Breakthroughs

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SPRING 2007

SCIENTIFIC DISCOVERY

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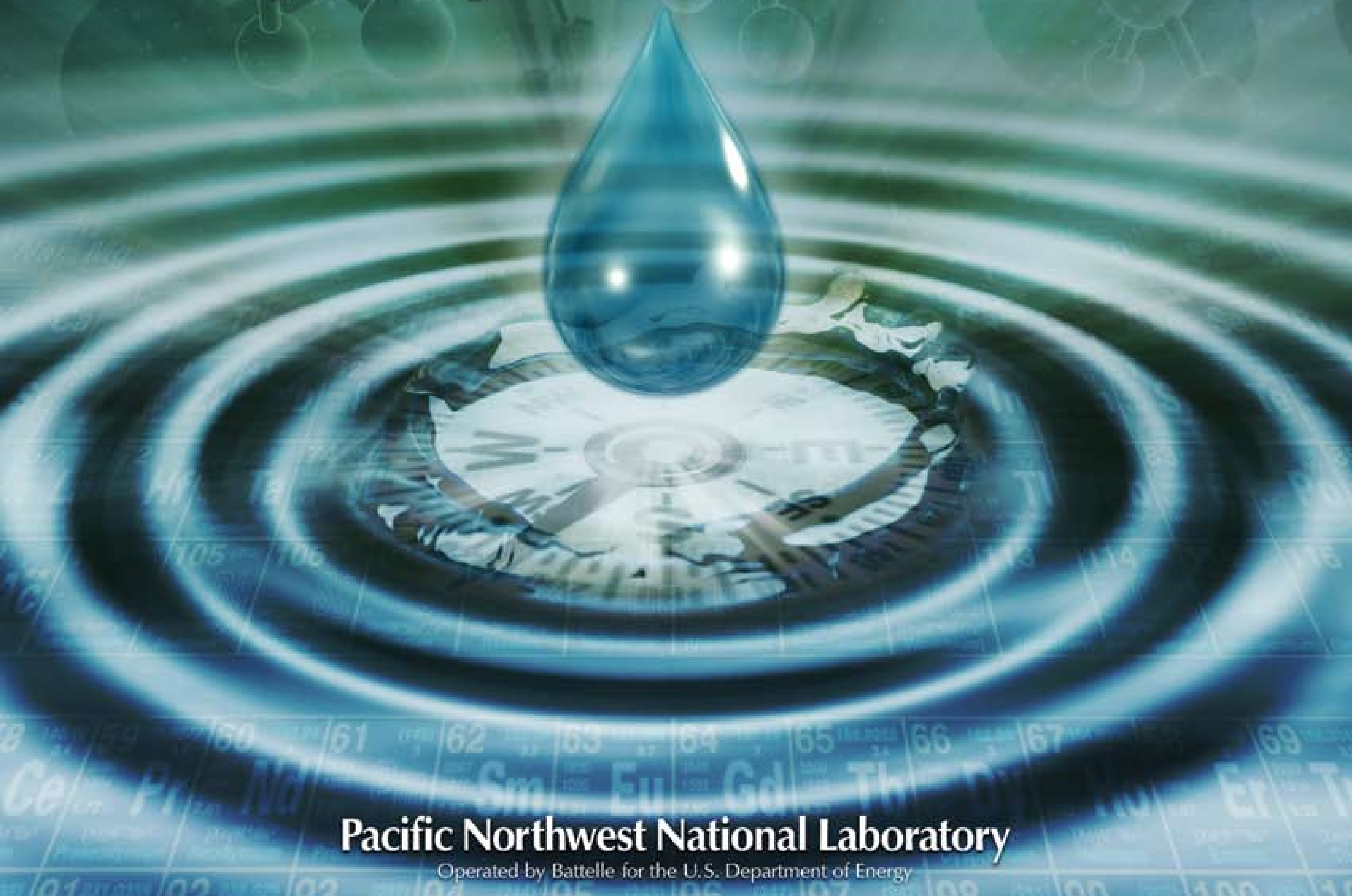

Pacific Northwest National Laboratory

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Breakthroughs

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editor's screen

Advancing frontiers, making progress

Over the past few issues, *Breakthroughs* has featured two of the four PNNL mission areas within the special section pages; those were energy and environment. In this issue, we focus on our discovery science mission. Fundamental research provides the foundation for the Laboratory's forays into unknown territory. Our mission: to advance science and technology that addresses our nation's most pressing energy, environmental and national security needs.

