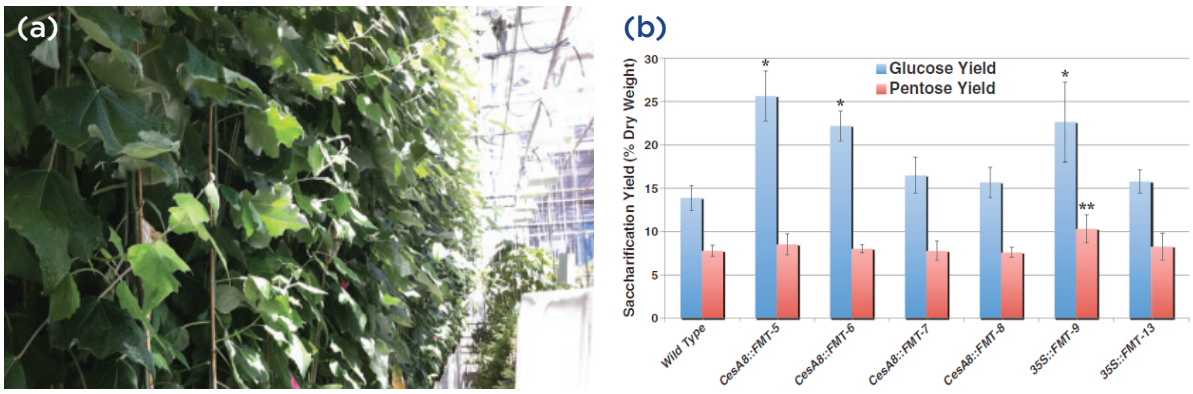
Lignin is an irregular phenolic polymer that is integral to the strength and function of plant cell walls. It is important in bioprocessing of plant biomass because it inhibits deconstruction of cell wall sugar polymers, such as cellulose and hemicellulose, into sugar monomers, a key step in biofuel production. The irregular structure and types of bond linkages within the lignin structure contribute to its recalcitrance to cleavage and hydrolysis. Interestingly, the enzymes that polymerize the lignin polymers are known to be promiscuous and can incorporate nonstandard monolignols if alternate precursors are supplied.

To exploit this promiscuity and construct a lignin molecule more amenable to hydrolysis, researchers at the Great Lakes Bioenergy Research Center genetically engineered poplar–an attractive biofuels feedstock–to biosynthesize ferulate conjugated monolignols in the developing cell wall of plant tissues that contain significant amounts of lignin (Figure 11a). Incorporation of ferulate monolignols into lignin results in the formation of ether bonds, which are more easily hydrolysable than native lignin bonds. Incorporation of the ferulate monolignols into structural tissues in poplar was confirmed using a suite of fluorescence techniques.

The modified plant biomass released up to double the glucose compared to the wild type poplar biomass in pretreatment studies (Figure 11b). These results demonstrate the utility of modifying lignin as a means to simplify processing and increase sugar yields from plant biomass for the production of biofuels. These improvements are important advances in overcoming the technical barriers to an economically viable and sustainable biofuels industry.

Figure 11 (a) Bioengineered poplar containing a modified form of lignin grows indistinguishably from non-engineered plants in greenhouse studies but (b) exhibits higher glucose yields relative to wild type poplar upon pretreatment in a biofuel production process.[13]

Credit: (a) From Wilkerson, C. G.; Mansfield, S. D.; Lu, F.; Withers, S.; Park, J.-Y.; Karlen, S. D.; Gonzales-Vigil, E.; Padmakshan, D.; Unda, F.; Rencoret, J.; Ralph, J. "Monolignol Ferulate Transferase Introduces Chemically Labile Linkages into the Lignin Backbone." Science (344:6179), 2014; pp. 90-93. Reprinted with permission from AAAS." (b) Pacific Northwest National Laboratory



Engineered Switchgrass Shows Increased Ethanol Production in Two-Year Field Trial

A major assumption in plant-based bioenergy research is that key plant cell wall traits can be genetically manipulated to reduce recalcitrance and increase biofuel yields per unit of biomass. A number of greenhouse experiments have shown promise, but few field studies have been completed to assess this assumption. Researchers at the Bioenergy Science Center (BESC), one of the DOE Bioenergy Research Centers, are the first to report a field study evaluating the biofuel potential of genetically engineered switchgrass (*Panicum virgatum L.*).

