RESEARCH FOR OUR ENERGY FUTURE

BROOKHAVEN NATIONAL LABORATORY

ON THE COVER
Energy research at Brookhaven National Laboratory is leading to advances that can transcend the limitations of current technologies and may enable completely new and vastly more efficient energy systems.

RESEARCH FOR OUR ENERGY FUTURE is published by the Community, Education, Government and Public Affairs Directorate of Brookhaven National Laboratory.

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U.S. DEPARTMENT OF ENERGY

Office of Science
U.S. Department of Energy

BROOKHAVEN NATIONAL LABORATORY

One of ten national laboratories overseen and primarily funded by the Office of Science of the U.S. Department of Energy (DOE), Brookhaven National Laboratory conducts research in the physical, biomedical, and environmental sciences, as well as in energy technologies and national security. Brookhaven Lab also builds and operates major scientific facilities available to university, industry and government researchers. Brookhaven is operated and managed for DOE's Office of Science by Brookhaven Science Associates, a limited-liability company founded by Stony Brook University, the largest academic user of Laboratory facilities, and Battelle, a nonprofit, applied science and technology organization.

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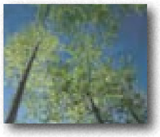
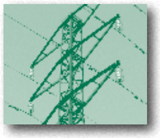
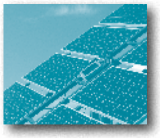
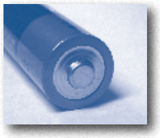




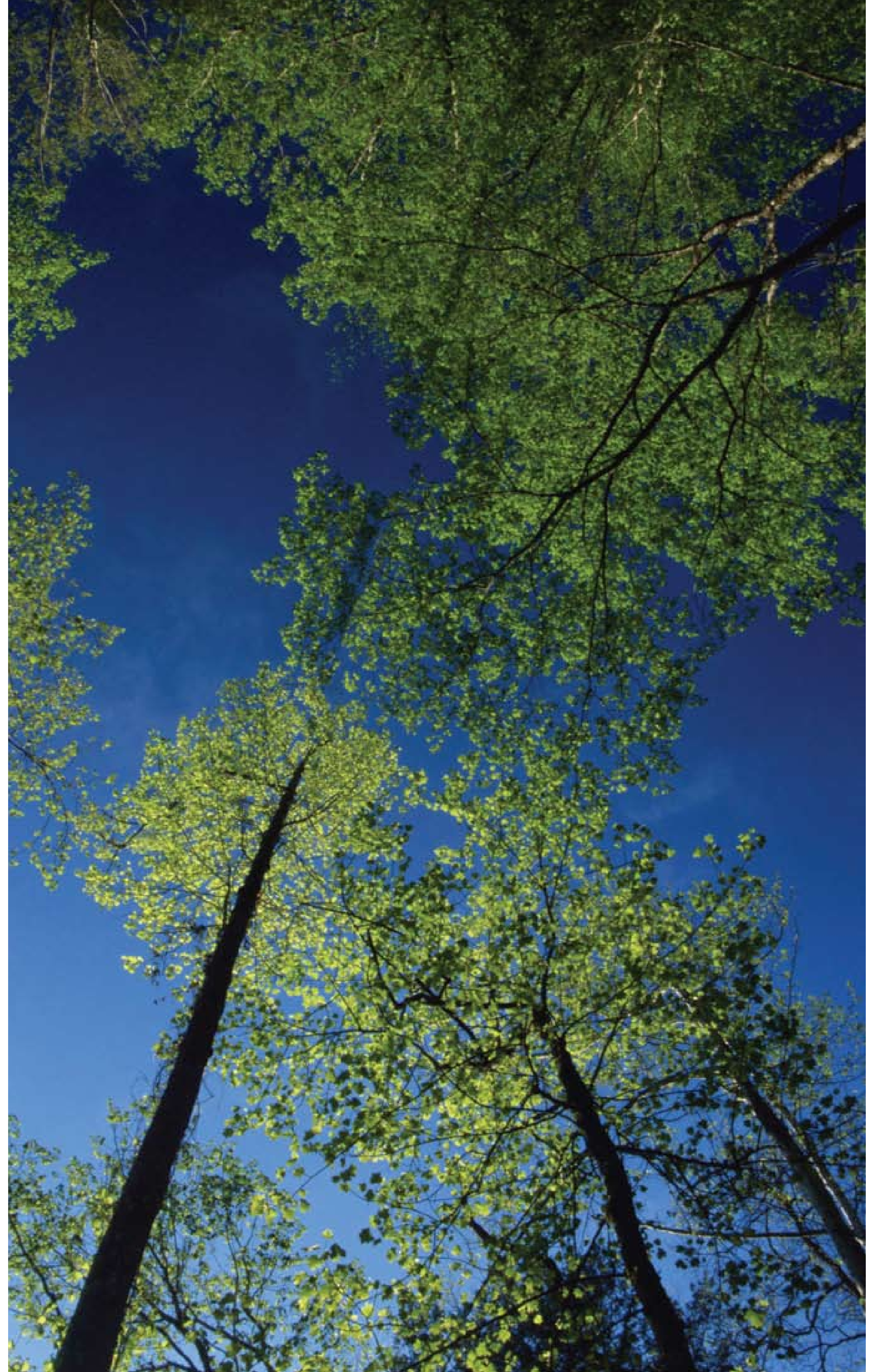




THE ENERGY CHALLENGE

Our nation faces a grand challenge: finding alternatives to fossil fuels and improving energy efficiency to meet our exponentially growing energy needs over the next century and beyond. The U.S. currently consumes about 3.5 terawatts of energy on a continual basis — think 35 billion 100-watt light bulbs burning constantly, or the output of 3,500 coal-burning power plants. And U.S. demand for energy will continue to increase, upwards of 50 percent for electricity alone by the year 2030. Science can meet this daunting challenge — not by making incremental improvements in existing technologies, but through fundamental, game-changing approaches fueled by an investment in basic research.

Right now, we derive the bulk of the energy we use from oil, gasoline, coal, and natural gas — non-renewable fossil fuels that, when burned, add carbon to Earth's atmosphere. Levels of human activity-generated carbon dioxide (CO_2) going into the atmosphere are at an all-time high, and CO_2 is the main "greenhouse gas" associated with climate change. In addition, our current dependence on fossil fuels means that we have no choice but to rely on imports, a large fraction of which come from increasingly unstable parts of the world.



It's crucial that we continue to develop new, renewable sources of energy, especially for high-demand applications like transportation and electricity generation. Most existing technologies for the former rely on products derived from petroleum. For electricity, we burn more than a billion tons of coal each year. To build a foundation for the 21st century and beyond, we clearly need replacements for these 19th century technologies — renewable replacements like solar, wind, hydro, or biofuel/biomass, among others.

The primary reason we use so much energy is the inherent inefficiency of our existing systems. In converting our current energy sources to their many end uses — to power our cars, support industry, and light and heat our homes and businesses — nearly 60 percent of the original energy is completely lost. In a time of dwindling supplies and rising costs, such inefficiencies are unacceptable.

Research conducted at national labs like Brookhaven is leading to advances that can transcend the limitations of current technologies and may enable completely new and vastly more efficient energy systems.

Brookhaven researcher Yimei Zhu with Brookhaven's state-of-the-art scanning transmission electron microscope (STEM). STEM was partially funded by a $1.8 million grant from the NY State Office of Science, Technology & Academic Research (NYSTAR), part of the State's effort to partner with Brookhaven, Stony Brook University, and other institutions in establishing the Empire State as a hub of nanotechnology development. STEM's ability to image material behavior at the atomic scale will significantly advance the Lab's energy-related nanoscience research.

THE ENERGY TECHNOLOGY PIPELINE

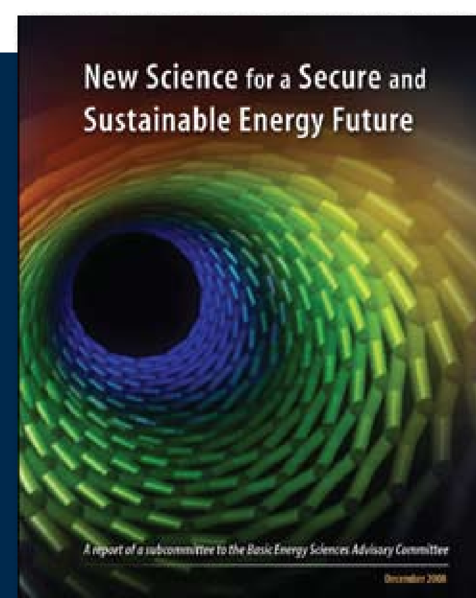
At Brookhaven, scientists develop new energy technologies through a very distinct process – an "energy pipeline" of sorts. Marketable technologies come out of the far end of the pipeline, but they begin with an idea or discovery typically developed through basic research, the cornerstone of innovation and our best opportunity to develop breakthrough solutions for our ever-growing energy needs.

Once scientists identify a technology or idea through basic research or "use-inspired" research (basic research focused on a desired outcome), they refine it as it moves through the pipeline, exploring potential applications and further developing and eventually deploying the technology. Basic research is the foundation, but keeping all of these aspects engaged is crucial in order to keep the pipeline flowing.

Brookhaven has renewable energy projects moving through each step of the pipeline. All these projects focus on one or more of the key aspects of the energy cycle: production, transmission, storage, and use.

Identifying Basic Energy Research Needs

The Department of Energy's Office of Science held a series of workshops involving top scientists from universities, industry, and national laboratories to identify the basic research needs for the nation's energy security. The "Basic Research Needs Workshop" series of reports identifies grand challenges and priority research directions that could provide breakthroughs in key scientific challenges to meet the energy needs of the 21st century. The Lab has aligned its energy strategy to take on these challenges. The reports can be downloaded at http://www.sc.doe.gov/bes/reports/list.html



When completed in 2015, Brookhaven's National Synchrotron Light Source II will provide the world's finest capabilities for x-ray imaging, providing unique opportunities for energy research.