Many of us can remember the days of elementary science courses that had us experimenting with blocks, beakers and bunsen burners in attempts to better understand our world. For many researchers, it was those early scientific dabblings that sparked their imagination and led them here to discover. Supporting science education continues to be a focus for PNNL as our nation attempts to recruit the next generation of scientists. By sharing some the progressive and (at times) unusual discoveries here, we hope to demonstrate the need for this basic knowledge that starts with something simple...and eventually ripples into a life-improving invention. — LT

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At a *glance*

Area students learn about economic espionage from PNNL expert

Globalization has given new wings to a very nasty problem. The Federal Bureau of Investigation defines economic espionage as anyone who knowingly performs targeting or acquisition of trade secrets to knowingly benefit any foreign government, foreign instrumentality or foreign agent.

Theft of intellectual property costs American businesses hundreds of billions of dollars each year. It stymies the development of new products from medications to movies and creates higher prices for whatever new goods are created. With companies doing more business overseas, the problem has become increasingly difficult to solve. Greg Curtis, counterintelligence officer at Pacific Northwest National Laboratory, may have a way to slow it down.

"I'm educating local students about the risks of economic espionage because students are the future users and developers of technology in this country," said Curtis. "If they know what to look for, they may be able to prevent future thefts."

Curtis is currently teaching classes at several Richland high schools. The course is four hours long and is taught over four days. ●

More room for RAM at EMSL

The William R. Wiley Environmental Molecular Sciences Laboratory, a Department of Energy national scientific user facility at Pacific Northwest National Laboratory, has added 4,000 square feet to the facility's supercomputing operations area. This is the first permanent expansion of EMSL since it was constructed in 1997.

The space was created to house a portion of EMSL's next-generation supercomputer and the facilities data archive. The new computer is targeted for operation in 2008.

"This new floor space will allow for nondisruptive migration of the existing system to the new system," said Kevin Regimbal, operations manager for EMSL's Molecular Science Computing Facility. "When received, the new computer will enable us to grant scientists larger allocations of resources and allow them to attack even larger scientific problems."

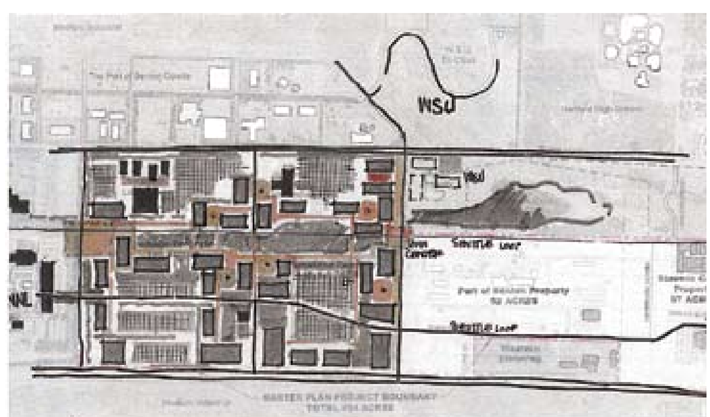
More EMSL expansions are planned in the future, including office and lab spaces and a radiological annex. ●

Richland Research District gets leg up from investors

Solaris Group, a representative of investors, is partnering with the City of Richland and the Port of Benton to develop parts of the Richland Research District surrounding Pacific Northwest National Laboratory's main campus. The Research District, a 1,600-acre area of land, contains more than 80 companies and 8,000 employees, including Washington State University Tri-Cities and PNNL.

