Oak Ridge National Laboratory
REVIEW
• MANAGED BY UT-BATTELLE FOR THE DEPARTMENT OF ENERGY •

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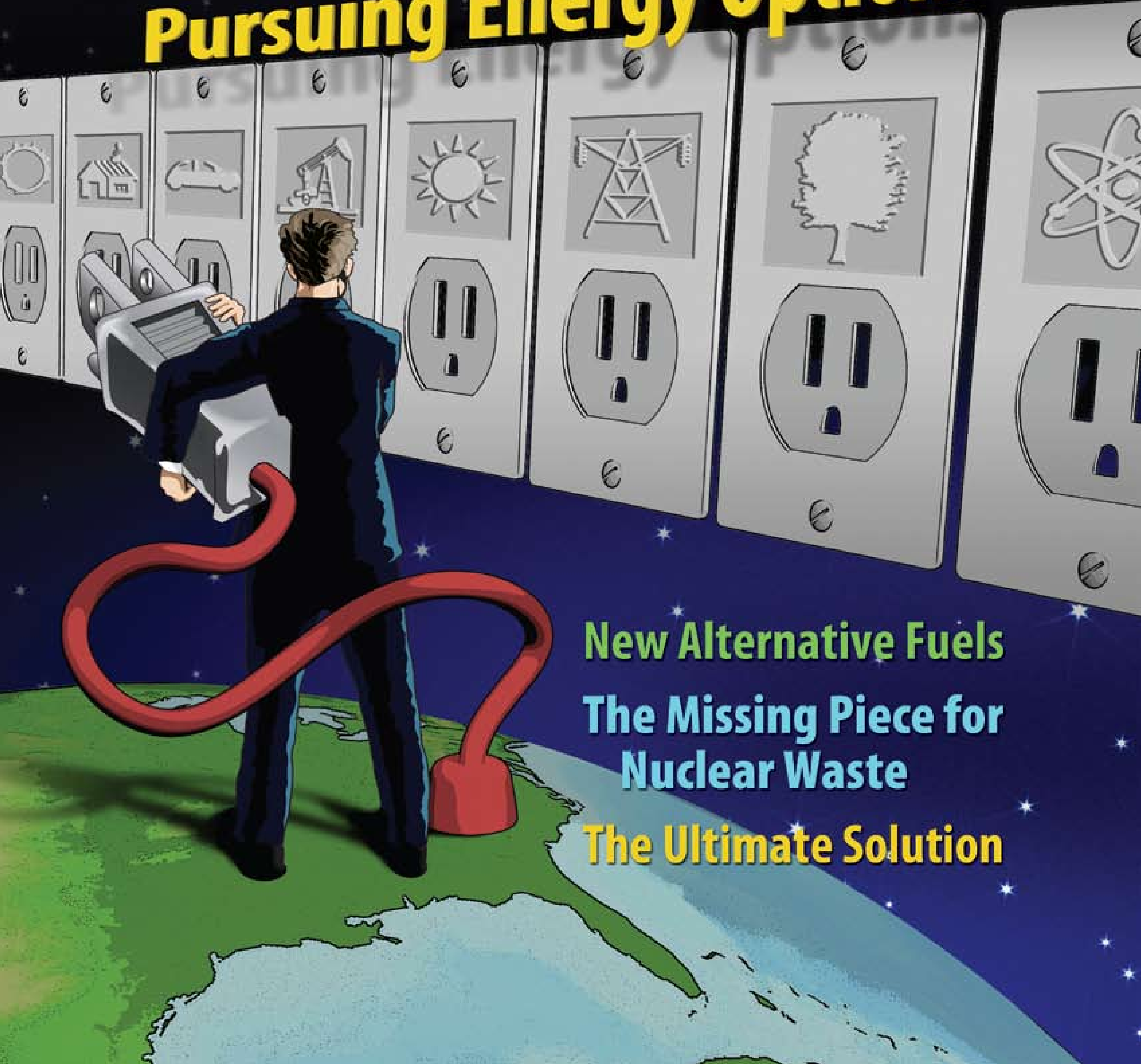
Pursuing Energy Options



New Alternative Fuels

The Missing Piece for Nuclear Waste

The Ultimate Solution

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Energy options at Oak Ridge National Laboratory

The South's
ENERGY LABORATORY

On occasion opportunity is more a product of fate than design. When, in 1942, Oak Ridge was chosen as one of three locations for the Manhattan Project, the decision was driven by the availability of cheap and abundant electricity and the remoteness of East Tennessee farmland. The idea that the new "national laboratory" would someday be a critical asset in the search for advanced energy science and technology was never considered.

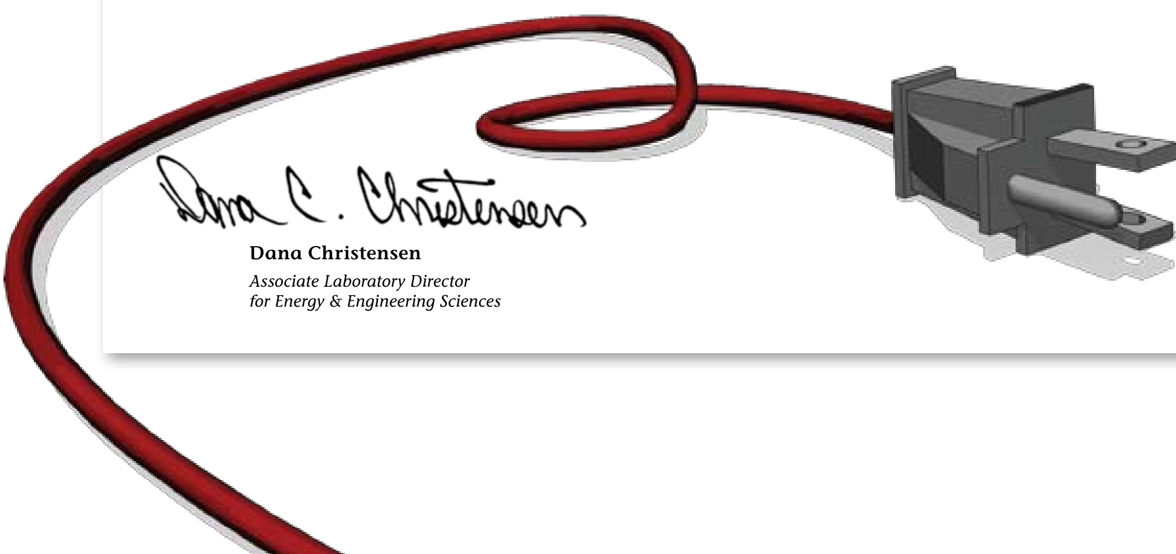
More than six decades passed, a time during which changes in America's research priorities resulted in similar changes for the mission of Oak Ridge National Laboratory. Today, the need to provide an adequate, affordable and environmentally sustainable sources of energy is a domestic priority with long-term consequences as important as the Manhattan Project. Once again, due to an entirely different combination of circumstances, ORNL is playing a leading role in building the research foundation required to develop a comprehensive set of energy options.

ORNL is the Department of Energy's only research laboratory located in the South. With the nation's largest energy research portfolio, the Laboratory has emerged as a major partner in the region's economic growth. Across the South, ORNL has established research partnerships with a growing number of universities and the private sector, with particular focus on multi-state utilities and the South's growing automotive industry.

This issue of the *ORNL Review* examines the Laboratory's energy mission, looking at each area of research in relation to the economy's energy sectors, with the Tennessee region as a demonstration center. Largely by coincidence, most of America's major energy challenges are represented in the region. The South is home to nuclear power plants that seek new materials for their reactors and a permanent solution for their spent fuel. The Tennessee Valley Authority owns one of the nation's largest systems of energy distribution and is looking for new ways to reduce emissions from coal-fired plants. The state of Tennessee has invested $72 million in biofuels research, including a refinery to test new cellulosic ethanol from processes developed at ORNL. The South is home to ten automotive assembly plants—two in Tennessee—and hundreds of suppliers that are reaching out for help with transportation and infrastructure technologies. Perhaps most ambitious of all, Oak Ridge is coordinating America's participation in ITER, the $12 billion, multi-national effort to design and build the world's first fusion reactor involving the governments of more than half the world's population.

The Department of Energy has determined, correctly, that no single technology will ever be the "silver bullet" required to meet the world's expanding energy demands or mitigate the impact of greenhouse gas emissions. Rather, the ability to provide America with adequate, affordable and sustainable energy will be based on an array of new technologies spread across the areas of energy generation, distribution and consumption. Because there is literally a testbed for each of these technologies in the Tennessee region, ORNL's research agenda increasingly is both shaped and strengthened by the confluence of accessibility and need.

Not unlike the Manhattan Project, ORNL's emerging role as a leader in energy research might be viewed as the product of fate. Regardless, the Laboratory's commitment—and expectations—are unchanged.



Dana C. Christensen

Dana Christensen

Associate Laboratory Director
for Energy & Engineering Sciences

News & Notes

Piece of Nobel Peace Prize

Left to right: David Greene, Tom Wilbanks, Virginia Dale, David Erickson, Paul Hanson and Rep. Zack Wamp (TN)

Former Vice President Al Gore is not the only Tennessean to share in the Nobel Peace Prize for "efforts to build up and disseminate greater knowledge about man-made climate change, and to lay the foundations for the measures that are needed to counteract such change." A co-winner was the United Nations' Intergovernmental Panel on Climate Change to which several researchers and a supercomputer at ORNL contributed. Tom Wilbanks, David Greene, Paul Hanson, Virginia Dale and Gregg Marland contributed to several reports of IPCC's four assessments. Wilbanks was a coordinating lead author of a chapter in the IPCC Fourth Assessment report on impacts, adaptation and vulnerabilities. Greene was a lead author for the "Transport" chapter of the IPCC Fourth Assessment mitigation report. Marland was a lead author of one of the first chapters on land use change and forestry and contributor to chapters for the panel's first three assessments.

Cheetah, the IBM high-performance computing system at the National Center for Computational Sciences, a Department of Energy user facility at ORNL, provided more than one-third of the simulations of Earth's past, present and future climate states for the joint DOE-National Science Foundation contribution to the first report of IPCC's Fourth Assessment, issued in 2007. David Erickson and John Drake were ORNL leaders of IPCC simulations on Cheetah in 2005. In a congratulatory letter to more than 2,000 scientists and policymakers who contributed to the panel's reports, IPPC Chairman Rajendra K. Pachauri of India wrote: "This makes all of you a Nobel laureate."

Superconducting Technology License Signed

SuperPower Inc., a Schenectady, N.Y., superconducting wire manufacturer, signed a license agreement to use an ORNL-developed technology that can lower the cost of producing superconducting wires for more efficient transmission of electricity.

The licensing agreement is part of a national effort led by the Department of Energy to research, develop and ultimately transfer energy technologies from DOE national laboratories to the global marketplace. Patricia Hoffman, DOE principal deputy assistant secretary for Electricity Delivery and Energy Reliability, said incorporating these high-temperature superconducting wires and power equipment into the nation's electric grid will help meet rapidly growing demand for energy in an energy-efficient, cost-effective manner.

At a press conference announcing the agreement, Hoffman said. "High-temperature superconductivity is a revolutionary and cross-cutting technology that can further the Administration's long-term effort to transform our nation's electricity infrastructure and provide a safe, reliable and affordable stream of electricity to all Americans."

Superconductors are special materials that have no electrical resistance at extremely low temperatures. High-temperature superconductors, discovered in 1986, lose resistance at warmer temperatures than conventional superconductors, although the temperatures are still very cold.

Cooled by cheap and abundant liquid nitrogen, high-temperature superconductors can be used to make lighter, smaller, more efficient, higher capacity power devices; relieve congested power line networks and increase power transmission capacity.

Two World Records

Fine print is much easier to read under a spotlight than a penlight in an otherwise dark room. The human eye needs a bright light—a high concentration of photons—to resolve the letters.

For scientists using neutron scattering to determine the arrangements and motions of atoms and molecules in a material, the concentration of neutrons in a beam is critical. The higher the concentration, the "brighter" the beam is. With a very bright beam, scientists can obtain experimental data not possible when working with less intense neutron beams.