PRODUCTION

By far, our largest source of untapped power resides in the sun, which produces a steady-state output of more than 386 billion *billion* megawatts. Scientists estimate that 600 million megawatts of this power — equivalent to the output of more than half-a-million typical coal-burning power plants — could theoretically be captured and used on Earth. Our focus in this area is improving the efficiency and lowering the cost of photovoltaic cells and finding new ways to use the sun to directly produce fuels through artificial photosynthes. We are also exploring advanced biofuels and fuel-cell catalysts.

TRANSMISSION

Just as important as generating energy is effectively transmitting it to end users. Our aging electrical grid faces significant capacity, reliability, quality, and efficiency challenges that can be met by basic research. Brookhaven scientists are working with new classes of superconductors, materials that carry electrical current with no resistance, to help meet these challenges. One superconducting cable made out of these materials could take the place of 10 conventional copper transmission lines.

STORAGE

Challenges in this area are linked to the inherent limitations of today's batteries, which, despite recent advances in the area of rechargeables, have been around in a basically unchanged form since Thomas Edison discovered the light bulb. Brookhaven researchers are studying new materials that can leapfrog over the limits of today's batteries. Nanoscience plays a large role here, as batteries (chemical storage) and capacitors (physical storage) based on nanostructured materials may become the new paradigm.

USE

Advances in materials, renewable fuels, storage, and energy delivery will transform everything from transportation to electronic devices to home heating and lighting. Some examples of "end-use" products that may emerge from this research include more powerful, efficient, and environmentally friendly fuel cells to power cars and homes, and high-efficiency, solid-state lighting to light our way and conserve power.

BROOKHAVEN'S VISION

Energy research represents a major growth opportunity for Brookhaven over the next decade. The Lab has identified several energy focus areas — including biofuels, complex materials, catalysis, and solar energy — that allow us to integrate our unique facilities with our scientific and technical strengths to address scientific "grand challenges" in energy. This brochure details Brookhaven's energy research portfolio.

We present a comprehensive, interdisciplinary approach to solve fundamental questions regarding U.S. energy independence, and to translate those discoveries into deployable technologies. The bottom line is that a long-term investment in basic research will enable paradigm-shifting advances in the energy arena. The potential payoff in improved energy efficiency and security is enormous, and is key to our nation's continued growth and success.

Energy Research Partners
Stony Brook University and Brookhaven

Brookhaven and Stony Brook University (SBU) are partners in the Advanced Energy Research and Technology Center (AERTC), a research facility created to develop alternative energy sources and protect natural resources by taking advantage of cutting-edge technologies. The Center, shown above, to be built at SBU and supported by $35 million in New York State funding, will be the largest facility of its kind on Long Island, and the centerpiece of a partnership among several academic institutions, research institutions, energy providers, and corporations.

AERTC's mission is to develop innovative energy research, education, and technology deployment with a focus on efficiency, conservation, renewable energy, and nanotechnology applications for new and novel sources of energy. More than 80 projects are already in development in such areas as renewable energy sources, fuels, and conservation.

AERTC's goals include reducing dependence on foreign oil imports, ensuring that the country is able to meet the increasing demand for energy in an environmentally sound manner, and developing a focus on renewable energy and nanotechnology applications for novel sources of energy. The Center will work to integrate basic research with wireless technology, modeling, simulation, testing, and evaluation for a seamless transition from concept to production to distribution. AERTC will also seek to improve the efficiency of existing fuels and the conservation of fuels — including oil and natural gas — that are in decreasing supply.

For more info, go to http://www.aertc.org.

KEY FACILITIES

Brookhaven Lab's one-of-a-kind user facilities support our energy research goals:

CENTER FOR FUNCTIONAL NANOMATERIALS

Brookhaven's *Center for Functional Nanomaterials* (CFN) provides state-of-the-art capabilities for the fabrication and study of nanoscale materials, with an emphasis on atomic-level tailoring to achieve desired properties and functions. Nanoscience has enormous promise in developing solutions to our energy challenges because the processes of energy production, conversion, and use — from the movement of electrons to the catalysis of reactions that convert energy from one form to another — all occur at the nanoscale. Basic research aimed at understanding the details of these processes and structures will enable scientists to design and engineer improvements to optimize efficiency and performance across the spectrum of energy production, transmission, storage, and use.

NATIONAL SYNCHROTRON LIGHT SOURCE AND NSLS-II

One of the world's most widely used scientific research facilities, the *National Synchrotron Light Source* (NSLS) provides intense beams of infrared, ultraviolet, and x-ray light to gain information about the electronic and atomic structures of materials, analyze very small samples, or study surfaces at the atomic level. Energy-related research at NSLS includes studies of the crystal structure of new materials, such as high-temperature superconductors and nanomaterials. The NSLS will be replaced in 2015 by the next-generation *NSLS-II*, which will be 10,000 times brighter than the existing NSLS and allow probing of nanomaterials for energy applications with unprecedented spatial and energy resolution.

NEW YORK BLUE SUPERCOMPUTER

The Brookhaven Lab/Stony Brook University *New York Blue* supercomputer, funded through a $26 million grant from New York State, is capable of 100 trillion calculations per second — about 10,000 times faster than a personal computer. It will be used to advance science in many areas, and particularly in nanoscale science and technology, where it will enable the complex calculations required to study the physical and chemical properties of nanoparticles being explored for their potential to foster U.S. energy independence.

BIOFUELS HARNESSING THE POWER OF PLANTS TO FUEL OUR FUTURE

Plants are efficient energy scavengers, using sunlight to convert carbon dioxide and water into carbohydrates and other products that fuel every living thing on Earth. When we burn fossil fuels to generate heat or electricity, we tap into this ancient source of energy, locked up long ago by the plants and animals that decayed to form those fuels. But dwindling supplies, high costs, and environmental consequences of fossil fuels, such as global warming, have inspired scientists to explore how plants might fuel our future more directly.

One key strategy is the exploration of biofuels — fuels produced directly by plants or derived from plant materials such as stalks, stems, seeds, and fruits. To optimize biofuel production, scientists must gain a better understanding of how plants accumulate biomass and other products in ways that will enable them to influence these processes and convert the plant materials to renewable biofuels. With expertise in plant genetics, metabolism, molecular biology, chemistry, and environmental interactions, as well as access to a suite of high-tech tools, scientists at Brookhaven Lab are poised to make important contributions toward this goal and our nation's sustainable energy future.

Poplar trees grow in many different climates and types of soil, including soil unfit for agricultural crops, making them ideally suited for biofuels production.

ALTERNATIVE PLANTS FOR ALTERNATIVE ENERGY

One of the best-known biofuels is ethanol, a form of alcohol produced by fermenting plant starches (e.g., corn), which can be used as a direct replacement for gasoline. But corn-based ethanol diverts an important food source — and the land it's grown on — for fuel production. A better approach would be to find ways to use non-food crops, ideally ones grown on non-agricultural land, as the source for ethanol or other biofuel production.

Brookhaven researchers are actively investigating several plant species, including various grasses, aquatic plants such as duckweed, and fast-growing poplar trees. Poplar has adapted to many different climates and many different types of soil, including soil unfit for agricultural crops. Brookhaven researchers are looking for ways to increase these plants' production of biomass and other products best suited for conversion to biofuels.

For example, through work originally designed to remove contaminants from soil, Brookhaven scientists have identified soil and plant-associated microbes that can improve plant growth on marginal soils. When bacteria equipped with the molecular "machinery" necessary to degrade environmental contaminants were introduced into poplar roots, the trees' biomass production increased significantly, even when no contaminants were present.

Understanding such microbial-plant interactions may yield ways to further increase biomass. With the world's largest collection of poplar-associated microbial species, Brookhaven stands to make significant advances in this area.

COMPOSITION COMPETITION

Another approach to improved biofuel production is to find ways to alter the composition of plant cell walls, the structural supports surrounding every plant cell. Like corn starch, plant cell walls can be broken down by enzymes into sugars suitable for fermentation into ethanol and other biofuels. But cell wall polymers (cellulose and hemicellulose) are much more difficult to "digest" than starch, making it necessary to find new enzymes for their efficient breakdown.

Using short- and long-lived radiotracers and sophisticated imaging technologies such as positron emission tomography and x-ray crystallography, Brookhaven scientists are exploring the factors that partition plant nutrients between production of lignin, a very recalcitrant cell wall compound, and hemicellulose and cellulose. The goal is to devise ways to tilt the balance toward more easily degraded cellulose, without compromising the structural integrity of the plants. Analysis of the plant enzymes involved in the production of cell wall materials, including structural studies at Brookhaven's National Synchrotron Light Source, can help identify molecular targets and genetic engineering mechanisms for achieving this goal.

Radiotracer techniques are also being used to investigate the allocation of nutrients such as carbon and nitrogen within a plant, and to learn how to influence these processes to improve plants as resources for biofuel production. Unlike in food production, where the goal has been to get plants to grow bigger fruits, sometimes at the expense of the plant as a whole, the goal in biofuel production is to increase plant size overall and maximize carbon dioxide fixation.

Increasing the rate of plant growth may also have benefits for cell wall construction, because lignin takes more time to form than does cellulose. So finding ways to increase nutrient uptake rates would likely favor the production of more easily degraded cellulose and hemicellulose over hard-to-digest lignin. Microbes, again, might play a role here simply by increasing growth rates to tip the lignin/cellulose balance, or possibly by directly affecting the production of these different materials.