Collectively, the investors have committed $80 million dollars to bringing mixed-use development to the area. Development is currently under way at the Research District. Solaris Group investors are funding Stevens Center, a fully-developed business park that is currently ready for tenants.

A 2006 study conducted by AngelouEconomics suggested that PNNL would be a primary draw for science and technology companies looking to locate to the Research District for collaborative opportunities. ●



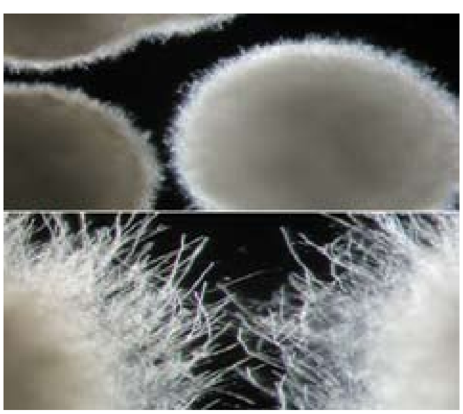
Architects for Solaris Group are developing a master plan that involves a pedestrian-friendly environment in the tradition of a university campus that fosters interaction and provides amenities, such as fitness and daycare facilities, that encourage people to enjoy being there.

science SPOTLIGHT

Taming the hairy mushroom

Fungi (yeasts, molds and mushrooms) have gotten a bad rap over the years. They have been blamed for infecting food crops and represent some of the most universal and costly pathogens known to man—both of which overshadow the important contributions fungi make, such as providing critical agricultural nutrients and compounds for antibiotics. Today, scientists at Pacific Northwest National Laboratory have developed the technology for truly harnessing the potential of fungi in our world.

Fungi, plants and animals represent the three non-bacteria phylogenetic kingdoms. Within the approximately 250,000 different species of fungi, about 75% are ascomycetes (approximately 90% of which are filamentous fungi, the remainder being yeasts) and 25% are basidiomycetes (commonly known as mushrooms). As a group, the fungi have an enormous impact on the United States and world economies. Yeast is used extensively in the baking and brewing industries, mushrooms are consumed as food all over the world, and filamentous (hairy) fungi are used for production of foodstuff and medicines and industrial production of enzymes and chemicals.



Ideal growth produces a pellet shape (pelleted morphology) as opposed to the wild threadlike, or hairy, growth that most often occurs in nature.

A group of six small fermentors allows researchers to grow quantities of fungi under the same conditions or to test multiple parameters simultaneously, vastly increasing the speed of conducting fungal experiments.

Filamentous fungi grow as long, multi-celled strands or filaments, and these filaments can combine to form larger masses like mushrooms. They are largely responsible for recycling biomass in nature and are the source for many important compounds, including organic acids, antibiotics and other therapeutics. Biomass is the largest renewable energy source in the United States and provides the only renewable alternative for liquid transportation fuel. Wood is still the largest biomass energy resource today, but other sources, such as food crops, residues from agriculture and forestry and even the organic component of municipal and industrial wastes, are quickly gaining momentum.

By combining traditional bioprocess research technologies with cutting-edge technologies such as molecular genetics, genomics and proteomics, scientists have developed new biomass processes using the filamentous fungi.

With state-of-the-art facilities and equipment, the PNNL fungal biotechnology research team applies established methods to evaluate and manipulate parameters to create novel fermentation processes using filamentous fungi to ensure that lab-developed techniques are relevant to industrial processes. This integrated capability is essential for developing the novel bioprocessing approaches necessary for efficiently converting biomass into industrial and energy products. Scientists use a variety of analytical instruments to understand the fungal system and determine products and by-products under different scenarios. A proteomics workstation rapidly identifies proteins critical to the efficient function of a given organism within a bioprocess. Multi-vessel fermentors and capillary electrophoresis equipment provide the fermentation and analytical capability critical for determining and creating the most efficient bioprocesses.