For that reason, in November 2007 ORNL researchers were excited to learn that the recently upgraded High Flux Isotope Reactor may have set a world record for cold neutron beam "brightness." The concentration of slow neutrons available for experiments at HFIR may have exceeded the cold neutron record established by the Institut Laue Langevin research reactor in Grenoble, France.

Lee Robertson, who leads the instrument development group and conducted the time-of-flight experiments designed to determine the brightness of the new cold source, said he and his colleagues measured a peak brightness exceeding ten trillion neutrons per unit solid angle per square centimeter per angstrom per second (the units in which source brightness is measured). Uncertainty about whether HFIR equaled or surpassed ILL's record stems from the lack of sufficiently detailed data on the brightness of other cold sources.

Recent experiments already performed on the two new world-class, small-angle neutron scattering instruments at HFIR range from experiments examining the nature of radiation damage in materials to studies of the structure of complex polymeric materials formed from branched chains (including "comb" structures that have long linear chemical chains with short attached side chains).

Before the recent upgrade, HFIR lacked the cold neutrons that have been available for years at other neutron scattering facilities. Cold neutrons are slower and have a longer wavelength than HFIR's thermal neutrons. Now that HFIR has a "cold source," which contains liquid hydrogen for slowing down the medium-fast thermal neutrons after they are reflected by the beryllium reflector surrounding the reactor core, experimenters can obtain more detailed information on biological and organic materials, such as proteins and polymers.

Meanwhile, the Spallation Neutron Source surpassed the world record for beam power for an accelerator-based source of neutrons. The SNS operated at 183 kilowatts last August; the previous record of 160 kw for beam power was held by the United Kingdom's ISIS facility. Although a world record, the beam power has reached only about 10% of ultimate capability at the SNS.

ORNL to Help Auto Industry

ORNL will lend a hand to the U.S. auto industry by supplying research and development work initiated through the U.S. Automotive Partnership for Advancing Research and Technologies, or USAutoPARTs, collaborative. The new R&D role was announced Jan. 17, 2008, at the North American International Auto Show in Detroit.

Made up of a consortium of federal, state and private partners, USAutoPARTs will perform pre-competitive, collaborative research to advance cost-effective emerging technologies and ultimately speed the commercialization of automotive technologies. Initially, research consortia will focus on advanced lightweight materials, electrical and electronic thermal management, and engine combustion and emission after-treatment. Signing a memorandum of intent to participate in the alliance were Michigan Governor Jennifer Granholm, Department of Energy Under Secretary Clarence Albright, and Neil De Koker, president and CEO of the Original Equipment Suppliers Association, or OESA. USAutoPARTs will be located in Shelby Township, Michigan, in a 56,000 square foot comprehensive vehicle R&D center with established laboratory infrastructure that will support up to 175 persons. The facility was previously occupied by the Delphi Corporation.

Through USAutoPARTs, automotive suppliers can take advantage of the unique expertise of the national laboratory system to aid them in developing technologies and components for America¹s next generation of automobiles in a cost-effective manner. Oak Ridge National Laboratory has some of the world's leading facilities for materials research and computational modeling, and is internationally recognized for its research in vehicle technologies.

Southern Solution

Demonstrating an energy future in our backyard

When the federal government built Oak Ridge National Laboratory as part of the Manhattan Project in 1943, the facility—established to demonstrate that plutonium can be separated from a reactor, which led to one of the nation's first nuclear weapons—was hidden in the hills of East Tennessee precisely so no one could uncover the top-secret operation. Even after the end of World War II, when the government's quiet project came to light, ORNL scientists often seemed to fit more comfortably in national and international venues or the halls of Washington, D.C., than in their rural southern backyard.

The past half-century, however, has brought sweeping economic changes to the South, attracting modern industry, new populations of transplants from the North and Midwest and unprecedented growth that is not expected to abate in coming decades. Changes have come to ORNL as well. In recent years, the Laboratory has been establishing partnerships with universities, economic developers and industries throughout the Southeast in an effort to raise the profile of the region as a center for research and development. As a result, ORNL is uniquely positioned to demonstrate future innovation of benefit to the nation—and the world—through collaborations closer to home.

At the forefront of these efforts is energy. The increase in energy demand, primarily a result of global population growth and the expansion of manufacturing into the developing world, is placing pressure on natural resources central to energy production. Simultaneously, environmental concerns and in particular greenhouse emissions are demanding reconsideration of fossil fuel combustion. Finally, global geopolitical instability is sending ripples throughout energy markets, causing policy action in many countries. For example, petroleum underpins global transportation, but cost and geopolitical instabilities in the Middle East have brought the hunt for new transportation fuels closer to home. Energy supply uncertainty, together with imperatives for environmental and national security, necessitates pursuing ways to do more with less and tap power sources that are locally available, renewable, and sustainable—i.e., the regional use of wind, sun or crops that can be transformed into electricity or transportation fuel. Nuclear power is poised for resurgence, and renewed interest in energy efficiency, particularly in buildings applications, has already begun to add value.

"The South offers an ideal testbed for demonstrating the economic potential for all of these energy production approaches," says Dana Christensen, ORNL associate laboratory director for energy and engineering. "Whether it be power generation, transportation, distribution or efficiency in energy use, including capitalizing on renewable energy sources, we have expertise across a broad spectrum of disciplines to address the problem, from basic research to commercial application."

The Laboratory is already hard at work. In May 2007, ORNL and seven southern universities announced creation of the Automotive Research Alliance in an effort to provide expertise to the South's 10 automotive assembly plants and more than 3,000 suppliers. With political and economic pressure to create lighter weight, more efficient vehicles, alliance organizers believe automakers will be eager to tap

into these local R&D resources, particularly if they are cost effective.

In June 2007, the Department of Energy awarded a $135 million bioenergy research center to a team led by ORNL, which includes such southern partners as the University of Tennessee, Georgia Tech, the University of Georgia, North Carolina State and the Samuel Roberts Noble Foundation in Oklahoma. In conjunction with the award, the state of Tennessee announced it would pump $70 million into a cellulose-based transportation fuels demonstration. The award has also spawned an effort known as the Bioenergy Alliance, drawing on the expertise of additional research institutions throughout the region and using the regional expertise of the Southern Growth Policies Board to generate even more bioenergy-related funding and research.

In October, the first annual Southeast Solar Summit was held at ORNL, attracting a capacity crowd of southern companies, researchers and decision makers interested in developing the nascent solar technology market. Plans are under way to capitalize on the intense interest in developing a solar demonstration project, tuned to southern applications.

A retirement community now under development in Crossville, Tenn., plans to rely on energy efficiency expertise at ORNL, expanding on a local near-zero-energy Habitat for Humanity housing development in Lenoir City, Tenn., by developing a "deep-green" community of 7,000 to 10,000 homes for retiring baby boomers seeking sustainable lifestyles. As the demand for green, energy-efficient buildings and products explodes across the country, ORNL is engaged in talks to partner with other regional developers as well for both residential and commercial projects.

ORNL is working with the Tennessee Valley Authority, the major power provider for seven southeastern states, on a number of fronts. Leaders at ORNL and TVA are partnering on technologies supporting nuclear fuel reprocessing, clean technologies for fossil fuel plants and energy efficiency that can help the federally owned corporation meet a demand that is expected to grow exponentially in the coming years. This revolutionary partnership combines the skills of a major electricity provider and economic development agency with the R&D resources of a major national energy laboratory to establish energy sustainability in our local economy.

Christensen envisions many more such partnerships with industry, universities, communities and other national laboratories.

"As a national laboratory, we must push the scientific and engineering boundaries toward finding cost-effective solutions to national and international challenges," he says. "Everyone, from federal laboratories to states to the private sector, must come together to solve the energy problem. No one energy technology can do it all; we need them all but only if each technology can be deployed in a safe and sustainable fashion. Only then will taxpayers truly receive a return on their investment."—*Larisa Brass*

"The South offers an ideal testbed for demonstrating the economic potential for all of these energy production approaches"

The Missing Piece

ORNL seeks to close the nuclear fuel cycle.

Two facts shape much of the discussion regarding America's nuclear power industry. First, increasing anxiety about the growing volume of greenhouse gas emissions from coal-fired power plants has made nuclear power a more palatable option for many policymakers. Second, if nuclear power is to occupy a larger portion of our future energy inventory, new technologies will be required to address increased amounts of spent nuclear fuel generated by additional reactors and reduce proliferation risks.

With these considerations in mind, in September 2007 U.S. Secretary of Energy Samuel Bodman and senior officials from 16 nations agreed to enhance international nuclear energy cooperation through the Global Nuclear Energy Partnership. The partnership's overreaching goal is to meet worldwide demands for more electricity while avoiding climate-altering carbon dioxide emissions and nuclear weapon proliferation.

Two major objectives of the GNEP concept encourage the safe expansion of nuclear power. One objective is the development of "grid-appropriate reactors" for use in developing nations whose electric grids cannot accommodate large, gigawatt nuclear plants. The other is the development of advanced spent-fuel recycling technologies that provide a reliable fuel source for fuel-supplier nations as well as all countries that operate power reactors. ORNL has leading roles within GNEP in both arenas.

Underscoring GNEP's international aspect, the deployment of new grid-appropriate reactors will require multinational partnerships that will develop new reactor technologies and designs to improve safety and reduce the risk that spent fuel will be used to make nuclear weapons. In addition to the technological and security challenges of nuclear power, GNEP will address the more fundamental issues of providing workforce and management infrastructures in a number of developing countries. Sherrell Greene, director of ORNL's Nuclear Technology Programs, says that ORNL has established relationships with several other DOE laboratories and a number of countries.

The Department of Energy's proposed permanent repository at Nevada's Yucca Mountain site for spent nuclear fuel from America's existing 104 reactors will have insufficient capacity to meet the needs of an expanded nuclear power industry. The two-part alternative to building additional repositories would involve processing the spent fuel to separate the components. A large fraction of the reprocessed fuel would be reused in other reactors. The remaining materials would be treated to reduce their radioactive toxicity and repository decay heat load.

Estimates indicate that the volume of waste sent to Yucca Mountain can be dramatically reduced, potentially allowing Yucca Mountain to meet U.S. repository needs throughout the 21st century.

Several studies have demonstrated that most of the spent fuel components can be recovered and recycled. Uranium represents about two-thirds of the U.S. spent fuel inventory, including residual fissile uranium-235 that can be recycled directly as fuel for heavy-water reactors or enriched again for use as fuel in light-water reactors. The next largest component—roughly one-quarter of the total volume—is the zircaloy cladding. ORNL is working with an industrial consortium to explore recovery of zirconium from the cladding for reuse.

About 1% of spent fuel consists of plutonium and minor actinides. The radioactive toxicity of the disposed wastes sent to Yucca Mountain can be reduced significantly by transmuting long-lived, highly radioactive actinides, such as plutonium, into isotopes that would not require disposal in a geological repository. This task can be accomplished by separating the elements from the reprocessed fuel stream, fabricating them into new "transmutation fuels" (containing uranium, plutonium, neptunium, americium and curium), or separate "mixed-oxide fuels" (containing uranium, plutonium and neptunium) and "transmutation targets" (containing only americium and curium). Neptunium is coupled with plutonium primarily to enable neptunium recycle, but also to contribute a safeguards benefit. Protactinium-233, the decay product of neptunium, emits an easily detected gamma ray that could impede attempts to smuggle plutonium from a nuclear facility. These fuels and targets would then be re-irradiated in commercial reactors to accomplish the transmutation mission.

Fission products represent only about 4% of the spent fuel components. GNEP seeks to recover and immobilize long-lived iodine-129 and technetium-99 and explore possible recovery and reuse of xenon and platinum-group metals. ORNL researchers are developing new storage and disposal approaches for the remaining intermediate-half-life materials, such as tritium, krypton-85, strontium-90 and cesium-137.

A variety of options includes relying upon a protocol of processing fuel only after the fuel has "aged" for a few decades to allow time for decay of much of the short-lived fission product inventory. Commercial-scale facilities to accomplish these specialized recycle separations and fuel fabrication processes are still in the planning stage, although several of the key processes have been demonstrated at the laboratory scale.