BREAKING DOWN WALLS

To facilitate the breakdown of plant cell walls and the separation of products for further processing into biofuels, Brookhaven scientists are also investigating novel chemical

Poplar plants at 10 weeks after being treated with endophytic bacteria (right) compared with control plants (left). The inoculated plants show increased root and shoot formation.

treatments. One such method uses "ionic liquids," an environmentally friendly solvent, to separate lignin from cellulose in solution. Ionic liquids offer many advantages over traditional solvents, including the ability to be used over and over.

The Brookhaven team is also looking to Nature for clues to efficient biomass degradation. In collaborative projects with the National Renewable Energy Laboratory, the Department of Energy's (DOE) Joint Genome Institute, and DOE's Bioenergy Science Center based at Oak Ridge National Laboratory, Brookhaven biologists are prospecting for microbes and enzymes already adept at breaking down biomass. In one project, they isolated the microbial communities degrading poplar biomass in a compost heap and sequenced over half a billion nucleotides of DNA from these microbes, looking for genes encoding the enzymes involved in biomass decomposition. Previously unidentified enzymes discovered through this process can then be cloned and tested to see if they surpass the ability of enzymes currently used to degrade cellulose and hemicellulose.

Brookhaven researchers also have extensive experience with *Clostridium* bacteria, a group of soil microbes that can be used in fermentation for the efficient conversion of lignocellulose feedstocks to biofuels.

OILING THE TRANSITION

Drawing on 15 years of research into plant oils and the enzymes that influence their production, another group of Brookhaven scientists is investigating whether plants might be coaxed into producing oil-based biofuels, such as biodiesel.

This research was originally directed at producing rare fatty acids and other non-petroleum oils as potential feedstocks for the chemical industry. But the same techniques — modifying enzymes in metabolic pathways to alter the end products — can be used to modify plant oils for the direct production of biofuels, or to alter the fatty acid composition of existing biofuels.

Since fatty acid composition affects many of the properties of biofuels — things like melting point and viscosity — the ability to strategically tinker with compositions could lead to improved properties.

Featured Publication
ALTERING PLANT OILS

While conducting studies to alter the placement of double bonds in fatty acids, a group of Lab researchers discovered a fundamental shift in an enzyme's function that could help expand the toolbox for engineering biofuels and other plant-based oil products. Placing double bonds in different positions allows scientists to change the structure of the fatty acids to make products with different potential applications. The ultimate goal is to engineer designer plant oils to be used as biofuels and/or raw materials to reduce the use of petroleum.

To try to change the position of a double bond, the Brookhaven team modified a desaturase enzyme, changing three of the 363 amino acids in its protein sequence. But when they tested the modified enzyme and looked for the expected product, it wasn't there. Instead of producing a shift in double-bond position, the enzyme modification had yielded three completely new products. This was a profound shift in enzyme function — like throwing a switch.

Understanding the mechanism for this dramatic change and applying that knowledge could have enormous benefits for scientists attempting to engineer designer desaturase-like plant enzymes. This would allow them to tailor-make feedstocks with optimal properties, instead of relying on the properties of preexisting raw materials.

Publication:
E. J. Whittle, A. E. Tremblay, P. H. Buist, and J. Shanklin, "Revealing the catalytic potential of an acyl-ACP desaturase: Tandem selective oxidation of saturated fatty acids," *Proceedings of the National Academy of Sciences 2008*, **105**: 14738-14743

> The effort to identify and tailor new energy sources from plant products could go a long way towards addressing our nation's future energy needs.

COMBUSTION TESTING

Scientists at Brookhaven also have extensive experience identifying optimal combustion properties through years of combustion testing for traditional fossil fuels, particularly oil, in conjunction with boilers and other technologies. This work, which has led to improved efficiency, reduced air pollutant emissions, and increased reliability, was recently expanded to include biodiesels. Any new biofuels developed through other research efforts at the Lab could easily be added to this program.

INTEGRATED APPROACH

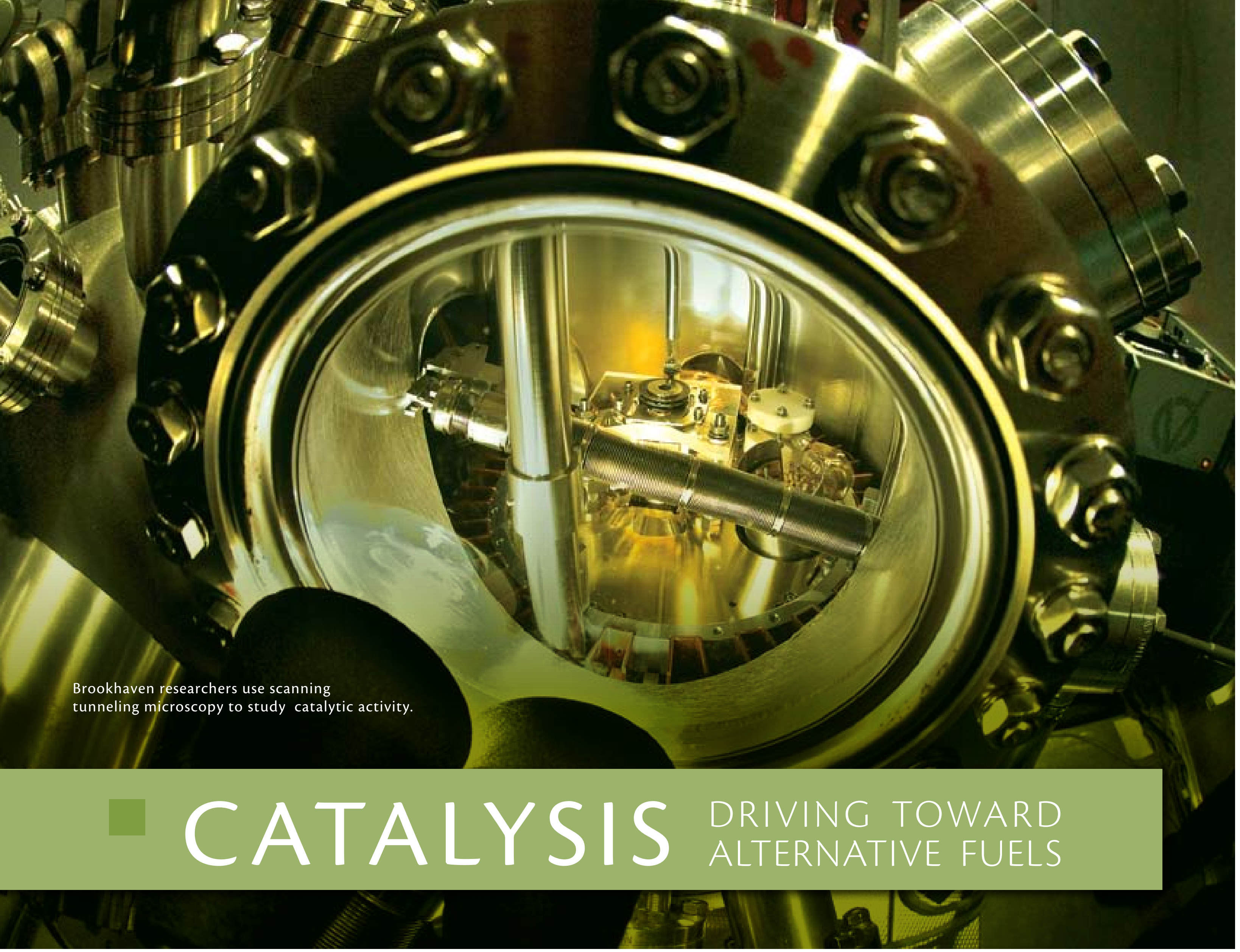
This multidisciplinary exploration draws on the strengths of many existing research programs across scientific disciplines and departments at Brookhaven Lab, and emphasizes the flexibility inherent in a national laboratory setting for maximizing the impact of such an integrated research program. Collaborative research with other DOE labs and nearby institutions such as Cold Spring Harbor Laboratory and Stony Brook University can only serve to help this research grow.

If successful, the effort to identify and tailor new energy sources from plant products could go a long way towards addressing our nation's future energy needs.

As an added benefit, converting to the use of plants as resources for carbon-based fuels will result in a more balanced carbon "budget" for our planet. That's because the carbon released by burning these fuels was only recently removed from the atmosphere, so returning it there has no net impact on global carbon dioxide (CO_2) levels. This is quite different from the release of carbon that was stored millennia ago in fossil fuels, which has been increasing atmospheric levels of CO_2 and altering our climate.

Biofuels may not reverse these changes. But if developed in sustainable ways, they will help bring us closer to the goal of a greener planet.

Finding alternatives to corn-based ethanol is one of the major goals of Brookhaven's biofuels research effort.



Brookhaven researchers use scanning tunneling microscopy to study catalytic activity.

CATALYSIS DRIVING TOWARD ALTERNATIVE FUELS

About 85 percent of the nation's energy needs are met by the combustion of fossil fuels such as oil, natural gas, and coal – finite resources that make the United States dependent upon other countries while polluting the environment through carbon emissions. In order to achieve energy security in an environmentally friendly manner, the nation's energy strategy must include alternative technologies based on renewable sources such as biofuels, and solar, wind, and nuclear power.

A central challenge, however, is the development of new processes and materials capable of tapping these sources and feeding the country's vast energy needs. A key part of the solution involves catalysis, the process of speeding up and directing chemical reactions.

In the effort to develop new, environmentally friendly, and renewable energy technologies, chemical fuels such as gasoline, diesel, and ethanol will continue to serve an important role. Chemical fuels are unmatched in their capability to store energy at high density, and they provide a very effective and economical way to transport and store energy over long distances for long periods of time, for example, as gasoline in a car. But most alternative energy sources do not directly create chemical fuels. Instead, a series of chemical conversions must first take place, assisted by various catalytic processes.