The research being conducted by PNNL scientists may dramatically enhance the production of valuable molecules and materials, having a tremendous impact on industry, medicine, agriculture and basic science. Because of this potential impact, a Fungal Biotechnology Review Board has been formed as an opportunity for industry to become involved in developing technologies relevant to their business. Members of the Fungal Biotechnology Review Board appreciate the access to world-class instrumentation and leading scientists in emerging and established scientific fields.

Together, PNNL and industry are taming the hairy mushroom—they are shaping the next generation of consumer products, medicines and biomass energy. Through better understanding, control and productivity, researchers are actively expanding the use of filamentous fungi. ●

PNNL aims to move fast chemical weapon agent sensing technique from lab-top to prototype

In the same amount of time it takes to download software or print a picture, you now can detect a chemical weapon agent. Needless to say, technology is cool.

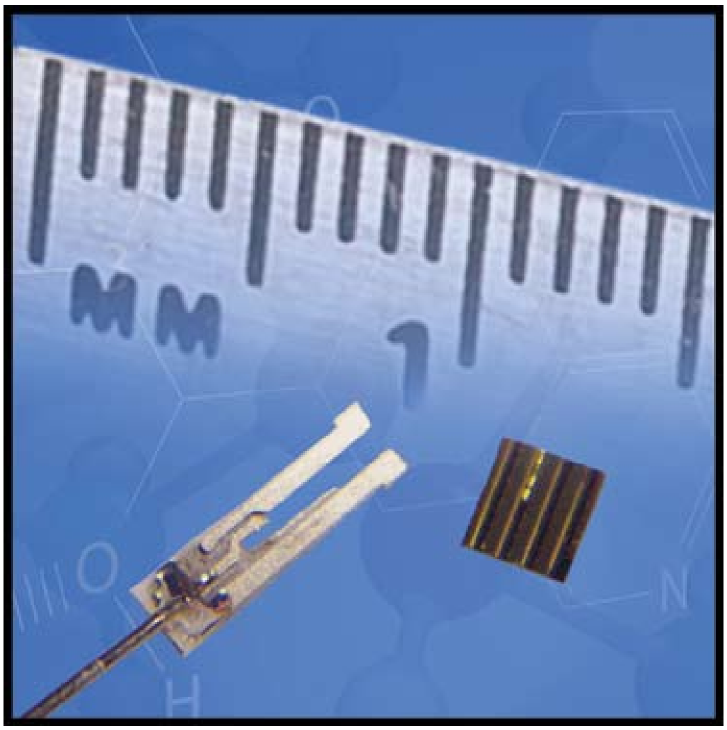
Researchers at Pacific Northwest National Laboratory have developed a sensor system that uses tiny lasers and tuning forks to detect chemical weapon agents at levels that can meet or exceed defense and homeland security chemical detection requirements. The system uses a technique called Laser Photo Acoustic Spectroscopy (LPAS) and a special sample concentrator, also developed at PNNL, that makes the technology extremely sensitive.

The new system, originally developed with funding from the Defense Advanced Research Projects Agency, is referred to as Quartz Photo-Acoustic Sensing, or QPAS. PNNL researchers are now free to pursue new clients to continue the systems development into application.

"The need for quick, accurate detection of harmful agents is not going to go away. We're excited about what we've developed and its applicability to a range of fields, such as homeland security, defense and, possibly, medical," said Michael Wojcik, a research scientist at PNNL.

LPAS is an exquisitely sensitive form of optical absorption spectroscopy, whereby a pulsed laser beam creates a brief absorption in a sample gas, which in turn creates a very small acoustic signal. A miniature quartz tuning fork acts as a microphone to record the resulting sound wave. In addition to LPAS, the technology uses infrared quantum cascade lasers, or QCLs.