"Previous advanced fuel-cycle R&D has been limited to a single portion of the overall process," says Jeff Binder, who leads the Coupled End-to-End (CETE) Demonstration to tie together all the process steps in support of GNEP. "ORNL's pilot project is a logical step toward creating a viable industrial-scale process, allowing us to identify any problems that could arise from linking together the individual process steps."

The CETE process originates at ORNL's Irradiated Fuels Examination Laboratory. There, commercial light-water reactor fuel rods are chopped into 1.5-inch segments. The fuel segments are heated in oxygen, which the uranium dioxide ceramic pellets bind with as they crumble into U_3O_8 powder. This "voloxidation" process drives off the fuel's volatile fission products, such as tritium, preventing contamination of the subsequent processing system.

The fuel powders are packaged and transported to the Laboratory's Radiochemical Engineering Development Center, where the powders are easily dissolved in nitric acid and the separations processes are tested using existing "mixer settler" contactors to perform several sequential solvent extraction steps. The initial step uses tri-butyl phosphate to perform one of the newly developed UREX+ uranium extraction processes. TRUEX and TALSPEAK processes are then used to separate americium and curium from the chemically similar lanthanide fission products. By changing the flow rate, acidity level, temperature and number of contactor stages, process performance can be optimized to produce the desired products.

Hot cells at the Radiochemical Engineering Development Center.

"In the first CETE campaign, spent fuel from the Dresden-1 Boiling Water reactor in Illinois was processed, and we produced a uranium stream, a uranium-plutonium-neptunium stream, an americium and curium stream and a fission product stream," Binder says. All these streams containing nitric acid will be turned into a solid to enable production of a fuel, target or waste form.

The CETE team uses a process developed at ORNL, called modified direct denitration, to drive out the nitric acid and convert the uranium and uranium-plutonium-neptunium products to an oxide powder that can be pressed and sintered into a high-density recycle fuel for irradiation in a reactor. Researchers perform analytical work using X-ray diffraction and a variety of other measurements to determine whether the chemistry of the powders will allow the particles to be compressed and heated to form high-quality fuel pellets. The goal is to process in one year 10 fuel pins, or 20 kilograms of heavy metal content of spent fuel.

Greene says the Department of Energy has engaged the commercial nuclear industry—General Electric, AREVA and General Atomics—and nuclear utilities such as the Tennessee Valley Authority to support development of spent-fuel recycle technologies and "advanced recycling reactors" that could produce electricity while transmuting the recycled actinides to less troublesome isotopes. "It's a multidecade program requiring a sustained effort," says Greene.

Developing technologies that can recycle spent fuel and greatly reduce the volume of nuclear waste requiring permanent disposal is among the most important scientific challenges facing a nation seeking long-term energy solutions. With a rich history of innovative nuclear reprocessing technologies and an array of unique capabilities, ORNL will continue to play a critical role in solving these challenges.—*Carolyn Krause*

Contact: greenesr@ornl.gov

A Different PATH

A talented team undertakes a novel strategy to developing

Oak Ridge National Laboratory microbiologist Tommy Phelps sees the untapped potential of bioenergy in shelves of bottles and beakers containing microscopic organisms that just might hold the elusive bug or enzyme capable of digesting large quantities of plant matter into ethanol.

Phelps's current batch of microbes, stockpiled in dozens of bottles of silt, rocks and soils, was collected from Yellowstone National Park, where the hot springs that draw millions of summertime visitors also nurture microscopic life in their boiling waters. These bugs, in turn, beckon microbiologists like Phelps, who seek a solution to transform Earth's abundant cellulosic sources into a modern energy supply. Yellowstone's warm waters offer the promise of microbes that can rapidly and efficiently degrade cellulose—the woody, leafy matter that makes up plants. Scientists hope to tap the power of these microbes for industrial-scale consolidated bioprocessing of plants, including trees and switchgrass, the species central to the BioEnergy Science Center's research efforts.

The hunt for this cellulosic "super bug" is part of a suite of efforts under way at the BioEnergy Science Center, headquartered at ORNL. Since being named one of three $135 million Department of Energy bioenergy research centers, researchers at ORNL and its partner institutions have quickly gotten to work. DOE's ambitious goal is to replace by 2030 one-third of the nation's transportation fuel with cellulose-based sources. At these centers, researchers are carrying out the targeted, fundamental science needed to bridge the gap between the potential of cellulose-based fuels and their reality.

In addition to ORNL, BioEnergy Science Center partners include the University of Tennessee, the University of Georgia, Georgia Tech, Dartmouth College, the National Renewable Energy Laboratory, ArborGen, Verenium Corp., Mascoma Corp. and the Samuel Roberts Noble Foundation, as well as individual scientists from other institutions.

"To develop what we call a consolidated bioprocess for cellulosic ethanol production, we are hoping to reduce the steps required to break down plant matter into sugars and ferment them into ethanol," says Martin Keller, the center's director. "By tapping nature, we hope to replace the current, and expensive, chemical processes with a microbe, enzyme or combination that consolidates multiple steps into one. That is the best path to economical, efficient bioethanol production."

Thus, October found Phelps and Keller on the hunt for microbes, a journey that will likely take them to various corners of the globe—through the center's partnership with Verenium—as well as locales closer to home in search of the best plant-processors that nature has to offer. Once collected, these microbes will be exposed to samples of poplar and switchgrass to test their ability to digest the cellulose. Then the most promising bugs will be put through a further gamut of tests to break down and map out their molecular function.

Current microbes and enzymes are relatively slow at attacking plant matter's complicated and protective structure. Researchers will determine precisely the genes involved in the interaction of the microbes and enzymes to break apart cellulose. Other genes responsible for producing undesirable products, such as acetic acids, will be knocked out in the hope of, ultimately, developing the perfect ethanol-manufacturing microbe. Particular enzymes will be isolated as well and genetically analyzed, with a focus on determining the ideal formula of enzyme or microbe and enzyme to serve as the vehicle for cellulosic ethanol production.

Microbes, however, are just a piece of the puzzle. Other researchers at the Oak Ridge center are going through similar steps to develop plants with qualities most conducive to processing into biofuel. Similar to the microbial work, researchers will analyze thousands of genetically modified switchgrass and poplar tree samples in order to discover and develop

alternative fuels

Researchers hike Yellowstone National Park, left, on the hunt for microbes that could potentially be used in bioenergy production. They analyze the samples back home in the lab.

the best varieties for ethanol production. As part of the process, the biofeedstock, together with the microbes and the enzymes, will be joined in a complex matrix of analysis and R&D in order to develop the best biofuel recipe.

On the biomass formation side, the partners will produce samples of plant material genetically altered to modify their cell walls for optimum breakdown into usable sugars. Such altered species might feature lower amounts of lignin—the substance that holds cellulose fibers together—or a reduction in the crystallinity of the cellulose. ArborGen and ORNL will be primarily responsible for creating and studying various altered trees, while scientists from the University of Tennessee, the University of Georgia and the Noble Foundation will take the lead in switchgrass research.

To find rapidly the most important effects and genes, researchers must screen thousands of samples for recalcitrance, says Brian Davison, the BioEnergy Science Center's lead scientist for characterization and modeling. "This task requires us to create a tiered, high-throughput characterization pipeline that reflects the complicated nature of plant recalcitrance, the resistance to breakdown into sugars. The screening must be realistic but practical because we can make improvements in the plants only if we are able to precisely measure their resistance—or lack of resistance—to processing. In other words, you get what you screen for."

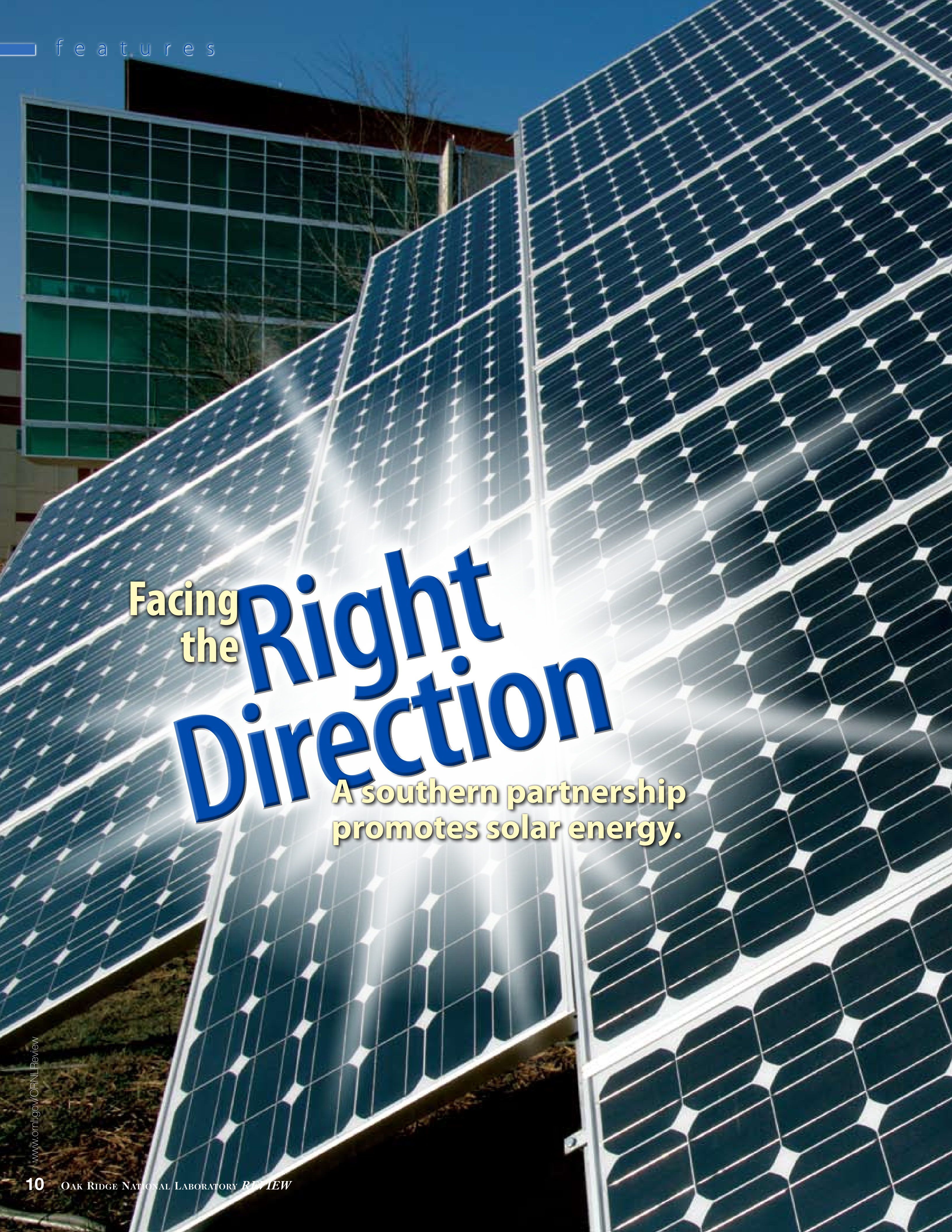
The samples will be delivered to the National Renewable Energy Laboratory, which will serve as a clearinghouse for cataloging, classification and detailed analysis. Assigned individual bar codes, the samples eventually will make the rounds of various institutions and be divided into separate samples—one ground for air drying, one to image, one shredded for pre-treatment and one frozen in its original state.

All samples will then undergo composition analysis, using state-of-the-art techniques such as analytical pyrolysis mass spectrometry or near infrared spectroscopy, to determine how much cellulose versus lignin is present. Next is a pretreatment with dilute acid to replicate the best current processing method developed by the University of California, Riverside. Following the pre-treatment the samples will be chemically assayed again to determine their response to the treatment. Finally, samples will undergo an enzyme digestion assay, which will test for reducing sugar release. This sugar release, along with the preceding measurements, will give researchers a pool of data on recalcitrance and enable subsequent studies to focus on the best samples and the genetic changes that lead to them.