BESC researchers had previously used inhibitory RNA (RNAi) to down-regulate caffeic acid O-methyltransferase (COMT), a key enzyme in the synthesis of lignin precursors. Switchgrass plants engineered in this way and grown in the greenhouse had less lignin and a shift in the quality of the lignin to a more hydrolysable form. These plants showed less recalcitrance and a greater percentage of cell wall sugars being converted to ethanol than control plants.

Figure 12 Field trials of a genetically engineered form of switchgrass demonstrate the ability of these plants to thrive under environmentally relevant conditions as a dedicated bioenergy crop.[14]

Credit: Baxter, H. L., Mazarei, M., Labbe, N., Kline, L. M., Cheng, Q., Windham, M. T., Mann, D. G. J., Fu, C., Ziebell, A., Sykes, R. W., Rodriguez, M., Davis, M. F., Mielenz, J. R., Dixon, R. A., Wang, Z.-Y. and Stewart, C. N. (2014), Two-year field analysis of reduced recalcitrance transgenic switchgrass. Plant Biotechnology Journal, 12: 914–924. doi:10.1111/pbi.12195

Since greenhouse results are not always replicated in the field, researchers wanted to learn if COMT- engineered switchgrass would show reduced recalcitrance and increased ethanol production when grown in the field (Figure 12). The two-year field trial in large part recapitulated the greenhouse results: the transgenic switchgrass plants had a similar reduction in the quantity of lignin and a shift in the quality of lignin; and a greater percentage of the cell wall sugars were released

with pretreatment, increasing ethanol yield by as much as 28% in the transgenic lines relative to controls. Furthermore, these results were collected from senescent tissues harvested at the end of the growing season, when crop yield is highest, compared to the young, green tissues used for the greenhouse studies. Finally, the transgenic plants were not more susceptible to rust (Puccinia emaculata) or other plant pests, which is an important characteristic for future agronomic application of this engineered plant species.

This important two-year field study affirms genetic engineering of the plant cell wall as a viable strategy for the improvement of plant biomass for the production of high-energy biofuels.

Modeling, Simulation, and Data Analytics of Complex Phenomena

Designing Better Biofuels

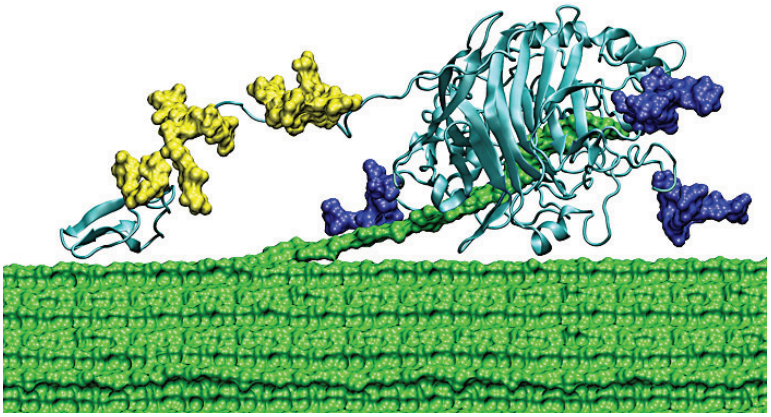
Inedible plant materials such as wood chips and switchgrass contain cellulose that can be broken down into sugars and converted into biofuels. This is a challenging process to commercialize because plant cell walls are recalcitrant, meaning they naturally resist being broken down into their constituent sugars. This trait has contributed to the challenge of producing biofuels from these organisms at a cost and pace that would make them competitive with petroleum-based transportation fuels.

To address this issue, a research team from the National Renewable Energy Laboratory is using Mira, the Argonne Leadership Computing Facility's 8.6 petaflops supercomputer, to conduct large-scale simulations of the physical behavior of cellulase enzymes. Naturally produced by some fungi and bacteria, these enzymes are an attractive modeling target because they effectively trigger the chemical changes necessary to degrade recalcitrant plant materials into sugars.

The research team is using the simulations to develop a molecular-level theory of enzyme "processivity" —the ability to catalyze consecutive reactions--that relates directly to the structural features of the enzymes (Figure 13). This work will provide accurate binding free energy values, a parameter difficult to experimentally determine, on various enzymes of importance to the biofuels industry, shedding light on a key parameter used to compare the function of enzymes.