To create QPAS, researchers paired multiple QCLs with the tuning forks, allowing simultaneous examination of a single sample at many infrared wavelengths. Nearly every molecule has unique optical properties at infrared wavelengths between 3 and 12 micrometers, and QCLs provide access to any wavelength in this region. "Because of this access and the fact that QPAS is almost immune to acoustic interference, the QPAS array has potential for excellent chemical sensitivity and selectivity," Michael said.



PNNL has demonstrated the ability of QPAS to detect gaseous nerve agent surrogates as part of a laboratory bench-scale sensor system consisting of the sample preconcentrator, an array of several QCLs and tuning forks and an automated computer data analysis program.

In one test of QPAS, researchers used diisopropyl methyl phosphonate, or DIMP, a chemical compound similar to sarin. QPAS detected DIMP well below the part-per-billion level in less than one minute. This miniscule level is similar to letting one drop of liquid DIMP evaporate into a volume of air that would fill more than two Olympic-size swimming pools.

While the new QPAS technology has big promises, it's small in stature, making it ideal for portable use in the field.

QPAS consists of several QCLs that can fit on a 3-by-3 millimeter chip, and tuning forks—identical to the kind used in wristwatches—measuring only 4 millimeters long, 2 millimeters wide and 0.3 millimeter thick.

A conceptual design for a battery-operated, prototype QPAS sensor, which includes 10 pairs of QCLs and tuning forks, would fit into a briefcase 12 inches long, 12 inches wide and 6 inches high—and the entire package would weigh less than 15 pounds.

"On an industry scale of one to nine, QPAS is at a technology readiness level of four," said Wojcik. "This means that while the technical components exist and initial testing is complete, the system still must be converted to a prototype. We're eager to take it to the next level." ●

PERSONALITY PROFILE

PNNL welcomes new Interim Laboratory Director

Mike Kluse

Starting the new year, Pacific Northwest National Laboratory had a change in laboratory directors. Len Peters, who had served as PNNL's laboratory director since 2003, transitioned into a new role with Battelle, which operates PNNL for the Department of Energy. Len's new assignment draws upon his extensive experience in education and science and technology management.

As laboratory director, Len guided PNNL to many successes while building upon its record as a world-class science and technology organization. PNNL business volume grew from $582 million to $750 million, and 330 staff joined its ranks. The Laboratory's safety and security culture improved significantly, earning recognition among its sister laboratories in the DOE system. Len also enhanced PNNL's partnerships with research universities in the region.

Mike Kluse, who has been serving as PNNL's associate laboratory director for national security, took over as interim laboratory director in January. Mike had been managing PNNL's national security business since transferring from Battelle's corporate headquarters in 1997.

Prior to his PNNL assignment, he served in a number of leadership positions since joining Battelle in 1976. Mike also served as an officer in the United States Air Force.

When Mike took over the helm as PNNL's interim laboratory director, he reaffirmed his commitment to keep the Laboratory focused on providing outstanding science and technology to meet national challenges in energy, environment and national security.

A top priority for Mike is to ensure the successful delivery of the Capability Replacement Laboratory Project—a multi-year effort to build new facilities and extend the life of existing ones on PNNL's campus. And since DOE announced it will recompete the contract to manage and operate PNNL, Mike also wants to help Battelle submit a winning proposal.

Building on a strong foundation of excellence in science and technology, management and operations, and community stewardship, Mike intends to keep PNNL moving forward as a world-class national laboratory. ●

NOTABLE *Achievements*

PNNL physicist named IEEE Fellow

Richard Kouzes

Pacific Northwest National Laboratory's Richard Kouzes, a nuclear physicist, was elected Fellow of the Institute of Electrical and Electronics Engineers (IEEE). This is the highest honor bestowed by the IEEE on individuals with an extraordinary record of accomplishments. Fewer than two percent of the organization's 356,000 members hold this grade.

A Laboratory Fellow, Kouzes holds a doctorate in physics from Princeton University. Currently working in PNNL's Computational and Information Sciences Directorate as chief scientist, Kouzes was previously the principal investigator and technical lead for the Radiation Portal Monitor Project. His guidance helped the project define the threat of illicit nuclear materials at U.S. borders and identify necessary monitoring equipment, leading to the successful deployment of radiation detection equipment along the country's borders.