Besides more detailed analytical examination with electron microscopy, nuclear magnetic resonance spectroscopy, microCAT scanning and new tools under development, samples that show promise in these tests will be exposed to experimental enzymes and microbes such as those discovered in Yellowstone—which will have undergone a similar rigorous genetic and systems biology analysis—to determine the ones that work best together. Meanwhile, the enormous volume of results from the thousands of biomass, microbe and enzyme samples scooting through the system will be fed into large databases maintained by the various partners and housed primarily at ORNL's Center for Computational Sciences. To make sense of these vast databases, frequent personal communication among the partners is critical. By the end of the 2007, team members had spent more than 40 days in face-to-face meetings to plan a truly cohesive research effort.

"We are developing a process that is standardized in order to methodically find and develop the plants, microbes and enzymes that will work the best while ruling out the ineffective ones," Keller says. Summing up the center's opportunity and challenge, Keller adds, "This is the first time anyone has taken this kind of systematic approach to the bioenergy problem."—*L.B.*

Contact: davisonbh@ornl.gov



Facing the Right Direction

A southern partnership promotes solar energy.

Solar array located on ORNL campus.

Facing the sun and located in the courtyard of Oak Ridge National Laboratory's new east campus, a gleaming symbol of ORNL's commitment to renewable energy is slowing down the Laboratory's electric meter. The attractive array of solar cells purchased from Arizona Public Services injects electrical power into the local distribution system, subtracting around 9000 kilowatt hours from ORNL's annual electric bill.

The device was dedicated Oct. 24, 2007, at the opening of the first Southeast Solar Summit, held at ORNL's new conference center. Sharp Electronics Corp. of Memphis, Tenn., manufactured the photovoltaic modules in the array.

On the roof of the largest research building along the courtyard perches a 700-watt solar system designed by JX Crystals. The combination of concentrating solar modules and a turntable tracker makes the photovoltaic system more efficient and less costly than conventional systems. In each module 24 reflectors focus sunlight onto 72 single-crystal silicon solar cells. The four 175-watt modules concentrate sunlight up to three times its normal strength, reducing by two-thirds the number of expensive silicon cells required to produce the same amount of electricity.

An inexpensive solar tracker keeps the modules facing the sun throughout the day, theoretically increasing the energy output as much as 35% in some regions. ORNL purchased and installed the system in September 2007. Data from the electrical performance and efficiency tests were jointly presented by ORNL's Curt Maxey and JX Crystals at a recent international conference in Germany.

The rooms at the top of a nearby four-story research building are illuminated by hybrid solar lighting. In this technology pioneered by ORNL, sunlight is piped into rooms through optical fibers, and intelligent sensors adjust artificial light levels needed by occupants during cloudy days. Sunlight Direct of Oak Ridge is commercializing this technology, which has entered the demonstration phase with installed systems at locations owned by Wal-Mart, Staples, Battelle and San Diego State University.

ORNL materials researchers using the plasma arc lamp hope to demonstrate elimination of defects from multicrystalline and amorphous silicon thin-film solar cells, which are less efficient than single-crystal solar cells but less expensive to make. Measurements of these processed materials will be made at the new Center for Advanced Thin-film Solar Cells. (See article on p. 25.)

The Department of Energy, not surprisingly, is a major driver behind ORNL's expanded research in solar energy. Craig Cornelius, acting program manager of Solar Energy Technologies in DOE's Office of Energy Efficiency and Renewable Energy, has indicated that greater funding for research to make solar materials more efficient and less expensive will be available to national laboratories.

Indeed, the fiscal-year 2008 budget recently enacted by Congress contained one of the largest funding increases in history for alternative energy research. ORNL, which boasts one of the world's leading materials research capabilities, proposes innovative basic technology research to help meet DOE solar materials challenges.

The Department of Energy has mandated that by 2013 7.5% of all energy used at national laboratories must be produced from renewable energy. ORNL plans to install more photovoltaic panels, perhaps as solar walkways and solar roofs over parking lots, and possibly biomass-fired boilers, to help achieve that goal.

Cornelius, who leads the Solar America Initiative as part of the President's Advanced Energy Initiative, has stated that DOE's goal is to make solar energy cost-competitive with conventional forms of electricity by 2015. DOE predicts that by 2015, solar energy will produce 15 gigawatts, enough to power 11.2 million American homes.

"Adding solar energy to our nation's energy mix will increase America's energy security by providing decentralized sources of clean power for the electric grid," he said. "Solar power will improve the environment by avoiding 191,000 tons per year of carbon dioxide emissions and boost the economy by promoting a U.S.-based solar industry."

The Tennessee Valley Authority is also pushing solar energy. Through a collaboration with ORNL, TVA recognizes that wide deployment of solar energy could help solve the peak power problem that threatens the grid's capacity during the hottest days of summer. In his talk at the summit, ORNL's Jeff Christian reported that, on the hottest day of 2007 in East Tennessee, he actually took a near-zero-energy house in nearby Lenoir City off the TVA grid. Meanwhile, the residents remained comfortable in the house with rooftop solar panels and energy storage in the basement. His experiment suggested that peak demand—and the expensive capacity needed to meet that demand—can be reduced if enough solar zero-energy households could do without grid power between 5 and 7 p.m. daily in summer when demand for power for air conditioning normally soars.

One challenge is to convince American consumers to purchase and install solar technologies. A recent survey of 500 individuals indicated that consumers tend to associate "green" with "more expensive" and are skeptical about corporations that they suspect are more interested in selling products than solving environmental problems. Tennessee Governor Phil Bredesen has encouraged the growth of a solar energy industry in the state through clean energy grants. For the time being, the relatively low cost of TVA electricity is a disincentive for homeowners to make the transition to solar technology.

Germany is the fastest growing market for photovoltaic cells because the government pays a premium price for electricity from solar panels. In the Southeast, the average amount of sunlight available for producing electricity is twice that available in Germany.

Back in Business with Water Power

After several years without funding, the Department of Energy's hydropower research program has been revived by Congress for 2008. The new "water power" program includes research on both conventional hydropower technologies and new ocean and instream hydrokinetic technologies. ORNL is the lead laboratory for the hydropower side of this new program. Total funding for the first year is $10 million, a large portion of which will come to ORNL.

ORNL's work will include technology development, demonstration and deployment, resource assessment, environmental studies, siting issues, strategic planning and analysis.

Hydropower provides more than 70% of the renewable electricity in the U.S., but that share has been declining in recent years as other renewables have been growing. The goal of the new DOE Water Power Program is to double generation to more than 500 terawatt hours per year by 2030, which would ensure that hydropower maintains an important place in the nation's renewable energy portfolio.

—L.B. ***Contact: smithbt@ornl.gov***

To boost U.S. solar capacity (which is responsible for one-eighth of 1% of U.S. electricity generation), other barriers must be overcome in addition to increasing efficiency and reducing cost. At the summit, attendees noted the need for a national net metering standard, more certified installers of solar panels and ways to dissipate the heat generated by concentration of sunlight on roof-mounted panels.

Many baby boomers about to retire have expressed strong interest in moving to "Deep Green" communities. One such planned community is Walden Reserve, which will be located on 6,000 acres of heavily forested ridges between Black Mountain State Park and Ozone Falls State Park, only 40 miles from Oak Ridge. Because houses will be surrounded with trees, the roofs will not have solar panels. However, a photovoltaic system is planned for an open field to help provide electricity to the self-contained community, which will have its own energy sources, water supplies and sewer system.

Walden Reserve is envisioned eventually to accommodate 20,000 residents and provide them with restaurants, a golf course, a spa, greenways for hiking and biking and other community amenities. The development of Walden Reserve is guided by 12 "bedrock principles" to ensure environmental responsibility. Developers hope the community will act as a testbed for "green" products and services.

"Projections call for more new home and building construction in the Southeast than in any other region," says Patrick Hughes, manager of ORNL's Building Technologies Program. "Our region has the opportunity to lead because volume begets affordability. Imagine if Walden Reserve succeeds in developing an entire all-electric community that contributes zero to TVA's peak period loads."

Hughes said one outcome of the summit was the recognition of the importance of policy and leadership. Germany leads the world as a market for solar cells for these reasons, even with a solar resource eclipsed by Tennessee's.

"The most exciting outcome of the summit for me was the evidence of some emerging leadership," he continues. "With the leadership from DOE, the state of Tennessee and TVA, people in this region can create remarkable communities of ultrahigh-efficiency, demand-responsive buildings powered in large part by solar and other forms of renewable energy."

Facing the sun may be the first step in the right direction.—*C.K.*

Contact: lapsamv@ornl.gov

Curt Maxey with concentrating solar modules.

GIVING BACK

Plug-in hybrid electric vehicles may have an unexpected value.

One car of tomorrow may not only get its energy from the grid but also may give "imaginary power" back to the grid. The plug-in hybrid electric vehicle envisioned by the Department of Energy would be plugged at night into a home wall outlet, connecting the car to a local electrical distribution system that would recharge the battery. The next day the car would travel using a combination of stored electric energy and fuel. According to a vision of Oak Ridge National Laboratory researchers, the car's charger would supply the grid with "reactive power," or non-active power, to help regulate local utility voltage.

To convert the alternating current from the local electrical distribution system to the direct current needed by the car's battery, a rectifier, or charger, is required. Conversely, an inverter is needed to convert direct current to alternating current. The car would use alternating current to power the drive motor. The rectifier, or charger, could be located either in the car or at facilities designed specifically to recharge batteries of plug-in hybrid electric vehicles parked for extended periods at, say, apartment complexes, hotels and parking garages.

Inverters have several uses, including the ability to inject reactive power to the grid or absorb this imaginary power from the grid. This helps regulate the voltage on distribution and transmission systems. Inverters can prevent "micro-voltage collapses" that frequently occur in the western United States. Such sudden voltage dips can cause dimming of lights, computer crashes, damage to equipment and destruction of semiconductor wafers during manufacture.

DOE researchers are working with the U.S. automobile industry to optimize plug-in hybrid engine, motor and battery performance for efficient vehicle operation. ORNL and University of Tennessee power electronics experts at the National Transportation Research Center are seeking to improve inverter design to make the device smaller, lighter and less expensive. ORNL is a member of the Plug-in Hybrid Development Consortium.

DOE also supports research on one way to reduce peak demands on the electric grid: deploy distributed energy resources—microturbines, fuel cells and photovoltaic panels—to provide electricity to both local buildings and the electric grid. The plug-in hybrid could be considered another distributed energy resource, but one that also stores energy.

One group of ORNL researchers is studying the effect of plug-in hybrid electric vehicles on the electric grid. Another group is examining ways to make inverters and chargers smarter so they can help distributed energy resources provide voltage regulation as well as electricity to the grid.

ORNL researchers led by Stan Hadley have found that the U.S. electric grid will operate more efficiently as more Americans charge the batteries in their plug-in hybrid vehicles after 10 p.m., when the electric load on the system has dropped to almost zero and the wholesale price for energy is least expensive. The researchers have analyzed the potential impacts of plug-in hybrid electric vehicles on electricity demand, supply, generation structure, prices and associated emission levels in 2020 and 2030 in 13 regions as specified by the North American Electric Reliability Council and DOE's Energy Information Administration.

Their study assumed that by 2020 a mixture of sedans and SUV plug-in hybrids would make up one-quarter of the cars sold. They performed calculations using the Oak Ridge Competitive Electricity Dispatch model, which was developed at ORNL over the past 12 years to evaluate a wide variety of critical electricity sector issues.

The ORNL researchers ran seven scenarios for each region for 2020 and 2030. In each scenario they assumed these vehicles plugged in starting at either 5 p.m. (early evening) or at 10 p.m. (nighttime) and remained until fully charged.

"We concluded that most regions must build additional electrical generating capacity or rely on demand response to meet the added demands from plug-in hybrid electric vehicles in the early evening charging scenarios," Hadley says. "This need will be critical by 2030 when plug-in hybrids will likely have a larger share of the installed vehicle base and thus exert a greater demand on the electrical system."