Many of the currently used catalytic processes, developed during the past century, were intended for the conversion of fossil fuel products. The next-generation catalytic challenges require complex steps to turn alternative energy sources into electrical energy that is then transformed into chemical fuels, or by directly converting carbon dioxide into useable fuel sources with the assistance of power from the sun. To meet these technical and theoretical challenges, researchers at Brookhaven National Laboratory are developing an atomic-level understanding of these chemical transformations and the catalysts that enable them.

NEW ROUTES TO RENEWABLE FUELS AND EFFICIENT USE

Making fuel from hydrogen

In contrast to burning fossil fuels such as oil and natural gas, the use of hydrogen molecules as a fuel produces no pollution. In addition, hydrogen atoms – a constituent of water – are widely abundant. However, finding simple, inexpensive ways to produce hydrogen fuel from water, and to store and efficiently use it, is technologically tricky.

Brookhaven scientists are developing catalysts to support a hydrogen-based economy. Many of these studies involve catalysts that assist in hydrogen production for fuel cells, which combine hydrogen and oxygen without combustion to produce direct electrical power and water.

Solar energy to fuels: mimicking Mother Nature

To find some of the world's best catalysts, look no further than your backyard, where Mother Nature has perfected sustainable and clean energy production. For this reason, Brookhaven Lab researchers are trying to design catalysts inspired by photosynthesis, the natural process by which green plants convert sunlight, water, and carbon dioxide into oxygen and carbohydrates. The goal is to design a bio-inspired system that can produce fuels like methanol, methane, and hydrogen directly from water and carbon dioxide using renewable solar energy.

For example, Brookhaven researchers have mimicked a step in photosynthesis called "water oxidation catalysis," one part of water splitting, a high-energy process that separates water into hydrogen and oxygen. Specifically, the scientists tested how a novel ruthenium complex catalyzes water oxidation to form oxygen. Finding efficient and inexpensive catalysts to assist in this reaction is crucial to making the process useful for hydrogen production for fuel cells.

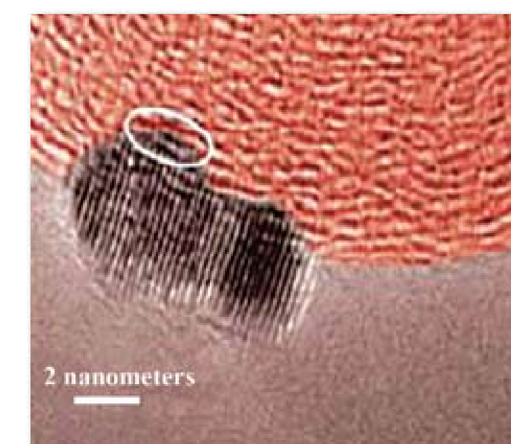
Renewable liquid fuels

While the major challenges to establishing a hydrogen economy are being worked out, scientists also are investigating the production and use of renewable liquid fuels such as methanol, ethanol, and butanol produced from carbon dioxide. Methanol, for example, may be used as a fuel in an easily adaptable internal combustion engine that exists today or in fuel cell-powered cars in the future. Brookhaven researchers are investigating catalysts that can efficiently and selectively produce these desired liquid fuels from renewable energy and starting materials such as water and carbon dioxide, or from the conversion of biomass.

New electrocatalysts for fuel cells

Brookhaven researchers also are working on projects that bridge basic and applied science. The best example of this work is the development of new fuel cell electrocatalysts, which convert hydrogen to electricity for use in electric vehicles.

Although platinum is the most efficient electrocatalyst for accelerating the oxygen reduction reaction in fuel cells, it is expensive, and not stable enough to be used during stop-and-go driving. Brookhaven scientists developed the first platinum monolayer fuel cell electrocatalyst, which has long-term stability and the same activity as the traditional model but 10 times less platinum, making it



A highlight of the Brookhaven catalysis effort is Radoslav Adzic and his research group's work on nanostructured electro-catalysts, like the gold/platinum/copper catalyst shown here. Synthesis techniques have been developed to place platinum atoms on the surface of nanoparticles to produce new catalysts that have higher stability, use less platinum, and are more resistant to impurities for hydrogen fuel cells. The new catalysts made at Brookhaven already meet the future targets the Department of Energy has set for fuel cell catalyst performance.

At Brookhaven, scientists are using expertise, world-class research instruments, and theoretical methods to drive these revolutionary processes to the next level.

much more cost-effective. Researchers are now studying several types of this monolayer catalyst in the laboratory and are working with several companies to test its performance in actual fuel cells. In addition, this research is advancing the development of electrocatalysts that allow the direct use of liquid fuels in fuel cells, taking away the need for the internal combustion engine. Research on electrocatalysts also could lead to the development of other applications, including methanol fuel cells, which could be used to power portable electronics such as computers and cell phones.

Catalysts for pollution reduction

When fossil fuels are burned, sulfur impurities within the fuels become sulfur dioxide, a major air pollutant and a source for the formation of acid rain. Industry uses metal-oxide catalysts in catalytic converters and smokestack scrubbers to help keep sulfur pollutants out of the atmosphere. But there's a new emphasis on making this process more efficient and less expensive.

Brookhaven scientists have worked with industry to help develop new catalysts that destroy sulfur dioxide more effectively, yet present no health or environmental hazards and are inexpensive.

UNIQUE TOOLS STEERING CATALYTIC SCIENCE

Illuminating discoveries

To characterize the state and activity of catalysts as they exist under reaction conditions, scientists use bright beams of x-rays at Brookhaven's National Synchrotron Light Source (NSLS). Capable of producing sample environments with extremely high temperatures and pressures, the NSLS is one of the world-leading scientific facilities for catalysis research.

These capabilities are continuously promoted, improved, and expanded by the Synchrotron Catalysis Consortium (SCC), an organization sponsored by the U.S. Department of Energy and made up of researchers from academic, industrial, and national laboratories. The SCC provides visiting researchers from around the world with: dedicated beam time at the NSLS for experiments using a technique called x-ray absorption fine structure; research staff to assist in the experimental set-up and data analysis; and training courses and help sessions. The consortium also aids in the development and testing of new hardware and software for catalytic and electrocatalytic research.

In addition to these techniques, Brookhaven researchers use a suite of investigative tools, including spectroscopy techniques in the Lab's chemistry department and powerful microscopes and other probes at the Center for Functional Nanomaterials (CFN). In the near future, the souped-up capabilities of the upgrade to the NSLS, the National Synchrotron Light Source II (NSLS-II), will allow scientists to characterize even more complex catalytic systems more efficiently and at higher resolution.

Catalysis on the nanoscale

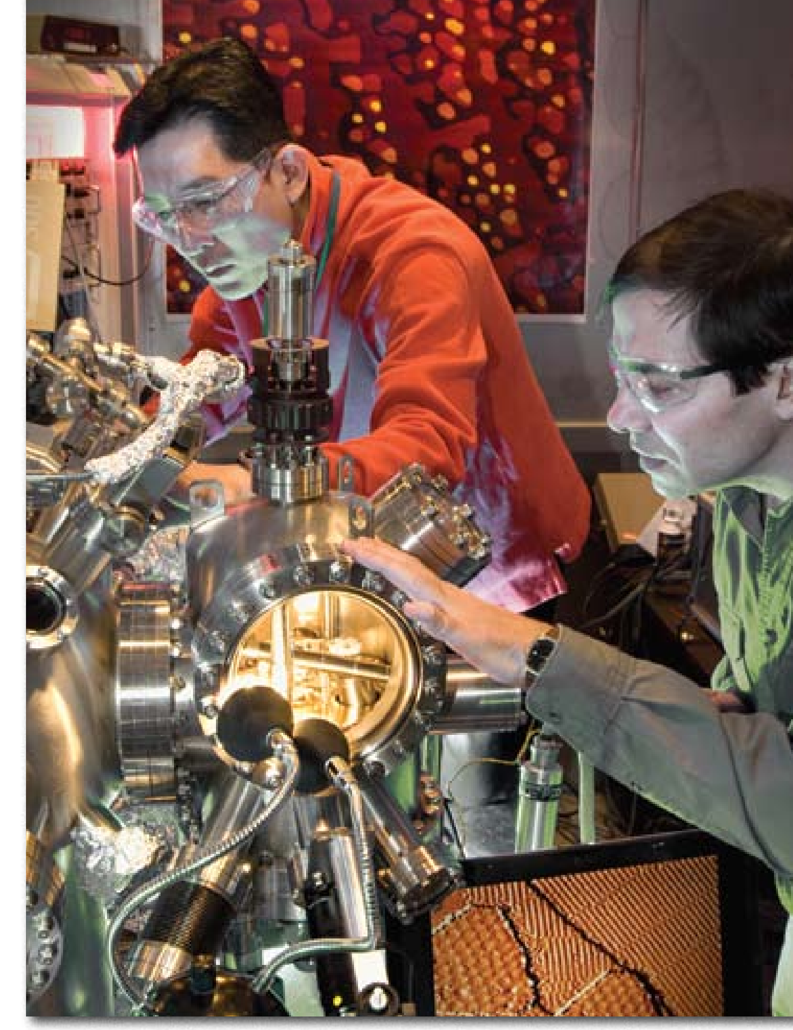
Materials on the nanoscale – on the order of billionths of a meter – have different chemical and physical properties than bulk materials. The gold in a wedding band, for example, is inert. But gold nanoparticles are actually highly reactive, and can play a role in numerous catalytic systems.

To study the activity and key reaction sites of catalysts at the nanoscale, Brookhaven scientists use the state-of-the-art fabrication and characterization instruments at the CFN and NSLS.