His participation with the IEEE Nuclear and Plasma Sciences Society extends more than twenty years. Kouzes has held key positions with the society's administrative and technical committees and has served as its webmaster for the past six years. ●

PNNL scientist recipient of esteemed DOE award

John Zachara

In March 2007, Pacific Northwest National Laboratory environmental chemist John Zachara was honored with the Department of Energy's prestigious Ernest Orlando Lawrence Award. Zachara joins the ranks of five other PNNL scientists recognized with this award for his exceptional contributions in research and development that support DOE and its mission to advance the national, economic and energy security of the nation.

Zachara took home a gold medal, a citation and an honorarium of $50,000 for his accomplishment in the Environmental Science and Technology category. With years of expertise in soil chemistry, his research of how toxic metals travel in the subsurface of the DOE's Hanford Site is helping provide science-based environmental solutions with broad applications. Zachara also has been instrumental in bringing teams of top scientists to Hanford to collaborate with PNNL and Hanford scientists to resolve complex issues of subsurface contaminant migration.

PNNL's newest awards showcase airline safety and blackout prevention

Researchers at Pacific Northwest National Laboratory have been recognized again this year by the Federal Laboratory Consortium for their efforts in commercializing PNNL-developed technologies. Adding to the growing collection of more than 60 FLC awards—more than any other DOE laboratory—PNNL was honored this year with two Excellence in Technology Transfer Awards for the development and commercialization of The Morning Report and the Grid Friendly Appliance™ Controller.

The Morning Report is an aviation safety tool that analyzes massive amounts of aircraft operational data to identify patterns and events that could indicate potential safety concerns during flights. The technology collects aircraft data such as speed, wing angle, equipment status and engine temperature from thousands of flights per day. The information is analyzed using sophisticated statistical algorithms, and the system generates a report for the next morning.

Although the data-intensive programs used by the Morning Report are quite complex, the technology itself is easy to operate with a simple desktop application. Safety inspectors use the report to rapidly pinpoint anomalies, share information with other decision makers and possibly prevent accidents.

The Grid Friendly Appliance™ (GFA) Controller is a unique technology developed to more cost-effectively manage the operation of the nation's electric power grid and prevent possible blackouts. The GFA, a computer chip measuring 2 x 2.5 inches, can be installed on household appliances such as washers, dryers, refrigerators, air conditioners and water heaters and has the ability to turn them off for a few seconds at a time when the frequency of the power grid suddenly drops.

GFAs can be programmed to autonomously react in fractions of a second when a disturbance is detected, allowing the grid to stabilize, then turns the appliances back on automatically. The controllers have been installed on hundreds of clothes dryers and water heaters throughout the Pacific Northwest as part of a year-long test-bed demonstration project.

Fundamental Science Director Doug Ray

In defense of discovery science

When Isaac Newton described gravity, there probably were people who asked, "But what good is it? Will it keep apples from bruising when they fall?" Today, of course, Newton's mathematical description of gravity provides a foundation for many applications, from the thrust needed to launch satellites into space to calculations of the deposition of airborne contaminants on the ground.

Discovery science advances the frontiers of knowledge. When scientists discover how the world works, others can apply that knowledge to many problems. Answering difficult scientific questions ripples far beyond a specific technology problem.

Additionally, scientific research can fill gaps in our understanding of real-world concerns. "Use-inspired" research informs technology development and deployment. Without new knowledge, technology solutions are impossible.

In this section of Breakthroughs, we feature ways PNNL strengthens U.S. scientific foundations for innovation through original research. We also speak to providing tools, techniques and user facilities that enable the discovery process to move forward.

By advancing the frontiers of knowledge, we can ensure that our nation's most pressing concerns—energy security, environmental quality, national and homeland security—are tackled.