Accommodating the peaks and valleys of electricity use is a major challenge for generators and transmission operators. Ideally, customers would reduce their consumption of electricity at peak load times in response to market prices or a utility's request. During hot summers, the demand for air conditioning between 2 and 6 p.m. can boost the peak load to the point that a utility must purchase power from another utility at a higher price. In sharp contrast, the grid on the same night may be so underutilized that energy is sometimes given away.

Nighttime battery charging would greatly benefit generation and distribution companies, who normally see their facilities used efficiently for only a few hours each day. Local distribution grids would see a significant change in their electricity usage patterns. For example, early evening charging would probably use a higher proportion of natural gas to coal than nighttime charging, with consequent effects on carbon dioxide and other emissions.

Limits have been placed nationally on nitrogen oxide emissions by power plants, but NOx caps do not exist for gasoline cars. Instead, each vehicle has a regulated emission rate per mile; more vehicles or more miles mean more emissions. The benefits of widespread usage of plug-in hybrids thus include reduced dependence on foreign oil and cleaner air.

Another potential advantage of wide usage of plug-in hybrids is that charging stations can help regulate local voltage. Researchers at ORNL's Distributed Energy Communications and Control laboratory plan to test this concept. Under Tom King's direction, John Kueck, Tom Rizy and Fran Li have been experimenting with a control system for an inverter and testing how well a smart inverter or rectifier can regulate voltage to improve power quality.

"Our goal is to show that distributed energy resources such as fuel cells, microturbines and arrays of solar cells can support the electric distribution system," Kueck says. "Our approach is a little different from the conventional electrical industry, which is calling for a massive retrofit of the communication and control system.

"We think distributed energy resources can be controlled by local, independent, autonomous, adaptable controllers that function independently without causing problems to the others. Local voltage regulation from a fuel cell or microturbine is much cheaper and simpler than a massive, hierarchical control system. The local control would still, however, be under utility supervision."

"Our goal is to show that distributed energy resources such as fuel cells, microturbines and arrays of solar cells can support the electric distribution system."

"We propose modifying the charger to control the local voltage as a service to the electrical system," Rizy says. "With this approach, utilities would not have to worry about voltages going too high or too low when numerous fuel cells, microturbines and photovoltaic arrays are connected to their distribution systems. The individual energy resource would control the voltage itself locally."

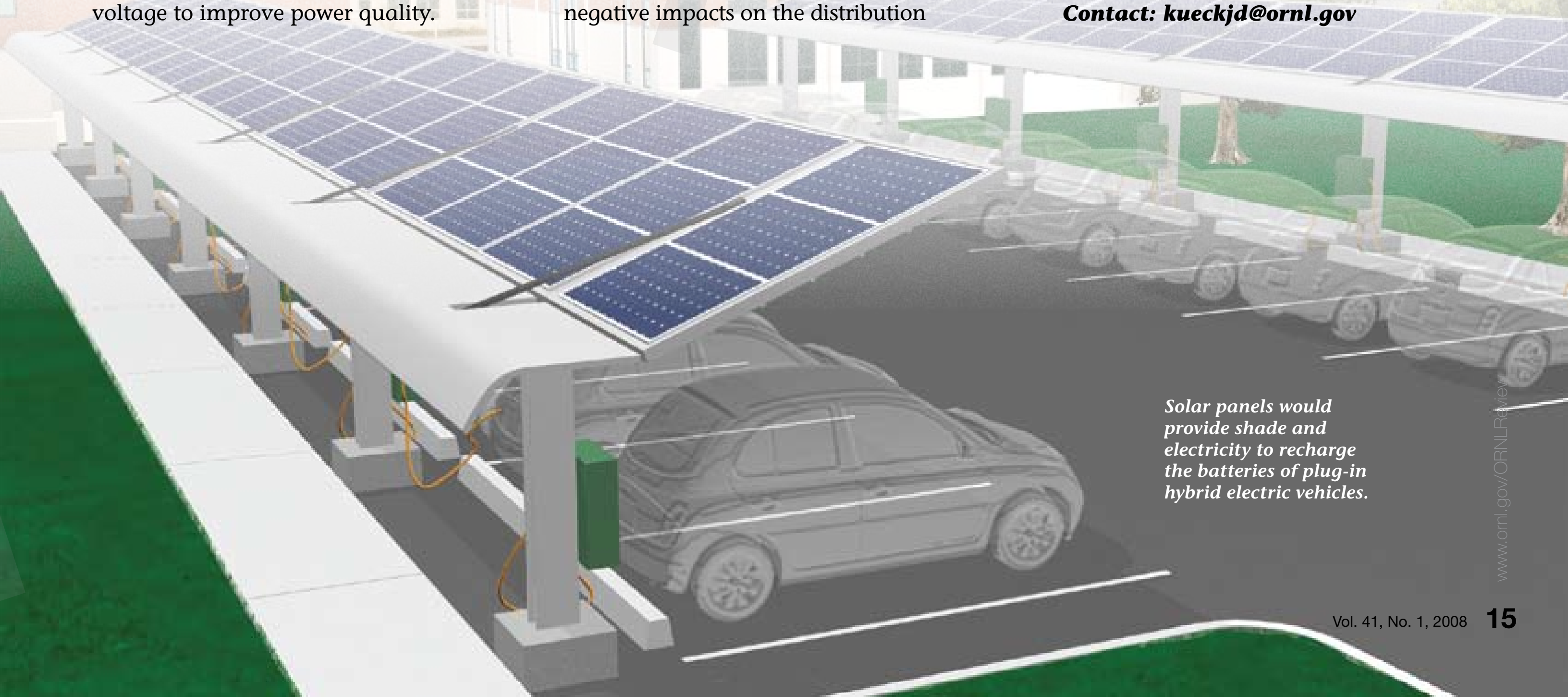
Smart chargers are needed to avoid negative impacts on the distribution system. For example, if several plug-in hybrid pickup trucks with 250-kilowatt batteries were recharged in 10 minutes on a feeder without a smart charger, the distribution system's reliability could be threatened. In one project, ORNL's Burak Ozpenici is examining possible rectifier designs that would perform rapid charging while providing reactive power compensation.

Yan Xu, a postdoctoral researcher at UT, is devising intelligent controls to enable the inverter or distributed energy resource to inject dynamic reactive power into the ORNL distribution system to regulate the local voltage. She has developed a definition of non-active power that facilitates real-time control.

In 2008 Kueck and Rizy will be testing ORNL's intelligent inverters with multiple distributed energy resources connected to a Southern California Edison distribution circuit. Both anticipate that grid-related tests down the road will involve plug-in hybrid electrical cars.

For years electric cars have been an impractical fantasy. This persistent image is giving way to the reality that, with support from the electric grid, they will be an integral part of America's automobile future that can also give back to the grid.—*C.K.*

Contact: kueckjd@ornl.gov



Solar panels would provide shade and electricity to recharge the batteries of plug-in hybrid electric vehicles.

Southern Teamwork

A new research partnership supports the South's automotive industry.

The group was an auspicious one. Congressional representatives from Tennessee, South Carolina and Alabama. Senior management from national laboratories at Oak Ridge and Savannah River as well as the University of Tennessee, Clemson University and BMW. They gathered on a makeshift platform in the Clemson International Center for Automotive Research, a symbol of the South's emergence over the last two decades as a powerhouse in automotive manufacturing. The event, part of the Tennessee Valley Corridor Southeast Partnership, was designed to bring together the region's collective transportation research talent to focus on ways to support continued growth of the automotive industry.

The gathering was symbolic of a growing realization that in matters of economic development, the South has learned the importance of teamwork. In the case of transportation, this regional teamwork has resulted in the cooperation of lawmakers, business leaders and research institutions on a broad array of initiatives, from creating new fuels to helping the world's auto manufacturers build lighter, stronger, more energy-efficient cars and trucks. As Peter Brown, associate publisher and editorial director at *Automotive News*, expressed in a keynote luncheon address to the group of business and government leaders gathered for the Tennessee Valley Corridor event earlier that day, "It is extraordinary coming from the North to see this level of cooperation."

Oak Ridge National Laboratory for years has been the leader in transportation research for the Department of Energy's energy efficiency programs. More recently, the Laboratory has sought to connect to the growing automotive presence in the Southeast. The region is now home to 3,000 automotive suppliers and 10 major automotive assembly plants including Toyota in Kentucky and Mississippi; BMW in South Carolina; Ford in Georgia; Mercedes, Hyundai and Honda in Alabama, as well as Saturn and Nissan—which recently relocated U.S. headquarters to Nashville—in Tennessee.

Surrounding these plants is a set of universities that, along with ORNL, represent extensive expertise in supply chain management, sustainable manufacturing, heavy vehicle research, power electronics, engines and high-performance materials. In 2007, ORNL and the University of Tennessee, along with six southern research universities, announced the Automotive Research Alliance, a regional effort to provide southern automakers access to unique research capabilities.

"We are looking for opportunities to increase and advance automotive research and development in the Southeast and ultimately in the nation," says Ben Ritchey, vice president of the Transportation Marketing Sector at Battelle Memorial Institute in Columbus, Ohio. Ritchey also serves as acting chief executive officer and president of the National Transportation Research Center Inc., the business developer for ORNL, UT and the other Automotive Research Alliance members.

Ritchey says the Alliance has multiple goals. "We want to motivate the development of new academic programs in university business and engineering departments that stimulate more automotive research," he explains. "We want to introduce new skills to the auto industry, such as computational modeling and simulation. Perhaps above all, we want to focus our research on leading-edge issues." To complement the extensive

transportation program at ORNL, the alliance is setting up centers of excellence, established around university partners. A Center of Excellence in Automotive Supply Chain has been launched through the University of Tennessee School of Business and a Center of Excellence in Sustainable Automotive Manufacturing is being led out of the University of Kentucky. Additional centers are in the offing.

"The purpose of the centers of excellence is to have industry contribute financially to the center," Ritchey says. "In exchange for that contribution, industry would select the nonproprietary research on which faculty and graduate and undergraduate students would work. An added benefit is access to students who are potential future hires. There is also the potential for crossover. If someone from Auburn is interested in and skilled in transportation logistics, Tennessee would be interested in including that expert in its own center of excellence. The entire initiative is based on the premise of aligning strengths among the institutions."

Research capabilities outside automakers' own R&D organizations are crucial to development of new technologies and products, says Tom Bologa, vice president of engineering, United States, for BMW of North America. Bologa represented BMW for two panel discussions held during the Tennessee Valley Corridor event and has helped capitalize the Clemson International Center for Automotive Research.

"We absolutely look to the outside because we can't possibly do it all," Bologa says, adding that the Clemson partnership will focus initially on production improvements at BMW's plant in nearby Aiken, S.C., and development of a skilled workforce. Eventually the partnership may broaden to other research challenges more directly related to vehicle performance.

"I can speak for the whole industry when I say energy efficiency is probably 80% of our focus when it comes to developing new technologies," he says. "How are we going to get the greatest energy efficiency possible? That is not going to be one technology. It is going to be a whole variety of things. We don't have the resources to track down all the needs that we have. There are so many things we are working on we just don't have the people to do everything."

On the R&D side, Thomas Kurfess, professor and BMW Chair of Manufacturing at Clemson, says Automotive Research Alliance partners' capabilities will complement each other. He had recently visited the National Transportation Research Center near ORNL where he says he saw several opportunities for collaboration.

"This is not an issue of competing but instead an issue of how we can work together," Kurfess says. "What I've seen is that, when we work together with our supposed competition, we all win. This is not one plus one equals two. The value is much greater. I think there are tremendous opportunities left and right."

Although the South's largest research laboratory, ORNL is not restricting automotive research efforts to the Southeast. The Department of Energy recently announced an initiative headquartered at automotive supplier Delphi Automotive's former R&D center in Detroit that pulls together ORNL, DOE, the Department of Defense and a consortium of automotive suppliers. Called USAutoPARTs, the effort will provide both expertise and facilities to second- and third-tier automotive suppliers, most of which cannot afford a program of in-house research.

"We are most effective as a national laboratory when our research can be applied to real-world problems that provide solutions and practical benefits for the nation's industries," says Ray Boeman, director of the National Transportation Research Center at ORNL. "By making our resources available, ORNL can play a direct role in supporting one of the most important sectors of the American economy."—*L.B.*

Contact: ritchey@battelle.org

Reducing the Appetite

ORNL and TVA are joining hands to reduce the South's energy demand.