For example, scientists have used data from x-ray techniques at the NSLS to study gold and copper nanoparticles for use in the water-gas shift reaction — a process that helps eliminate impurities in hydrogen production for fuel cells. While metal nanoparticles alone are not useful in this reaction, when they are supported on the metal cerium oxide, they have tremendous catalytic activity. In addition, the team discovered that although gold nanoparticles continue to show the greatest catalytic activity, copper is almost as reactive and its cost is much lower.

Computing power

Building off of the work done in the laboratory, Brookhaven scientists use advanced computational methods to model optimal catalysts for particular reactions and to apply theory to validate the results. Special help comes from New York Blue, an IBM supercomputer located at Brookhaven as part of a cooperative effort between Stony Brook University and the Laboratory. Brookhaven scientists also use supercomputers at Lawrence Berkeley National Laboratory and in-house operations to build a framework for designing the best catalysts for the job.



Chemists Joon Park (left) and Jose Rodriguez study catalysts that could help improve the performance of fuel cells.

CATALYZING NEW ENERGY INNOVATIONS

One of the most important missions of energy research is to develop methods for exploiting, converting, and optimizing existing and recently developed energy sources. Catalysis serves as a crosscutting enabling science in this quest, with the potential to lead to renewable, efficient, and inexpensive alternative sources to bring the nation out of its current energy crisis. At Brookhaven, scientists are using expertise, world-class research instruments, and theoretical methods to drive these revolutionary processes to the next level.

Featured Publication

PRODUCING PURE HYDROGEN

A major problem facing fuel cell technology is that the hydrogen-rich materials feeding the reaction often contain carbon monoxide (CO), which deteriorates the expensive platinum-based catalysts that convert hydrogen into electricity. Brookhaven researchers study catalysts that assist in eliminating these impurities through the "water-gas shift" (WGS) reaction, a process that combines CO with water to produce hydrogen gas and carbon dioxide. The ultimate goal is to find the catalysts that will help convert nearly 100 percent of the CO into carbon dioxide, an important step toward achieving a hydrogen-based economy.

Toward this effort, a group led by Brookhaven examined the nanoscale catalysts gold-cerium oxide and gold-titanium oxide. These catalysts usually consist of gold nanoparticles dispersed on a ceria or titania surface. But to get a better idea of how the catalysts work, the researchers studied the "inverse models," ceria or titania nanoparticles on gold. Using powerful x-rays at Brookhaven's National Synchrotron Light Source, in addition to scanning tunneling microscopy and calculations, the group found that although pure gold is inert for the WGS reaction, it becomes extremely active when combined with ceria or titanium. This high activity is due to the catalysts' nanosized oxides, which are able to break apart water molecules – the most difficult part of the WGS reaction.

Publication:

J.A. Rodriguez, S. Ma, P. Liu, J. Hrbek, J. Evans, and M. Pérez, "Activity of CeOx and TiOx Nanoparticles Grown on Au(111) in the Water-Gas Shift Reaction," *Science*, **318**: 1757-1760 (2007).

COMPLEX MATERIALS

UNUSUAL PROPERTIES MAY LEAD TO NEW SUPERCONDUCTORS

The energy systems we rely on today were designed at the start of the last century and are based on scientists' understanding of the properties of basic materials — simple metal wires for conducting electricity, insulators for holding in heat.

In recent years, scientists have discovered an array of unusual and dramatic properties in materials with more complex composition. Certain layered materials that act as insulators at room temperature, for example, can carry electrical current with no resistance when doped with a small amount of impurity and cooled below a certain temperature. Other complex materials convert small amounts of heat into electric currents. Though similar effects had been observed in some simple materials, the effects in complex materials appear to be significantly enhanced.

Today's scientists are looking for ways to harness these dramatic new properties to create the transformational applications needed to meet the energy challenges of our future. Understanding high-temperature superconductors, for example, and tailoring them for applications such as zero-loss power lines could lead to $120 billion in cost savings per year, with five times the power-carrying capacity for the U.S. electrical grid.

Brookhaven Lab, with world-renowned scientific expertise and a suite of high-tech tools for probing the mysteries of complex materials, is eager to meet that challenge.

A new Long Island Power Authority transmission system uses the first generation of a high-temperature superconductor wire technology first studied at Brookhaven Lab.

THE ELECTRON CONNECTION

Understanding the startling properties of complex materials has changed the way scientists think about condensed matter — the regular arrays of atoms making up most of the materials around us.

As is the case with simple materials, a lot of the properties of complex materials depend on the movement and interactions of electrons among atoms. In ordinary metals, despite the huge number of electrons, the interactions are fairly straightforward and can largely be understood by a model in which the electrons are considered to be independent from one another.

But in complex materials, electron interactions extend beyond the immediate neighbors. You tend to get "ordering" phenomena — such as alignments or alternations of individual electron spin directions (magnetic order), or periodically spaced clusters of charges (charge order) — that extend over a large area. And sometimes properties of individual electrons, like spin and charge, act independently of one another.

Scientists must understand the complexity of these interactions if they are to tap into these new materials' potential for energy-saving applications.

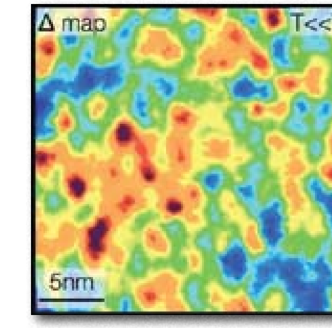
SUPER CURRENT CARRIERS

Brookhaven Lab has a world-class research program aimed at understanding high-temperature (high-T_c) superconductors.

Unlike ordinary conductors, in which electron interactions build up a significant amount of heat as electrical current moves through, superconductors carry current with no resistance. That means none of the energy is lost.

Metallic superconductors, discovered nearly a century ago, operate at temperatures near absolute zero (0 Kelvin or -273 degrees Celsius), requiring costly cooling systems. But the newer complex materials discovered within the past two decades transition to superconductivity at warmer temperatures — hence their designation as high-T_c. Their discovery has sparked the hope of finding or designing materials that perform this current-carrying magic at room temperature.

The key, of course, is to understand how they do it.



Scanning tunneling microscope image of high-temperature superconducting material.

INTRIGUING STRIPES AND OTHER CLUES

The basic idea behind superconductivity is that electrons, which ordinarily repel one another because they have like charges, pair up and move with fluid-like properties to carry current with no resistance. But what causes the pairing in high- T_c superconductors remains one of the great mysteries of condensed matter physics — and a key quest for Brookhaven researchers.

Brookhaven physicists have probed the interactions of electrons with vibrations in the crystal lattice making up the material — which are known to cause electron pairing in conventional metallic superconductors — as well as how changes in the spin alignments, or magnetic polarities, of adjacent electrons might contribute to electron pairing. Recent studies indicate that electrons pair up at a temperature higher than that at which superconductivity sets in. This may offer more clues to the superconducting mechanism and suggest ways to push the superconducting transition closer to room temperature.

Another particularly interesting finding has been the discovery of a pattern of alternating regions of charge and spin order known as "stripes" in certain superconducting materials. Many theorists have long assumed that such stripes should be incompatible with superconductivity because their static pattern implies that the charges are localized in relatively fixed positions, rather than able to move freely to carry current. Brookhaven's measurements suggest that stripes — though perhaps in a more fluid, hard-to-detect form — may, in fact, be essential to superconductivity.

The development of superconductors that could be used in real-world applications, particularly power transmission, could transform the U.S. energy landscape.

Brookhaven scientists are also investigating the role of dimensionality in determining the extreme physical properties of complex materials. Recent studies show that the ability to carry current in the high-temperature superconducting materials, which are made up of many layers, is much greater *within* the layers than between them. This will have important implications for those manufacturing high-T_c power lines, who will either have to find ways to maintain this dimensionality over very long distances — or discover new superconductors that operate equally well in all directions.

Another area of investigation is the role of variations in the composition of the superconducting materials. Scientists need to understand how to deal with patches of irregularity if such patchiness impedes superconductivity.

OTHER MATERIALS

In addition to high-T_c superconductors, scientists at Brookhaven are studying a range of other potentially useful complex materials. These include:

- Materials that exhibit an enormous thermoelectric effect — that is, convert a small amount of heat into a large electric current. Brookhaven scientists are collaborating with automobile manufacturers to see if such materials could be incorporated into auto-exhaust systems to recover some of the energy lost as heat in auto exhaust and use it to recharge electric batteries, for instance.

- Heavy fermion superconductors, which show some similar characteristics to other high-T_c superconductors, albeit at much lower temperatures. These materials may offer further clues to how the high-T_c superconductors function.

- Soft condensed matter, which may have applications in new kinds of solar cells.

TOOLS OF THE TRADE

To investigate the properties of complex materials, Brookhaven scientists employ a suite of high-tech tools and techniques.

Electron photoemission spectroscopy: At the National Synchrotron Light Source (NSLS), a source of high-intensity light at various wavelengths, scientists use beams of visible light to "kick" electrons off their sample materials and measure the electrons' properties to reveal how their interactions with the sample changed them. This gives information about the material's overall electronic structure.

X-ray scattering: Performed at the NSLS and elsewhere, but this time using beams of x-rays, which scatter off the sample. Changes in the rays' energy and momentum reveal details about the ordering of complex materials.

Neutron scattering: Similar to x-ray scattering, only using beams of neutrons. Performed at neutron facilities around the country, including the National Institute for Standards and Technology and the Spallation Neutron Source at Oak Ridge National Laboratory. This technique provides information on the magnetic and charge ordering.

Scanning tunneling microscopy: Uses a probe to allow electrons to flow either into or out of a material to give information about the electronic structure at a particular "real-space" point on the sample.

Electron microscopy: Uses high-energy electrons as a beam to scatter off the material's crystal lattice. Techniques include real-space imaging, electron-energy loss spectroscopy, and phase-sensitive microscopy to provide insight into the structure of complex materials with atomic resolution.