EMSL—a national scientific user facility marking 10 years of science

On October 1, the Environmental Molecular Sciences Laboratory (EMSL), a national scientific user facility operated by PNNL for the Department of Energy, will celebrate its tenth year of operation. Under the leadership of Allison Campbell, EMSL provides scientists worldwide with experimental and computational capabilities and onsite scientific expertise to address environmental molecular research. EMSL houses, under one roof, computational, nuclear magnetic resonance (NMR), mass spectrometry, and optical and imaging capabilities that focus on research in four science themes: atmospheric aerosol chemistry, biological interfaces and dynamics, geochemistry/biogeochemistry and subsurface science, and science of interfacial phenomena. These instruments often are not available to researchers elsewhere. Campbell discusses the past decade and the scientific direction of EMSL.

How has EMSL progressed scientifically during the past decade?

EMSL has become a true problem-solving environment where multiple experimental and computational capabilities are used together to address critical scientific challenges.

Our Scientific Grand Challenge concept is an excellent example where multiple instruments are used to address environmental and energy concerns. They involve teams of users from multiple institutions that focus on significant scientific challenges requiring EMSL capabilities for considerable periods of time. Two Scientific Grand Challenges are under way. One in the area of biogeochemistry is using integrated capabilities to understand how organisms exchange energy and electron flux with minerals—such as uranium—in soils, sediments and subsurface materials. Research results have implications for contaminant remediation. Another Scientific Grand Challenge addresses membrane biology and takes advantage of several capabilities to understand the network of genes and proteins that govern the structure and function of membranes and their components responsible for photosynthesis and nitrogen fixation in cyanobacteria, or blue-green algae. Results can positively impact bioenergy research. Both projects have published in prestigious journals such as *Journal of Bacteriology*, *Public Library of Science Biology* and *Proceedings of the National Academy of Science*.

Our focus on science themes is also designed to encourage researchers to take a multi-instrument approach to a scientific problem. For example, a combination of computational and experimental capabilities helped users from Washington State University and the University of Nebraska discover a class of gold atom clusters that are the first-known metallic hollow equivalent of the carbon buckyball. This breakthrough research was featured on the cover of *Proceedings of the National Academy of Science*. NMR and computing capabilities combined with computational chemistry software are providing users from Washington State University and the University of Alabama with an understanding of how biological systems effectively convert sunlight into chemical energy, to obtain insight into development of novel solar energy alternatives.

These are just a few examples of how EMSL's integrated problem-solving environment helps users answer questions critical to DOE missions and the nation.

What are examples of capabilities EMSL has developed and/or deployed to enable user science?

EMSL has a history of developing and/or deploying "marquee" and state-of-the-art instruments supporting research important to DOE and the nation. The facility footprint was designed with the 900-MHz NMR spectrometer in mind. The system was delivered in 2002 and today remains one of the world's highest-performance wide-bore NMR systems. The system has supported several leading-edge research projects, such as a University of Washington study of mutations in proteins implicated in breast and ovarian cancers and Penn State-led research designed to gain an understanding of how strontium contaminants—the most abundant radionuclide in Hanford Site tank waste—can be contained in clay soils.

Another area where our instrumentation has become increasingly robust is mass spectrometry. A powerful 12-tesla magnet, one of a handful in existence, joined our suite of mass spectrometers in 2004. Our users depend on these systems for proteomic studies of biological and national security importance. For example, a study conducted by users from PNNL and UCLA identified nearly 8,000 different proteins in a mouse brain; in turn, this information is being used to study the connection between cell damage and neurodegenerative diseases such as Parkinson's and Alzheimer's. PNNL researchers also are using these capabilities to conduct one of the largest studies of vaccinia virus, a poxvirus nearly identical to smallpox; the study is expected to support development of improved antiviral drugs and vaccines to combat poxvirus outbreaks potentially resulting from a biological threat.