Vermont, Oregon, Washington, Hawaii, Maryland, Connecticut, and New Jersey. The eclectic group is "America's Greenest States," a list produced by *Forbes* magazine last fall.

To find southern representation, however, keep reading—all the way down to number 20, Florida; 23, Virginia; 29, Georgia and 36, South Carolina. Tennessee, Arkansas, Kentucky, Mississippi, Louisiana, Alabama and West Virginia make up seven of the bottom eight on the "Greenest States" list.

Energy consumption is one of six factors incorporated into the tally, closely linked to other "green" standards, including air quality and carbon dioxide emissions. Kateri Callahan, president of the Alliance to Save Energy, used a bit of hyperbole to summarize the situation in a recent presentation to Oak Ridge National Laboratory employees: "The South is the Gobi Desert of energy efficiency."

From Callahan's perspective, while bioenergy, nuclear and other expanding energy options are important, "the potential of energy efficiency is probably greater than any other resource." She views the confluence of record prices for oil and increasing anxiety over carbon emissions as a "perfect storm" that makes the attitude of both the market and the public ripe for fundamental change.

Recognizing these trends, Oak Ridge National Laboratory researchers are developing an array of energy-efficient appliances, testing energy-saving building materials and refining a zero-energy home that literally will produce more energy than it consumes. As world energy demand collides with the growing public desire for a carbon-constrained environment, ORNL increasingly is recognized as a source of expertise for cities, states and utilities looking to trim bulging energy waistlines. The Tennessee Valley Authority has joined state and local government as well as non-profit energy efficiency advocate groups in asking the Laboratory to provide input for policy, incentives and technologies to transform the desert of consumption into an oasis of energy efficiency.

Twenty minutes from the ORNL campus, the City of Knoxville has launched an energy and sustainability task force to create a plan for citywide energy savings and carbon emissions reductions. "Once we started thinking along these lines, it didn't take us very long to realize that we were pretty well positioned with energy expertise all around us," says Madeleine Weil, Knoxville deputy director of policy development who put together the task force. Dana Christensen, ORNL associate laboratory director for energy and engineering research is a member of the task force. ORNL researchers sit on three of the body's four working groups.

"We quickly determined that Knoxville has a tremendous opportunity to emerge as a leader in energy use and sustainability, and we plan to take advantage of that," Weil says. ORNL is helping the city develop a proposal for an energy services performance contract to improve efficiency in all city facilities. Working with another group, ORNL's Patrick Hughes has submitted a white paper outlining a weatherization program for private homes.

Perhaps more than any single energy initiative, ORNL's zero-energy homes project has generated interest among local, state and federal officials seeking practical and affordable options for residential energy conservation. TVA has helped fund construction of five near-zero-energy homes (current utility costs are actually about 40 cents a day) at a Habitat for Humanity development in nearby Lenoir City. The project was the focus of a recent visit by Tennessee mayors from Knoxville, Chattanooga, Memphis and Nashville.

Demonstrating a renewed commitment to energy efficiency, the TVA board recently named Joe Hoagland, former senior advisor to TVA President Tom Kilgore, to a newly created post of vice president for energy efficiency and demand response. Hoagland's first task is to determine how much energy savings TVA needs to achieve in order to meet growing energy demands over the next 20 years.

Times have clearly changed. "In order to meet the goals of low cost and reliability, energy efficiency and demand response are now tools as much as our assets that generate electricity," Hoagland says,

adding that TVA's strategy also incorporates environmental concerns. "A megawatt not produced is a green megawatt."

When Hoagland came to his new post last fall, he was asked to determine what was needed to generate 1,200 megawatts of energy savings, or the equivalent of one large nuclear or coal-fired power plant, by 2013. "As we begin to understand the situation better, I'm not sure that is going to be enough. I expect that we will need to cut back more, much more," he says.

Meeting the challenge will require TVA to adopt a combination of tactics, including new technologies, rate restructuring, education and customer incentives to achieve the required savings. The agency has signed a memorandum of understanding with ORNL as a first step in what Hoagland envisions as a growing, and necessary, partnership with the Laboratory.

"ORNL has a broad expertise in energy efficient technologies to help us do things better," he says. "Oak Ridge researchers have unique experience in designing zero-energy homes, creative construction techniques, new insulation technologies and a sophisticated set of energy efficiency standards. Perhaps most important to us, they actually play a key role in developing the technologies."

In Nashville, state government is hoping to build on the recognition recently gained from a $72 million Tennessee Biofuels Initiative led by the University of Tennessee. The state's investment was designed to complement $135 million from the Department of Energy to support a new BioEnergy Science Center, headquartered at ORNL, With these two projects, Tennessee has quickly achieved status as a national leader in developing alternatives to petroleum-based transportation fuels derived from sustainable, renewable sources growing in fields and forests.

"State government has a strong history of partnership with the national lab," says Ryan Gooch, a graduate of Oak Ridge High School who was appointed in 2007 to serve as director of energy policy with the Tennessee Department of Economic and Community Development. "I think with time Tennessee can become a leader in energy and energy savings initiatives by tapping into ORNL's energy and renewable research expertise, which is second to none."

Those leading the charge say that creating the kind of energy savings that can make a real dent in demand will require the coordinated effort of government at all levels along with power generators, utilities and consumers.

"A lot of things have to come together," Hoagland says. "We must target market incentives. We will need to price electricity based on when people use it. We must alter habits through incentives, whether they be rebates or funding for energy efficient improvements. At the same time the state must guide the market by setting standards and codes that require the use of energy efficient building practices and materials. Most important, we have to work all those tracks simultaneously."

If these initiatives prove successful, the potential impact is enormous. ORNL researchers believe that fully one-half of the South's anticipated increase in energy demand can be met through energy efficiency. If that prediction proves accurate, the ranking of green states is likely to change.—*L.B.*

Contact: hawseyra@ornl.gov

"A megawatt not produced is a green megawatt."

THE ULTIMATE SOLUTION

Coordinating America's participation in an international fusion energy experiment

An international project that seeks to demonstrate one of humankind's few abundant clean energy options will be both a scientific and cultural experiment. Oak Ridge National Laboratory is playing key roles in the U.S. contribution to the International Thermonuclear Experimental Reactor (ITER) fusion energy project through ORNL's expertise and experience in fusion technology and management of large projects.

Assigned the leadership role by the Department of Energy, ORNL is guiding the U.S. participation in the international partnership to design and build ITER, a multi-billion-dollar fusion research device too large and complex for any single nation to develop. The six other partners are China, India, Japan, Russia, South Korea and the European Union. ORNL is joined by DOE partners Princeton Plasma Physics Laboratory and Savannah River National Laboratory in working on ITER, a top priority of DOE's Office of Science.

ITER will be built in Cadarache, France, with scheduled completion in 2016. Plans call for ITER to operate 20 years to demonstrate the scientific and technical feasibility of magnetically confined burning plasmas on a large scale. ITER represents a meeting of nuclear particles as well as a meeting of the minds. In a burning plasma, two types of fast-moving hydrogen nuclei—deuterium and tritium—bounce off each other and occasionally fuse after overcoming their natural repulsion. The result is the production of helium nuclei and neutrons. The electrically charged helium nuclei slow down in the plasma, keeping the plasma hot. ITER will not produce electricity but will provide considerable heat that can be converted to electricity.

Ned Sauthoff, manager of the U.S. ITER Project Office in Oak Ridge, says that DOE Undersecretary for Science Raymond Orbach's decision in 2005 to locate the U.S. ITER project office in Oak Ridge, "had a lot to do with ORNL's success in coordinating the construction of the $1.4 billion Spallation Neutron Source. Oak Ridge was recognized for its capability of delivering large projects on cost and on schedule. One of Oak Ridge's core competencies is the management of large-scale scientific projects.

"The ITER team includes many of the people who were working in the same positions for the SNS. Carl Strawbridge, who had been deputy manager of SNS, is now deputy manager of the U.S. ITER Project Office."

Many ORNL employees, as well as current staff in DOE's headquarters and Oak Ridge Office, proved with the seven-year SNS project their leadership capabilities and the ability of their management tools to control costs and schedules and manage risks. "I am most proud of our team members," Sauthoff says. "They are experts in their technical or management field, they have experience that is directly relevant and they work together well as an integrated team."

ORNL, which hosts one of the world's broadest fusion energy research programs, has also contributed leaders in fusion science and technology to help guide the

design and construction of ITER. Their expertise will be required for a facility 10 times larger than the world's current largest fusion research device, the Joint European Torus in the United Kingdom.

"Our signature is the integration of research across the spectrum of science and technology issues facing the development of fusion energy as an economical, commercial source of electricity," says Stan Milora, leader of ORNL's fusion energy researchers. For the U.S. ITER Project Office, Milora is director of the Virtual Laboratory for Technology and chief technologist.

"ORNL's fusion core competencies are atomic physics, plasma theory and simulation, experimental plasma physics, integrated fusion systems, technology and materials research and concept innovation, such as the Quasi-Poloidal Stellarator, or QPS, that we hope to build and operate at ORNL later this decade. We collaborate with major fusion laboratories around the world, especially those engaged in research on tokamaks, stellarators and spherical tori."

The U.S. labs—Oak Ridge, Princeton and Savannah River—will build hardware for ITER and ship it overseas to France. The United States through ORNL will provide magnets including materials from Japan, superconductors for the large magnets, radiofrequency heating components to heat the plasma, plasma-facing materials that remove heat, vacuum components, power supplies, cooling water systems and pellet injectors for refueling the plasma (a technology that was pioneered by Milora). Princeton will provide instrumentation for diagnostics and electrical power systems. Savannah River will deliver ITER's tritium processing systems.

If ITER proves viable, fusion power plants built in 40 to 50 years will provide electricity without producing high-level radioactive waste or carbon dioxide, a greenhouse gas that contributes to global warming. A fusion plasma consists of super-hot gases of deuterium and tritium. The sun is powered by fusion, with gravity confining its plasma. In ITER, superconducting magnets will confine the plasma, which will be heated to more than 100 million degrees by shooting in radio waves and neutral particle beams (using technologies developed at ORNL) and by fusion reactions themselves.

"What we are trying to do at ITER is move from an externally heated system to a self-heated regime," Sauthoff says, explaining that commercial fusion power plants must be self-heated to be efficient. ITER will demonstrate plasma "burns" lasting from minutes to an hour in which deuterium from seawater and tritium nuclei combine to form helium nuclei, or alpha particles (two protons and two neutrons), which deposit energy in the plasma as they slow down. The helium "exhaust" is extracted from the plasma vessel, and deuterium and tritium recovered from the exhaust are recycled back to refuel the plasma.

Another significant scientific difference is the size of ITER's plasma vessel, which is at least 10 times as large as today's largest fusion research device. Just as coffee retains its heat longer in a big pot than in a small cup, the plasma in ITER is expected to stay hot longer than the plasma in smaller fusion devices, helping sustain fusion reactions. A third difference is the influence on plasma stability of energetic particles sailing through the plasma and stirring up waves.

> "If ITER proves viable, fusion power plants built in 40 to 50 years will provide electricity without producing high-level radioactive waste or carbon dioxide…"

DOE Undersecretary for Science Orbach is the leader of the U.S. delegation on the 28-member ITER Council. The four-person U.S. delegation includes a member from the State Department. Sauthoff says the State Department views ITER as a major positive activity in foreign relations, a successful cultural experiment in which countries are working together for a common goal.

To make ITER a truly successful scientific experiment, researchers must produce a stable, self-heating plasma, the long-term key to abundant and affordable clean energy.—*C.K.*

Contact: sauthoffnr@ornl.gov
Contact: milorasl@ornl.gov

DANA Christensen

sees energy production through green-colored glasses. A product of the 1960s and 70s, with degrees in chemical engineering and environmental management, the associate laboratory director for energy and engineering sciences started his career in the water treatment business.