MATERIALS SYNTHESIS

An important key to advancing complex materials is a strong capability in materials synthesis. Brookhaven has a wide array of advanced synthesis capabilities.

For example, a unique *molecular beam epitaxy* system developed at the Lab enables layer-by-layer synthesis of atomically smooth films as well as multilayers with perfect interfaces. Using this device, Brookhaven researchers recently produced two-layer thin films where neither layer is superconducting on its own, but which exhibit a nanometer-thick region of superconductivity at their interface. These materials might be useful in devices such as superconductive transistors and eventually in ultrafast, power-saving electronics. The technology may also help improve the ability of layered superconductors to carry super-current between layers.

Other Brookhaven researchers have become experts in growing single crystals of complex high-T_c materials, supplying researchers at Brookhaven and other research institutions with samples for their studies. Such high-quality, single crystals are at the very heart of scientific research successes in the field of condensed matter experimental physics.

There are also important economic reasons for being on the cutting-edge of new-materials design: Applications tend to be developed in close proximity to the innovators, so nations that discover new materials stand to benefit by being first to market. Right now, the U.S. is behind several countries in new-materials development. Brookhaven scientists hope to do their part to change that.

Brookhaven Lab superconducting cable researchers: (from left) Vyacheslav Solovyov, Department of Condensed Matter Physics & Materials Science (CMPMS); Tom Muller, Physics Department; and Masaki Suenega, CMPMS.

LET IT FLOW

The development of superconductors that could be used in real-world applications, particularly power transmission, could transform the U.S. energy landscape. In addition to huge cost-savings, the higher capacity enabled by superconducting cables would help overcome urban power bottlenecks in today's power grid, reducing the potential for blackouts and other power interruptions. It would also improve the cost-effective control of power flowing across the national grid and extend the operating life of existing high-load power lines. Furthermore, zero-loss transmission would enable the transfer of solar energy generated in parts of the U.S. where sunlight is most abundant to those where it is not, thus making other energy-saving technologies more practical and affordable.

Featured Publication

ELECTRON PAIRING IN HIGH-TEMPERATURE SUPERCONDUCTORS

Brookhaven physicists have found ways to sharpen images of the energy spectra in high-temperature superconductors to reveal previously unobserved details about electron pairing. These new imaging methods confirm that the electron pairs needed to carry current emerge above the transition temperature, before superconductivity sets in.

The findings rule out certain explanations for the development of superconductivity in these materials, and lend support to other, competing theories. Honing in on the mechanism for high-temperature (high-T_c) superconductivity may help scientists engineer new materials to make use of the current-carrying phenomenon in transformative applications such as high-efficiency transmission lines in the U.S. power grid.

To search for pre-formed electron pairs, the Brookhaven team bombarded a copper-oxide material, held at temperatures above and below its transition temperature, with beams of light from the National Synchrotron Light Source, and analyzed the energy spectrum of electrons emitted from the sample. This technique allowed the scientists to look for symmetry in a so-called pseudogap they'd previously observed in the energy spectrum of some high-T_c materials well above the transition temperature. Symmetry in this gap would be a clear indication of electron pairing above the transition temperature. The Brookhaven team demonstrated that the pseudogap does indeed exhibit this symmetry, indicating that electrons are forming pairs before the material becomes a superconductor.

Publication:
H.-B. Yang, J. D. Rameau, P. D. Johnson, T. Valla, A. Tsvelik, G. D. Gu, "Emergence of preformed Cooper pairs from the doped Mott insulating state in Bi2Sr2CaCu2O8+É¬," *Nature* **456**, 77 - 80 (06 Nov 2008)

SOLAR ENERGY

HARNESSING THE SUN'S POWER FOR FUEL AND ELECTRICITY

The average power need of the world's energy economy is 13 terawatts — a thousand trillion watts of power — and by 2050, that amount is expected to double. Fossil fuels and other non-renewable sources are not the answer to the world's ever-expanding need for energy. Also, burning oil, coal or natural gas pollutes the atmosphere and contributes to global warming, which threatens the long-term viability of the earth and its inhabitants.

Efficient utilization of energy from the sun may provide a solution to this important problem. The amount of clean, renewable energy derived from the sun in just one hour would meet the world's energy needs for a year. If we can convert solar energy to fuels with only ten percent efficiency — and use two-tenths of a percent of land in the world for that purpose — we can meet more than 60 percent of the world's need for energy. While no single source will solve the energy problem, converting solar energy to fuels could be a large part of the solution.

Currently, solar energy is converted to electricity only for use in specialized applications such as calculators and satellites, primarily because it is more expensive than fossil-fuel based alternatives. Use of solar energy for heating homes and commercial buildings is becoming more popular with increasing fuel prices; however solar heating is still relatively expensive and not completely reliable, compared to conventional fuels.

Brookhaven scientists are working on both converting solar energy to fuel and improving the efficiency of solar cells using inexpensive materials to lower the cost of energy produced by these methods.

ARTIFICIAL PHOTOSYNTHESIS

In the natural process of photosynthesis, plants convert energy from sunlight, carbon dioxide, and water to carbohydrates and oxygen. Brookhaven scientists are working at converting solar energy to fuel by mimicking photosynthesis in the laboratory.

By achieving better than one-percent efficiency in "artificial photosynthesis" in the laboratory — a better efficiency than that of plants — scientists could produce significant amounts of clean, renewable energy, but the challenges to overcome are difficult. While plants use chlorophyll to absorb sunlight, scientists use a photo-electrochemical cell to absorb light and to separate charges. The separated charges initiate complex chemical reactions that store the solar energy as fuels such as hydrogen or methanol. Brookhaven chemists are working on finding stable, visible-light absorbing materials for the cell's anode.

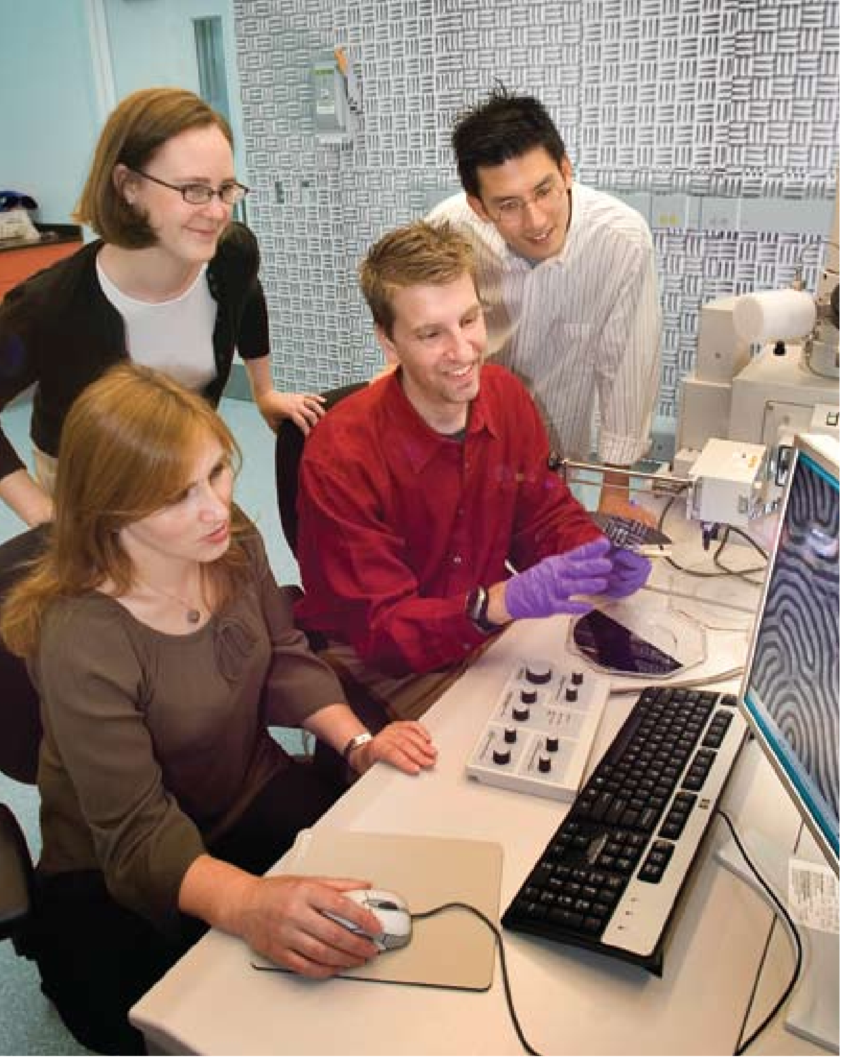
Another challenge is finding efficient catalysts to drive the complex chemical processes needed to mimic photosynthesis in the laboratory. Catalytic processes must coordinate multiple electron, proton, and atom transfer processes to form new high-energy chemicals from thermo-dynamically stable precursors. This artificial photosynthesis challenge is linked to the broader chemistry challenge of using catalysts to activate stable, small molecules for chemical reactions.

CATALYSTS FOR TWO REACTIONS

Catalysts are needed in two separate reactions in artificial photosynthesis to produce solar fuel, such as molecular hydrogen from water. A crucial step in the process is water oxidation — one part of "water splitting," or breaking water into hydrogen and oxygen. Water splitting requires a large amount of energy from sunlight and effective metal catalysts to activate the very stable water molecules. The process occurs as two separate "half-reactions." In one, water oxidation produces molecular oxygen along with protons and electrons; in the other, these protons and electrons are combined to make molecular hydrogen.

Brookhaven scientists, working with collaborators from the Institute for Molecular Science in Japan, have found a novel catalyst that appears promising for water oxidation: a ruthenium complex with bound quinone molecules. This compound efficiently catalyzes water oxidation to form oxygen through a very unique pathway in which the bound quinone molecules are actively involved.