Figure 13 A putative picture illustrates the mechanism by which processive cellulose enzymes interact with and degrade crystalline cellulose. The catalyst is arranged on the crystalline surface like a lawn mower. The five functional units (yellow and blue) function synergistically to degrade the crystalline cellulose (green). The broken chain is then directed to the entrance of the active site tunnel in the enzyme where the cellulose chain is hydrolyzed to cellobiose. The binding free energy of cellulose to the active site tunnel is a key metric needed to evaluate the efficiency of a catalyst.[15]

Credit: Gregg Beckham (National Renewable Energy Laboratory)



This project is providing tailored improvements to making biofuels based on available plant material. The process of screening for and testing new enzymes is greatly accelerated compared to conventional experimental approaches. This is a milestone towards rational design of novel biofuel enzymes.

Finding the Path to Sustainable Biofuel

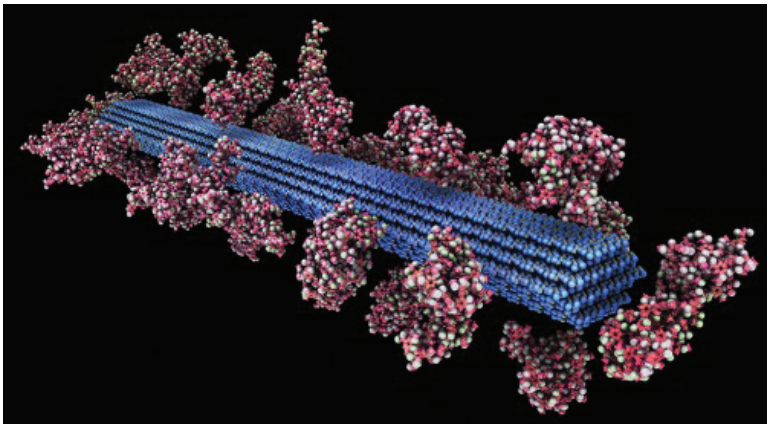
Cellulosic ethanol derived from biomass makes use of one of the most abundant organic compounds on Earth—cellulose—for renewable energy. However, producing this advanced biofuel requires costly treatments that hinder its market competitiveness.

Researchers at Oak Ridge National Laboratory are working to uncover the structure and interactions of molecules in the plant cell wall in order to find ways to make ethanol as cheap as gasoline and help biofuel producers meet U.S. renewable energy goals.

Using Titan, a 17.6-petaflops supercomputer at the Oak Ridge Leadership Computing Facility, the researchers were able to scale up a molecular dynamics simulation to monitor a 30-million atom system tracking the interactions of cellulose, hemicellulose, and lignin, a strengthening agent within the plant cell wall and one of the major obstacles to efficient biofuel production (Figure 14). Their research resolved the highly folded structure of lignin down to 1 Å (angstrom), about a million times smaller than the human eye can see, and led to the discovery that less organized non-crystalline cellulose fibers bind less frequently with lignin, making them easier to break down during biofuel processing.

Figure 14 A visualization depicting the interaction between a cellulose fibril (blue) and lignin molecules (pink). Computer simulations of the atomic-level interactions within the plant cell wall give biofuel researchers new information that contributes to the development of sustainable cellulosic ethanol.[16]

Credit: Jamison Daniel (Oak Ridge National Laboratory)



These insights contribute an atomic-level understanding of plant matter that helps direct the efforts of biofuel researchers, aiding in the design of new pretreatment methods, new types of biomass, and new enzymes that can harvest more energy from plant material.

In the future, the research team intends to create a simulation tool that can reliably predict the outcome of genetic modifications to plants for biofuel production, significantly speeding up the development of sustainable cellulosic ethanol.

Pore Models Track Reactions in Underground Carbon Capture

Deep saline aquifers are common underground geological formations of salty water found in sedimentary basins. They are viewed by many as the best deep geological feature for carbon dioxide (CO_2) sequestration. However, the effect of CO_2 sequestration on the geochemistry of these formations, and the resulting impact on CO_2 migration, remains poorly understood.