"When I entered the workforce, I had an environmental ethic that I had grown up with. I really wanted to improve the environment," he says. Although his career veered away from traditional environmental management work into the nuclear business at Los Alamos National Laboratory, Christensen says he has always approached his work with sustainability in mind. These days, that is a good thing. Christensen manages a broad portfolio of energy research programs at Oak Ridge National Laboratory—from nuclear power to coal-fired electricity production to bioenergy—at a time when sustainability and environmental awareness are no longer red-haired stepchildren to energy production.

"I've had this little thread in my career that is founded more in environmental management," he says. "As I've worked with industry, in the nuclear weapons and nuclear power business and in my current job, I always ask a basic question, 'How can we make energy to power our economy but do it in a way that doesn't destroy our environment?'"

In an interview with the *ORNL Review*, Christensen presented his unique perspective on energy and the Laboratory's role in shaping America's future energy options.

Given your roots in environmental management, how has your perspective of the nation's energy problems evolved and affected the way you are now managing one of the nation's largest energy programs at ORNL?

When you're young and fresh out of school, you're thinking altruistically about what is important to you. What you quickly realize is that energy makes the economy go and that without adequate energy the economy collapses. If you understand the premise that energy is essential then you ask, 'How can we minimize the impact that energy production and consumption have on the environment?' Over the years, my whole view of this question just turned over. I came out of school thinking we have got to tackle the environmental issue. But the challenge is not really an exclusively environmental issue. The real challenge is an energy issue and an environmental issue that go hand in hand.

Now, because of climate change, addressing environmental issues is imperative. We simply must deal with the emissions of fossil fuel into the atmosphere. There are no two ways around it. Part of the solution to the greenhouse gas issue means building more nuclear power plants. That is just a given. The hang-up is, what are we going to do with the spent fuel? This is a critical question we have been ducking for 50 years. The history of this issue is no different than safety. We can look back and see that America's industrial practices often changed for safety reasons. Now they are going to have to change again, and change pretty dramatically, this time for reasons of environmental quality.

Do you see ORNL being uniquely positioned to find environmentally friendly energy solutions?

The laboratory has an outstanding scientific summary basis that extends beyond fundamental science. We can make prototypes and develop techniques and technologies and model systems. If

we capitalize on that capability to make prototypes, the next step is to increase our involvement with industry and move that discovery science, discovery and demonstration science, out into a commercial demonstration mode. That entire process is what the Department of Energy, and particularly the agency's energy technology side, are looking for—stronger interaction with industry to move technology out into the marketplace. Oak Ridge is extremely well positioned to do that. We have some type of working relationship with hundreds of industrial firms across the country. Many of those industries have employees who work on-site or close to our campus. This part of the country, the Mid-South, is a growing industrial region. We see a lot of industry, particularly in the automotive sector, with manufacturers locating their headquarters and production sites in the region. Increasingly these companies are looking to ORNL to help them solve their research and development problems. The fate that 65 years ago located the Laboratory in East Tennessee made it possible for us today to apply our research capabilities on an industrial scale to U.S. industry.

You and others at ORNL have spoken about this new dimension for ORNL as the "Lab of the South." What does that mean?

We happen to be a very strong laboratory and we happen to be the only national laboratory located in the South, which is home to a sustained increase in population, industry and the utilities needed to service this growth. The "Lab of the South" concept says simply that at ORNL we should leverage our unique resources to help both the region and the nation. No other institution in the South has both the breadth of research capabilities and the network of partnerships that exists in Oak Ridge. I view this as an opportunity and a responsibility.

Virtually everyone agrees that there is no single solution to the energy challenge. How, when you are going forward with research on multiple fronts, do you come out with a coherent suite of technologies that are practical?

You've asked the really tough question. One answer is that ORNL, unlike many institutions, is a multi-program laboratory. We work with a variety of sponsors that focus on different energy sectors with unique milestones. We have to keep our eye on the real goal, which is to produce energy in an efficient way that supports the American economy without damage to the environment. When we work with the Department of Defense, we are seeking to produce energy for battlefield applications, and in so doing helping underwrite science that will eventually migrate into the marketplace. When we work with the Department of Homeland Security on technology that helps track and understand the movement of materials around the globe, the process enables us to continue to invest in technologies that can be applied in the marketplace for the energy industry. In contrast, private industry usually is seeking to solve a problem that is generally short-term in nature. Our researchers working with industry thus gain a better understanding of a world with different expectations. This combination of long-term, innovative research with industrial partnerships makes ORNL the perfect place not only to determine some of the best energy strategies for our nation's future—but also to back those strategies with sound science.

Extending the Half-Life

Computer modeling may make it possible to lengthen the life of nuclear reactors.

For the past 40 years, researchers at Oak Ridge National Laboratory have been testing reactor vessels, the critical part of nuclear power plants where nuclear reactions take place under extraordinary pressure. Specifically, they study the various steels the reactors are made of to assist the Nuclear Regulatory Commission in developing safety regulations for the plants. In the 1970s, ORNL researcher Richard Bass and his team employed large steel specimens weighing more than one ton to simulate the response of components to the pressure and temperatures caused by nuclear reactions inside commercial power plants. Today, the labs once housing ORNL's heavy-section steel technology program are closed. Bass and his colleagues now carry out large-scale simulations on high-performance computers.

The results of this transformation have had a significant impact on the nuclear power industry. A computational tool developed at ORNL, known as the Fracture Analysis of Vessels of Oak Ridge, or FAVOR, is proving to be a key factor in a proposed change in regulation that could double the operational life expectancy of nuclear power plants in the United States.

Most of the nation's 104 nuclear power facilities, which provide approximately 20% of the U.S. electricity supply, face expiration of their 40-year Nuclear Regulatory Commission licenses within the next 10 to 20 years. Using ORNL's research, the NRC recently issued a revised regulatory rule central to the agency's efforts to approve 20-year license renewals for many of those plants. Analysis and reliability tools developed at Oak Ridge indicate that an additional 20-year renewal will be feasible for many plants, extending their total lifetime to 80 years and making a significant contribution to the nation's energy demands. The economic impact of this extension is estimated in the hundreds of billions of dollars.

"All of the nuclear plants in operation today were approved by the NRC to be built in the 1960s and 1970s," Bass says. "While some were constructed in the 1980s, most plants have licenses due to expire within the next decade. We are looking at a replacement cost of billions of dollars for each plant, in addition to the time required to build and license a new facility and the associated reduction in power capacity when an existing plant is closed. With a projected renaissance in the nuclear power business, the extension to current licenses should provide enough time to build new plants that will replace aging ones and meet the growth in electricity demand."

Since the 1960s, ORNL has, with NRC funding, tested a variety of reactor vessels and their materials to help the agency create guidelines for operation and safety of the vessels. Results from that research contributed heavily to the first rulemakings in the 1980s and 1990s for assessing pressurized thermal-shock scenarios. Those rules, however, were conservative, partly because detailed information about the vessels and their response to a variety of stresses was not fully understood. As more information about the equipment has become available and modeling and computational tools have become more sophisticated, ORNL researchers have been able to reevaluate with much greater accuracy the probability of these events. The result is the ability to determine which vessels can operate longer than allowed by their current regulations with no compromise of safety.

ORNL is working with other national laboratories and research institutions to create a similarly comprehensive analysis tool that will encompass all pressure-bearing components of a nuclear plant, providing detailed findings about the condition of the plant as a whole. Bass says the capabilities developed at ORNL will be available for developing regulations for an anticipated increase in the number of new plants planned for construction in years to come.—*L.B.* ***Contact: bassbr@ornl.gov***

A Renewed Interest

A new ORNL process seeks to improve solar cells.

Research priorities are indeed cyclical. In the 1980s, Oak Ridge National Laboratory was a leader in the development of solar-cell fabrication techniques. The work's focus was laser processing, using light from a pulsed high-power laser instead of high-temperature heat to create solar cells. For a brief time in 1986 under Richard Wood's leadership, ORNL's 19.5% single-crystal silicon solar cell fabricated with laser processing held the world record for efficiency in converting sunlight's energy into electrical energy.

After 1987, the programmatic direction of the Department of Energy, and subsequently ORNL, changed. The Laboratory abandoned research on photovoltaics, or PV. Twenty years later, the challenges of the changing energy sector are putting ORNL back into the PV business.

DOE's Solar America Initiative recognizes that materials researchers at ORNL and other national labs could help industry raise solar-cell efficiencies and lower the costs of manufacturing PV materials and devices. As a result, ORNL researchers are encouraged to request funding for solar projects.

Through a project sponsored by ORNL's Laboratory Directed Research and Development program, researchers led by Ron Ott demonstrated that pulsed thermal processing using the Laboratory's plasma arc lamp could increase the collection efficiency of thin-film amorphous silicon solar cells by introducing a nanocrystalline microstructure within the amorphous material. As a result of this successful LDRD-funded collaboration with a leading manufacturer of thin-film amorphous silicon solar cells, the ORNL researchers received funding from the Defense Advanced Research Projects Agency. Their mission for DARPA is to help develop methods to increase solar-cell efficiencies on polymer substrates, reduce fabrication costs and improve productivity.

This type of thin-film solar cell is fabricated using amorphous silicon-germanium alloys consisting of three layers. Amorphous, or noncrystalline, materials are considerably cheaper to manufacture but are less efficient than standard crystalline silicon solar cells. The top layer is pure amorphous silicon, while the underlying layers consist of different silicon-germanium alloys. Each layer absorbs a different portion of the solar wavelength range.

The amorphous silicon-germanium layers are deposited on a metal substrate along with a transparent conducting layer that forms the topside electrical contact, as well as an anti-reflective coating that reduces the amount of light reflected from the cell. The entire device is placed under a protective cover layer. All the cells are then connected to make a PV module.

The Oak Ridge team believes the solar cells' efficiency might be improved by changing the amorphous silicon to nanocrystalline silicon. To explore this idea in the DARPA project, Ott will "flash" amorphous silicon thin-film specimens with the plasma arc lamp.

"We have shown that pulsed thermal processing will initiate solid-phase crystallization, which will introduce a nanocrystalline structure with fewer defects and higher efficiencies," says Ott, ORNL's program manager for solar energy technologies. "Our process will produce a purer structure faster than what an in-situ, deposition process can provide."

ORNL seeks funding from DOE to work with Georgia Institute of Technology on improving the university's process for increasing the efficiency of multicrystalline silicon solar cells. Georgia Tech researchers add to multicrystalline ribbon-grown silicon cells a hydrogen-containing silicon nitride antireflective layer. The researchers have tried using currently available rapid thermal annealing to drive the hydrogen from the antireflective layer into the multicrystalline silicon to "passivate," or reduce, defects and increase electron travel distances.

"They found their process cannot heat silicon nitride to high enough temperatures fast enough to force the hydrogen into the multicrystalline silicon," Ott says. "Pulsed thermal processing has higher heating rates and higher processing temperatures that should take the material to the next level in efficiency."

The findings are encouraging enough to warrant further funding. To characterize these new PV materials, ORNL has invested in the Center for Advanced Thin-film Solar Cells, managed by Jay Jellison. The center will house several instruments to measure solar-cell efficiency, spectral response, thin-film thickness and other parameters used to evaluate the record-breaking potential of PV materials.—C.K. Contact: ottr@ornl.gov.—C.K.

Contact: ottr@ornl.gov

Mouse-Like

Research on mice may help explain why humans become addicted.

Do differences in response to stress drive people to drink alcohol or take illegal drugs to the point of becoming addicted? What is the relationship among genes, gut microbes and intestinal disease? Why are some people more sensitive to pain than others?

These are some of the questions being addressed by a national group of researchers in collaboration with Oak Ridge National Laboratory geneticists in the Collaborative Cross project. ORNL's mouse genetics research facility, the William and Liane Russell Functional Genomics Laboratory, is the North American site of the Collaborative Cross. The laboratory houses the ultimate reference mouse population that models the diversity of humankind and provides a unique tool for understanding human disease and testing potential treatments.

The ORNL laboratory is a pathogen-free facility with cryogenic storage that contains 18,000 mice with space for up to 80,000. The state-of-the-art facility, which opened in 2004, began hosting the Collaborative Cross project in May 2005.