Another catalyst is needed for producing molecular hydrogen. Some bacteria employ hydrogenase enzymes to catalyze the production of hydrogen from water. These very efficient enzymes contain the earth-abundant metals iron and nickel in their active sites. Currently, platinum is the metal of choice as the catalyst for hydrogen production, but Brookhaven scientists are exploring the use of less expensive and more abundant alternatives, including cobalt, inspired by the hydrogenase examples.



Working at the scanning electron microscope at the Center for Functional Nanomaterials are: (seated) Brookhaven Lab researchers Raluca Gearba and Charles Black, and (standing) Katy Bosworth, Cornell University, and Brookhaven's Chang-Yong Nam.

Brookhaven researchers are also developing an understanding of how catalysts work in the complicated processes needed to replicate photosynthesis, including carbon dioxide transformation to fuels. If they can find catalysts that are both efficient and inexpensive to do the job, then they may bring the world a big step closer to tapping the sun's energy.

ELECTRICITY FROM THE SUN

Scientists at Brookhaven's Center for Functional Nanomaterials (CFN) are working on converting solar energy to electricity using new materials and new methods for controlling the structure of these materials. The research involves overcoming challenges to using inexpensive, organic materials or nanostructured inorganic materials in efficient solar cells.

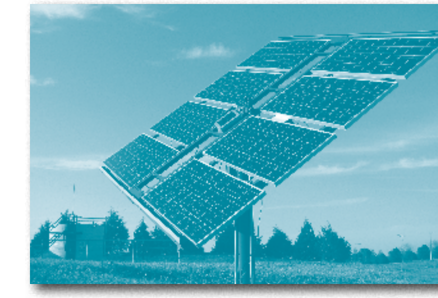
Today, only a small fraction of the electricity we use is generated by solar cells because these devices are made of crystalline silicon, an expensive material. Over the lifetime of a solar panel — about 30 years — the average cost of electricity is about five to ten times higher than electricity generated by conventional fossil-fuel based methods. If solar cell manufacturing costs could be reduced to one-tenth of their present value, these devices could provide cost-competitive electricity and thus be deployed on a more widespread basis.

Brookhaven scientists are studying low-cost polymer materials for possible use in solar cells. Their goal is rooted in both basic and applied science: They want to understand how the materials function and determine if they may be suitable for improving solar panels for the marketplace.

At the CFN, the scientists use sophisticated tools to determine how the materials function on the nanoscale (one nanometer is a billionth of a meter). In complementary studies at Brookhaven's National Synchrotron Light Source, x-rays are being used to probe the structure of organic semiconducting polymers, an essential part of solar cells.

Compared to conventional silicon solar cells, polymer solar cells are lightweight, flexible, disposable, potentially better for the environment, and less expensive to fabricate.

The amount of clean, renewable energy derived from the sun in just one hour would meet the world's energy needs for a year if it could be efficiently harnessed.



MAKING SOLAR CELLS FROM POLYMERS

Solar cells made of polymers are composed of electron donor- and acceptor- materials. When sunlight hits the electron-donor region of the cell, excitons — electronically excited pairs of electrons and holes, spaces where electrons previously resided — are created. To break the bound state of the electron and hole to create a current, the exciton must pass through an interface, which is constructed with two thin materials sandwiched together. A polymer-based material in the interface, the donor, absorbs photons, or energy from the sun, and the acceptor material, a fullerene, a carbon molecule in the shape of a nanotube, attracts the electron. An electric field at the interface of the solar cell is able to rip apart the electron and hole to create an electric charge needed for electrical power.

If the excitons move efficiently and quickly, and separate so that electrons are freed from holes, they will create a current. The cell's electric field provides the voltage, which, when combined with current, gives power to the solar cell. Brookhaven scientists are focusing on how to get excitons to find an interface before they are scattered and lost. The exciton must travel a distance of ten nanometers to get to the interface and the conducting metal wires that protrude from each side of the cell. By fabricating new architecture for the interface and the wires, researchers can give the interface a jagged surface and make the wires protrude like fingers, pointing in the direction of the excitons. Then the excitons have a shorter distance to travel, and more surface space to which they can bind.

Using sophisticated fabrication techniques at the CFN, the scientists can correlate structure and function. If they are able to build a more efficient solar cell using polymers on the nanoscale, they may revolutionize the solar power industry, leading the way to clean, renewable, economical electricity powered by the sun.

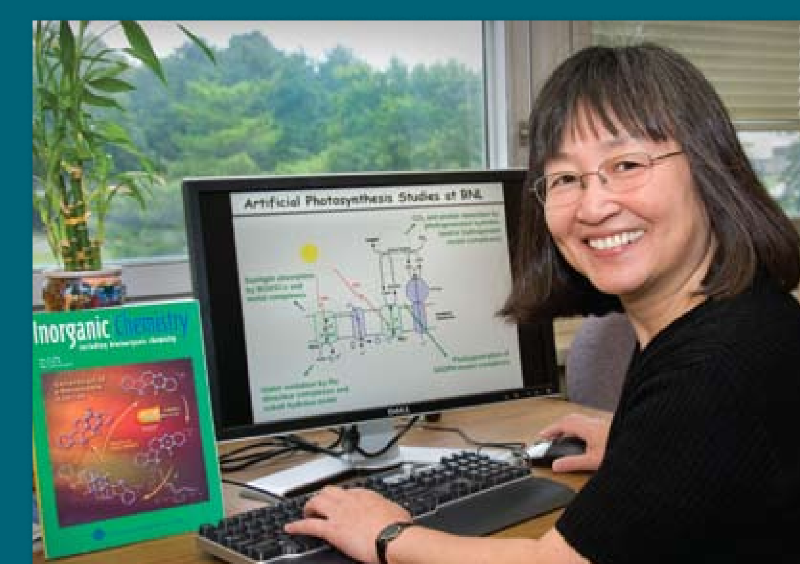
Featured Publication
ARTIFICIAL PHOTOSYNTHESIS

In the final stage of photosynthesis, plants convert carbon dioxide in the atmosphere into carbohydrates. A close collaboration of experimentalists and theorists from Brookhaven Lab and the Institute for Molecular Science in Japan have been trying to mimic that process with the goal of converting carbon dioxide into a clean, renewable fuel using sunlight.

The researchers submerged a light-absorbing ruthenium catalyst that mimics an important substance in photosynthesis in an aqueous solution containing an electron donor. When irradiated with visible light, the catalyst produces a renewable hydride donor that can transfer a negative ion of hydrogen to a hydride-acceptor molecule.

The researchers found that the catalyst was able to pool the energy from two photons — units of light energy — in the hydride donor. This catalyst is able to store two electrons generated by light and a proton as the hydride donor, which it can then transfer to an appropriate acceptor molecule. This process opens the door to light-induced, catalytic hydride-transfer reactions for transforming carbon dioxide to methanol.

Publication:
D. E. Polyansky, D. Cabelli, J. T. Muckerman, T. Fukushima, K. Tanaka, E. Fujita, "Mechanism of Hydride Donor Generation Using a Ru(II) Complex Containing an NAD+ Model Ligand: Pulse and Steady-State Radiolysis Studies," *Inorg. Chem.*, **47** 10 (2008).



Etsuko Fujita

Jason Graetz (left) and Yusuf Celebi assemble a high pressure hydrogen reactor to study the formation of aluminum hydride.

ADVANCED STORAGE SYSTEMS

TAPPING INTO FUEL CELLS AND BATTERIES

Imagine being able to drive a forty-mile round-trip commute every day without ever going near a gas pump. As the United States moves towards an energy economy with reduced dependence on foreign oil and fewer carbon emissions, development of alternative fuel sources and transmission of the energy they provide is only part of the equation. An increase in energy generated from intermittent renewable sources and the growing need for mobile energy will require new, efficient means of storing it, and technological advancements will be necessary to support the nation's future energy storage needs.

A change toward alternative transportation – hydrogen fuel-cell vehicles, hybrid electric vehicles, plug-in hybrid-electric vehicles and electric vehicles – is essential for reducing oil dependency. Brookhaven National Laboratory conducts leading-edge research into two of the most promising technologies to move us closer to making such vehicles feasible, affordable and safe: solid-state hydrogen storage and lithium batteries.

Brookhaven scientists are conducting basic electrochemical research to significantly improve the efficiency and reliability of fuel cells and batteries. They have launched a concerted effort of basic and applied research for the development of improved energy-storage materials and systems with high energy densities, fast cycling rates and long cycling lifetimes in efficient, economical and safe media. The overall goal is to establish a comprehensive, cross-disciplinary energy-storage program that includes basic and applied experimental and theoretical efforts on energy storage for mobile and stationary applications. Brookhaven aims to establish a continuum of scientific expertise capable of bridging gaps between synthesis of new energy materials, the preparation and testing of new materials, characterization, and finally, developing models and identifying structure-property relationships.

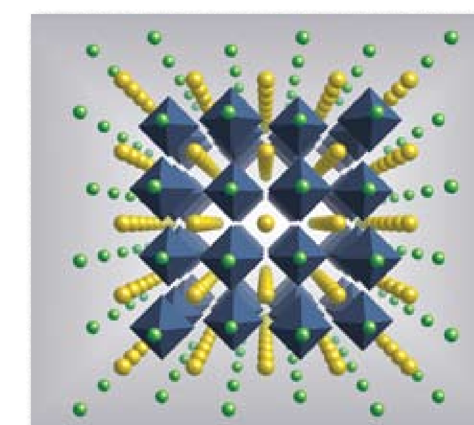
The Center for Functional Nanomaterials (CFN) and the National Synchrotron Light Source (NSLS), and its successor, NSLS-II, are crucial Lab assets and a major component of its energy storage effort. Brookhaven has the tools to become a world leader in energy storage through its capacity to develop synchrotron-based and microscopy-based capabilities to study energy-storage materials, specifically lithium electrodes, electrolytes and metal hydrides. Using the Lab's unique facilities, researchers will develop energy-storage programs in lithium batteries, electrochemical capacitors, metal hydrides, and chemical hydrogen carriers.