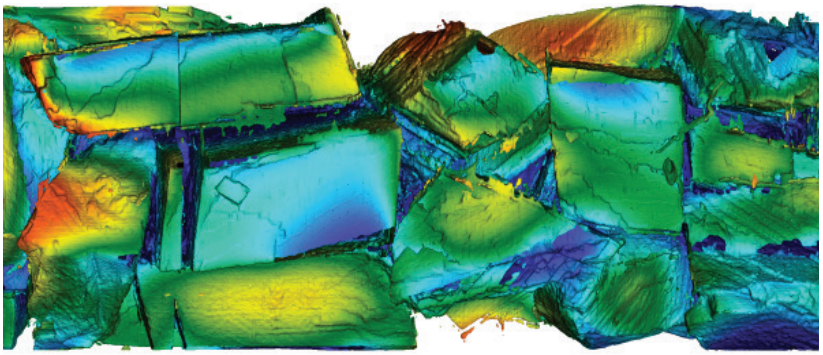
LBNL researchers have developed a unique method for modeling the effects of sequestering CO_2 deep underground in saline aquifers. The aim is to better understand the physical and chemical interactions between CO_2, rocks, and the minute saline-filled pores through which the gas migrates.

Unlike macroscale models, which are unable to resolve microscale features, the research team has used fluid dynamics algorithms to model the physical and chemical reactions happening at single micron resolution. In

simulations run at the National Energy Research Scientific Computing (NERSC) center at LBNL, a tube of calcite a millimeter wide and less than a centimeter long was modeled at 1 micron resolution (Figure 15). The pore-space geometry used in the simulations was based on experimental data. The results have demonstrated that the mineral dissolution rate depends on the pore structure of the aquifer, helping to resolve experimentally observed discrepancies in mineral dissolution rates between field and laboratory measurements.

Figure 15 The computed pH on calcite grains at 1 micron resolution. This level of detail is necessary to better understand the effect of CO_2 injection on the surrounding rock structure.[17]

Credit: David Trebotich (Lawrence Berkeley National Laboratory)



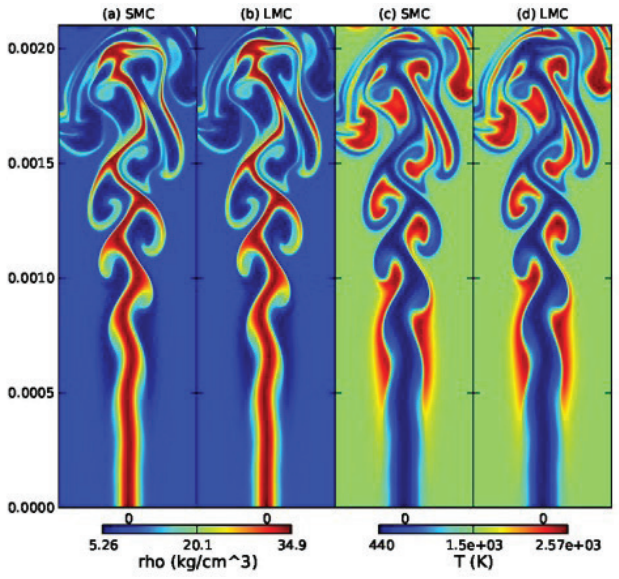
Long term, these efforts are paving the way to models that will be able to simulate the fate of a CO_2 plume over hundreds of years and kilometers in distance. The models of microscopic underground pores being developed could help scientists evaluate methods to store CO_2 produced by power plants. Other emerging applications for this code in the oil and gas industry include modeling flow through fractured shale and analyzing blowout preventer failures.

Optimized Algorithms Boost Combustion Research

More than 80 percent of energy consumed in the United States occurs via the burning of fossil fuels in transportation, heat, and stationary power generation systems. Research into new fuels and more efficient engine technologies offers enormous potential for savings as well as for pollutant reduction. Shortening the design cycle of new fuels optimally tailored to both meet emissions standards and work with new fuel-efficient engines requires fundamental advances in combustion science.

Figure 16 Fine-tuned turbulent combustion simulations aid in the design of more fuel-efficient combustion systems.[18]

Credit: Matthew Emmett and Weiqun Zhang (Lawrence Berkeley National Laboratory)



Modeling and simulation have become integral parts of the combustion design process. A good simulation can inform experimental design to ensure the return of high-quality experimental data and enhance the analysis of physical phenomena. A research team from LBNL has fine-tuned turbulent combustion simulations that will aid in the design of more fuel-efficient combustion systems. The team has developed new algorithmic

features to streamline turbulent flame simulations. In tests of the enhanced code run at NERSC, they achieved a dramatic decrease in simulation times, with methane flame simulations running six times faster than previously possible (Figure 16). The new algorithms are designed to scale up to the new many-core architectures that will power the next generation of supercomputers.

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