"Biologists usually work on small projects, but Oak Ridge has the big science project experience to host a large-scale biology user resource," says Elissa Chesler, project manager for the Collaborative Cross and leader of ORNL's systems geneticists. "ORNL offers the added benefit of high-performance computing to manage and analyze data from the mouse experiments."

Chesler says that the biology community is excited now that more than 9,000 mice bred for the Collaborative Cross project are available for experiments. The project has attracted funding from the Ellison Medical Foundation, the Department of Energy and the National Institutes of Health.

The ORNL team is collaborating with Virginia Commonwealth University in looking for connections between anxiety and alcoholism. Better understanding could lead to treatments for both disorders. The study recently identified a region of a mouse chromosome that appears to alter significantly the effects of alcohol on anxiety.

Not surprisingly, as the work progresses, new questions arise concerning the role of stress in alcohol addiction. Do alcoholics have an abnormal stress response? Does the same genetic variation that causes stress also cause alcoholism? Do people drink for different reasons?

Chesler evaluates a variety of studies about the genetics of mouse behavior. Her colleagues have found that many mice dislike the taste of grain alcohol commonly used for alcohol addiction tests. She now is collaborating on a genetics study of mice that consume beer, which has a taste more palatable than the stronger alcohol. She says mice show high levels of stress when picked up by humans and placed in commonly used memory tests, suggesting that traditional ways of handling and testing mice probably should be modified in the Collaborative Cross.

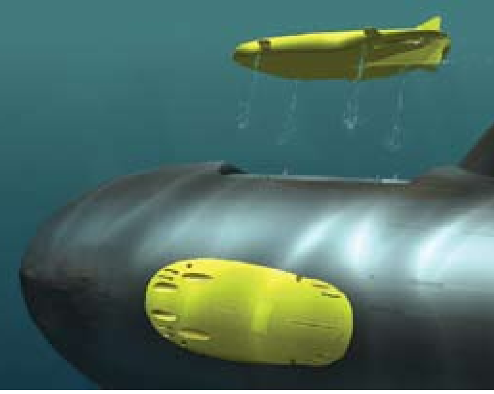
With members of the microbial ecology group, Chesler is examining whether genetic variation in Collaborative Cross mice contributes to differences in the composition of bacteria in mouse intestines. Gut microbes have been shown to influence diet, sensitivity to pain, inflammation, Crohn's disease and Celiac disease.

In one mouse study at ORNL conducted with the University of Pittsburgh School of Medicine, researchers look for genes that cause some people to be more sensitive to pain than others. The goal is to identify ways to design new drugs for more effective treatment of unique types of pain.

For years geneticists have sought a better research tool for understanding complex human traits—such as obesity, rates of aging and pain sensitivity—that are influenced by multiple genes and their interactions with the environment. Researchers have long desired an ultimate reference mouse population, not one bred from historic research populations derived from "pet" mice. "Those mice traditionally were selected based on a behavioral trait rather than randomly," Chesler explains.

The Collaborative Cross, proposed in 2001, uses a rigorous breeding scheme to maximize the genetic diversity of inbred strains of mice. Aided by software developed by Ken Manly, a visiting scientist from the University of Buffalo, eight "founder" mice with eight different genomes have been randomly bred at ORNL. Ultimately, through years of inbreeding, a thousand different strains of mice will be generated, perhaps providing answers to some of humankind's most intriguing questions.—*C.K.*

Contact: cheslerej@ornl.gov



Modeling Metal Fuels

Simulations show the promise of nanostructured solid-state boron as a fuel.

Gasoline, ethanol, hydrogen and other fluid fuels burn well in air. But in airless environments, solid fuels may work better. Specially designed metals may have the right stuff for fueling tomorrow's submersible vehicles and high-altitude, low-speed aircraft, as well as providing electric and propulsive power for hypersonic spacecraft.

Because metals are high-density energy carriers, their combustion can produce tremendous heat. Combustion of metal particles a few billionths of a meter across requires such low activation energy that even a nine-volt battery can provide enough heat for ignition. Because nanoparticles have considerable surface area, they may collect sufficient oxygen to combust. Thus, nanoparticles require a thin layer of surface rust to prevent self-ignition, a process akin to dry hay catching fire on a hot day.

Researchers at Oak Ridge National Laboratory have studied nanoparticles of iron and aluminum. Compared with gasoline, iron produces twice the energy per unit weight and aluminum yields three times as much. But boron spectacularly provides five times the energy. Unlike hydrocarbon fuels, which produce nitrogen oxides, carbon dioxide and soot upon combustion, ORNL-engineered metallic nano-fuels emit no pollutants.

Supported by ORNL's Laboratory Directed Research and Development (LDRD) program, computational chemist Bobby Sumpter helped investigate solid-state metals as fuels. He and theorists Vincent Meunier, Bill Shelton and Mike Drummond used computers to simulate nanoscale combustion. Simultaneously, experimentalists Parans Paranthaman, Solomon Labinov, Louis Qualls and David Beach carried out numerous laboratory studies that put the fundamental theory, initially proposed by Labinov, to the test.

Previous ORNL experiments explored how iron nanoparticles burn, how efficient particle combustion is and how likely nano-fuel combustion by-products can be recycled by chemical reduction. That work spawned the world's first paper about metal fuels, published in a 2007 issue of *Journal of Energy Resources Technology*.

The computational work employed the Cray X1E Phoenix and SGI Altix Ram supercomputers at the National Center for Computational Sciences, ORNL's leadership computing facility, to simulate combustion of boron (B) and boron oxide. Just as stop-action photography reveals events frame by frame, simulation shows every step of combustion at the atomic level. Using models based on quantum mechanics, the center's supercomputers simulated a process that in the real world lasts five trillionths of a second. The supercomputers required only two days to simulate the process with B_{12} oxidation and two weeks to mirror it with B_{80}.

Boron normally clusters in 12-atom icosahedral structures or flat sheets, each of which oxidizes differently. The researchers sought a material that could resist melting, or loss of structure. They modeled B_{12} and B_{24}, as well as the particularly stable B_{80}, discovered in 2007 through predictions by theorists at Rice University.

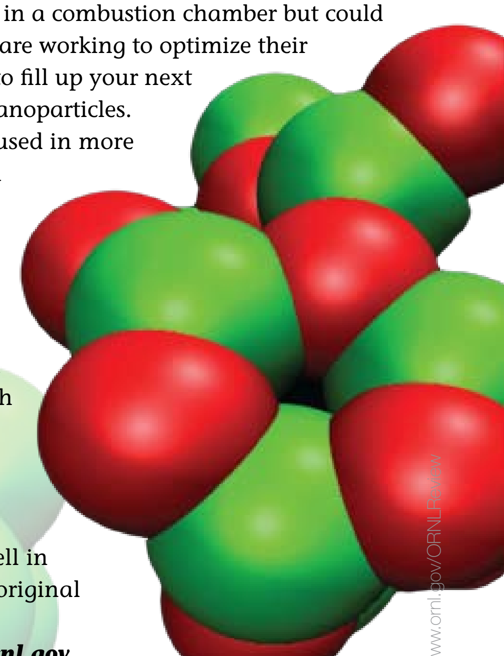
Adsorption and subsequent chemical reaction of just one oxygen molecule was enough to destroy the original structure of B_{12}, the simulations showed. Although B_{80} tolerated several oxygen molecules, it too ultimately lost its structure. Drummond, Meunier and Sumpter published their initial theoretical studies in spring of 2007 in the *Journal of Physical Chemistry A*.

Computation has confirmed that combustion of solid-state boron nanoparticles will produce considerable heat, reaching temperatures around 1,300°F. The calculations indicate that a boron particle could be generated with enough adsorbed oxygen for complete combustion. Thus, in theory, boron could work as either an aerobic or anaerobic solid-state fuel.

Armed with that knowledge, the ORNL experimentalists succeeded in burning boron in a combustion chamber but could not sustain the flame. They are working to optimize their test setup. But don't expect to fill up your next car's fuel tank with boron nanoparticles.

Boron will probably be used in more specialized applications. "A major problem with boron is that the nanostructure is lost during the oxidation process," Sumpter says. "Thus, we can't easily recycle it by using chemical reduction, as is the case with iron." Currently, the LDRD team is computationally exploring the encapsulation of boron nanoparticles in an iron or aluminum shell in an attempt to preserve the original nanostructure.—*Dawn Levy*

Contact: sumpterbg@ornl.gov



...and the WINNERS are...

Accomplishments of Distinction at Oak Ridge National Laboratory

Vinod Sikka received the ***Director's Award for Outstanding Individual Accomplishment in Science and Technology*** at UT-Battelle's Awards Night on Nov. 16, 2007. He also received ORNL's Inventor of the Year Award. Sikka's work with nickel aluminides, infrared-based process heating and computationally designed stainless steels and cast irons has resulted in 41 patents and commercial products with sales in the billions of dollars. Honored with a ***Director's Award for Outstanding Team Accomplishment*** were participants in the international effort to sequence the poplar tree genome: **Stan Wullschleger, Udaya Kaluri, Lee Gunter, Frank Larimer, Philip LoCascio, Tonming Yin, Gwo-Liang Chen, Ed Uberbacher** and team leader **Gerald Tuskan**. The ***Director's Award for Laboratory Operations*** was bestowed on **Ronald Crone** for leadership in the High Flux Isotope Reactor's recent successes. **Jeff Christian** received the ***Director's Award for Community Service*** for his effective communication of building technologies research and development—most notably, zero-energy housing—to the public.

ORNL Director **Thom Mason**, **John Budai** and **Krzysztof Rykaczewski** have been elected ***fellows*** of the ***American Physical Society.***

Saed Mirzadeh received the American Nuclear Society's 2007 ***Seaborg Medal Award***, named for Glenn T. Seaborg, the Nobel-prize winning nuclear chemist who co-discovered plutonium and many transuranium isotopes and chaired the U.S. Atomic Energy Commission from 1961 to 1971.

Ho Nyung Lee is one of eight Department of Energy scientists to receive the ***Presidential Early Career Award for Scientists and Engineers***. The PECASE award, one of the nation's top honors for young scientists, was presented Nov. 1, 2007, in a White House ceremony. Lee, an experimental physicist in ORNL's Materials Science and Technology Division, focuses on controlling interfaces in artificially layered complex oxides and on understanding collective phenomena arising from the atomic-scale coupling within complex transition-metal-oxide superlattices and across heterogeneous interfaces.

Herb Mook, a leading ORNL neutron scientist, and **Peter Cummings**, a Vanderbilt University chemical engineering professor who directs the Nanomaterials Theory Institute of the Center for Nanophase Materials Sciences at ORNL, have been elected **fellows** of the ***American Association for the Advancement of Science.***

Amit Goyal has received the ***"Pride of India" Gold Award***, one of 24 natives of India to receive this prestigious award.

Thirty-two ORNL researchers and technology transfer managers won six awards, including project of the year and three excellence in technology transfer awards, from the ***Southeast Federal Laboratory Consortium***. Winning inventions were a new superconducting wire, a method for finding defects in semiconductors, a device that uses acoustics to detect chemical residue from a distance, high-temperature electronics for use in oil drilling and a high-power search engine.

Frank Kornegay was honored by the Earth and Atmospheric Sciences Department of ***Purdue University*** as a ***distinguished alumnus.***

Vinod Sikka

next issue

online extras

www.ornl.gov/ORNLReview

on the web

ORNL at the Auto Show
- Video, slideshow and more info about DOE's deal with auto suppliers

How to make a superconductor
- Watch researcher Mike Gouge demo power transmission lines of the future.

Showcasing the sun:
- Video tour of researcher Curt Maxey's solar test project

Reference desk:
- View papers associated with the research projects mentioned in this issue.

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Writer—Larisa Brass
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Illustrator—Andy Sproles
Photographers—Charles Brooks, Curtis Boles, Jay Nave, Michael Sarnacki
Web developer—Dennis Hovey

Editorial office telephone: (865) 574-7183
Editorial office FAX: (865) 574-9958
Electronic mail: krausech@ornl.gov
Web addresses: www.ornl.gov
www.ornl.gov/ORNLReview/

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