HYDROGEN IN A SMALLER PACKAGE

Storage is one of the more challenging technological barriers to the development of hydrogen-fueled vehicles. Since hydrogen is a gas at ambient pressure and temperature, it has an extremely low volumetric density. On an energy basis, one kilogram of hydrogen is equivalent to about one gallon of gasoline. So if we use hydrogen as our energy carrier, the fuel weight would be only about one-third of gasoline. However, even a few kilograms of hydrogen onboard would occupy a volume much greater than the car. We need a way of storing the hydrogen in a lightweight and compact package. Existing storage technologies such as compressed gas and cryogenic storage have limited capacities, are too expensive and will not meet the targets established by the Department of Energy (DOE).

Solid-state hydrogen storage has the greatest potential for meeting the requirements for onboard storage that will be needed to make fuel cell-powered vehicles a reality. Brookhaven has two programs on solid-state hydrogen storage. The first, funded by DOE's Basic Energy Sciences under the Hydrogen Fuel Initiative, investigates the process of hydrogen uptake and release in complex hydrides and is trying to identify how atoms and molecules move around during the charge and discharge process. The second program, funded through the DOE's Office of Energy Efficiency and Renewable Energy under the Metal Hydrogen Center of Excellence, is developing hydrogen-storage materials for automotive fuel-cell applications.

Brookhaven researchers are developing new solid-state hydrogen-storage materials — metal hydrides and chemical hydrides — that have the potential to meet the requirements for onboard storage. In solid-state storage, atomic hydrogen is stored among the atoms of a host material. The complex hydrides, such as sodium aluminum hydride, can store around five percent hydrogen by weight, and are just one class of materials being investigated at Brookhaven. Other materials of interest at Brookhaven include aluminum hydride, which is a fine powder composed of more than 10 percent hydrogen. The unique feature of this material is that it is completely stable at room temperature, but will rapidly release hydrogen upon heating to around 80°C. The challenge is that once the hydrogen is released, it is difficult to get it back in, and extremely high pressures are necessary to "recharge" the material with hydrogen. Brookhaven scientists are working to develop alternative, low-cost methods to regenerate aluminum hydride under moderate pressure and temperature conditions.



An example of a "tunable" hydrogen storage material developed by Brookhaven researchers. By controlling the ratio of different alkali metal ions (yellow and green balls), scientists can tailor the pressure and temperature at which hydrogen is released from the material.

Researchers are also developing new materials with higher hydrogen capacities that release

Brookhaven has the tools to become a world leader in energy storage.

hydrogen at lower temperatures and are tailored to an automotive fuel-cell system. They are also interested in using Brookhaven's NSLS and CFN to study catalysts in these materials. These results will be used to develop new metal hydrides and catalysts with improved properties.

BETTER, CHEAPER, SAFER BATTERIES

One of the more promising near-term ways of reducing our dependence on foreign oil and our energy-related emissions is the development of economical, plug-in hybrid electric vehicles. However, in order to meet the driving range and performance expectations of most consumers, these types of high-power mobile devices will require better, cheaper lithium batteries with new electrodes composed of inexpensive materials that can accommodate more lithium without compromising the system size, weight or cycle life.

Two Brookhaven programs have been researching materials for lithium batteries for nearly a decade. These two programs, Applied Battery Research and Batteries for Advanced Transportation Technology, are both funded by the DOE's Office of Energy Efficiency and Renewable Energy. The programs aim to develop new batteries with longer cycling and calendar life, higher capacity, low cost and improved safety characteristics. Research accomplishments include development of new electrolytes and electrolyte additives for lithium batteries, and development of numerous x-ray absorption and diffraction technologies for battery and fuel cell material studies using the unique DOE-funded facilities located at Brookhaven, such as the beam lines at the NSLS.

Brookhaven scientists are preparing new nanoscale electrode materials capable of higher lithium capacities and rapid cycling rates. Alternative high capacity anodes (the negative electrode) have the potential to double or triple the cell capacity, but these materials are plagued by large volume changes and phase transitions that limit the cycle life. In general, a number of challenges arise with the structural changes, like volume expansion and phase changes, that accompany an increase in lithium density. These changes tend to damage the electrode during cycling making them unsuitable for rechargeable lithium batteries. Electrodes prepared from nanocrystalline powders and nanofilms may be able to sustain large volume changes without particle breakup. These electrodes exhibit improved cycling characteristics as a result of their nano-scale dimensions, which means the battery can be cycled more often without losing capacity. In addition, the nano-scale particle dimensions also promote fast cycling rates, which means higher power capabilities and less time needed to recharge the battery. The new nano synthesis and characterization facilities at the CFN will give Brookhaven a unique opportunity to explore atomic- and molecular-level processes.

On the other side of the battery, the researchers are looking at improving the positive electrode (cathode) by developing materials that can "host" more lithium. In a typical cathode, the negative charge from the lithium is donated to a metal ion in a process called reduction. Normally, there is one metal atom for every lithium atom that is cycled in the battery. Since the metal atoms are heavy, this ultimately limits the capacity of the host material. The Brookhaven team is developing new cathode materials with metal ions that can accommodate two or more electrons to significantly increase the electrode capacity and ultimately reduce the size and weight of the battery.

David Lacina and Weimin Zhou prepare a LabVIEW program to measure the hydrogen uptake and release from a complex hydride in solution.

ON THE ENERGY HORIZON

Brookhaven scientists have embarked on a number of new initiatives designed to move forward their fuel cell and battery programs. These include internally funded studies and proposals on the frontier of our existing science.

A new Laboratory Directed Research and Development project on energy will focus on nanoscale electrodes for lithium batteries. This project includes efforts in materials synthesis, electrochemistry, and microscopy. The goal is to understand how electrode morphology and microstructure affect and are affected by lithium charging and repeated cycling using high-resolution electron microscopy and microanalysis.

A proposal for an Energy Frontier Research Center on hydrogen storage materials, titled "Interfacial Thermodynamics at the Nanoscale," has been submitted. This effort is being led by the California Institute of Technology and includes partners from Carnegie Institution, University of California-Irvine, and HRL Laboratories. A number of other national and international collaborations are already in place for the hydrogen storage programs.

A second proposal for an Energy Frontier Research Center on lithium batteries, titled Northeastern Chemical Energy Storage Center, was also submitted. This effort is being led by Stony Brook University and includes partners from Rutgers, Massachusetts Institute of Technology, Binghamton University, Lawrence Berkeley Laboratory, Argonne National Laboratory, and the Universities of Michigan and Florida.

The development of improved hydrogen storage systems will usher in a new type of fuel-cell car that closely resembles the vehicles on the road today with one important difference: no tailpipe emissions. Similarly, if batteries can be made to power electric hybrid plug-in vehicles for a 40-mile range, there will be a significant increase in the demand for these vehicles. Fundamental and applied research efforts in energy storage and alternative energy carriers like these at Brookhaven are crucial if the nation is to meet the challenges of our energy future. Success will mean elimination of the need for petroleum for most U.S. commuters and significant reduction of our energy-related emissions and dependence on foreign oil.

Featured Publications

STORAGE

The success of hydrogen as our energy carrier of the future will require breakthroughs in the technologies we use to produce, store and use hydrogen. One of the most demanding challenges is hydrogen storage, which has been identified as the bottleneck in the development of hydrogen-fueled vehicles. The difficulty is that hydrogen is a gas under ambient conditions and is difficult to store in a compact and lightweight package. Scientists at Brookhaven are working toward developing solid-state hydrogen storage materials in which a metal or compound is used to "host" hydrogen atoms. This group is developing new storage materials and catalysts to enhance hydrogen uptake and release. Instruments at the National Synchrotron Light Source and the Center for Functional Nanomaterials are being used to prepare new materials and develop a better fundamental understanding of reversible hydrogen storage in the solid state.

Publications:

S. Chaudhuri, J. Graetz A. Ignatov, J. J. Reilly, and J. T. Muckerman, "Understanding the Role of Ti in Reversible Hydrogen Storage as Sodium Alanate: A Combined Experimental and First-Principles Theoretical Approach," *J. Am. Chem. Soc.*, **128** 11404 (2006).

E. Muller, E. Sutter, and P. Zahl, C. V. Ciobanu, P. Sutter, "Short-range order of low-coverage Ti/Al(111): Implications for hydrogen storage in complex metal hydrides," *Appl. Phys. Lett.*, **90** 151917 (2007).

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FUTURE RESEARCH IMPACTS

Brookhaven Lab scientists envision applications that will transform conventional methods of powering our homes, offices, and vehicles.

Catalysis

Nanocatalysts enable efficient fuel-cell reactions to power electric cars

Biofuels

Renewable plant oils used to replace petroleum as fuel

Complex Materials

Reliable superconducting power grid efficiently charges batteries in plug-in hybrids

Storage

Enhanced lithium-ion battery packs power plug-in hybrids; new materials safely store hydrogen to power fuel cells

VEHICLE FLEET


Catalysis
Efficient production of hydrogen for use in distributed fuel cells
Complex Materials
Superconducting power grid transmits electricity efficiently; solid-state lighting offers low-cost, long-life illumination
Biofuels
Renewable replacement for imported petroleum to generate heat and hot water through efficient combustion
Solar Energy
Photovoltaics and solar panels for electricity generation
OFFICE BUILDING

BROOKHAVEN
NATIONAL LABORATORY

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