Our researchers and users are also increasing the productivity and sensitivity of our mass spectrometers by developing award-winning systems to manage and store massive amounts of data generated by experiments as well as capabilities that significantly accelerate proteomic analysis and provide unprecedented accuracy and depth of data.

What does EMSL hold for the future?

▲ EMSL Director Allison Campbell

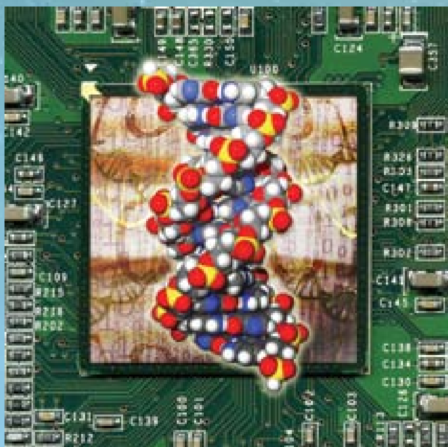
EMSL will continue to contribute substantially to DOE missions by combining computational science expertise with experimental observation. Our users will continue to address critical environmental problems by investigating fundamental questions related to reducing emissions, cleaning up the DOE weapons complex, and stabilizing waste forms. We will play a major role in the post-genomics arena by developing advanced tools that enable scientists to determine protein expression levels rapidly and with high accuracy. EMSL's research measurement science and the development of tools and techniques for detecting and characterizing biological and chemical species are vital to our nation.

We will execute a recapitalization effort aimed at maintaining EMSL at the scientific forefront. The effort will extend over the next 5 to 8 years at a cost of $50 million to $70 million. User and stakeholder input has resulted in a refreshment plan that will bring enhanced capabilities in nuclear magnetic resonance; mass spectrometry, such as the world's first 21-tesla system; an operando transmission electron microscope, which will help users unravel the mechanisms of interfacial reactions of importance in environmental remediation and catalysis; and a next-generation supercomputer.

We also recently celebrated our first permanent expansion—space where a portion of our new supercomputer and data archive capabilities will be located. In March, we broke ground on a new office wing that will house nearly 100 staff and users. We will also continue to work with our client to develop radiological capability and further expand the facility.

With continued growth of EMSL and its capabilities, we expect another decade filled with great science.

SCIENTIFIC DISCOVERY



Researchers in the Biopilot project are developing new and innovative software to help solve data-intensive computational problems in biological research.

Data-intensive computing laying foundation for biological breakthroughs

Biological breakthroughs to solve society's most challenging problems require innovative tools and a "different way" to analyze the enormous amounts of data being generated.

Finding this way is the goal of the Data-Intensive Computing for Complex Biological Systems (Biopilot) project—a joint research effort between the Pacific Northwest National Laboratory and Oak Ridge National Laboratory funded by the Department of Energy's Office of Advanced Scientific Computing Research. The two national laboratories are teaming to support areas of biological research in urgent need of data-intensive computing capabilities.

Recent advances in high-throughput technologies have generated an explosion of biological data. "Conventional software isn't able to efficiently deal with such massive data sets," said project lead T.P. Straatsma, a PNNL senior scientist. The Biopilot project is developing innovative and robust software solutions to address large-scale, data-intensive computational problems in biology and to make these new capabilities available to the biology community.

"To really understand biological systems, we must integrate its complex networks and pathways for a coherent understanding of the system," Straatsma said. "The more different types of data you can integrate, the deeper are the biological insights. Our goal is to create an integrated suite of highly flexible, very adaptable computational tools for large-scale data sets that will be used to address specific challenges facing DOE and our society."

Researchers in the Biopilot project are focusing on three areas: peptide protein identification and quantification algorithms for mass-spectrometry proteomics, massively parallel solutions for high-throughput comparative genomics, and large-scale integration of molecular and network modeling and simulation with bioinformatics approaches.

"The ability to process and analyze massive amounts of data and information in real time is powerful in making breakthroughs and solving complex problems," Straatsma said. "The Biopilot project will play a major role."

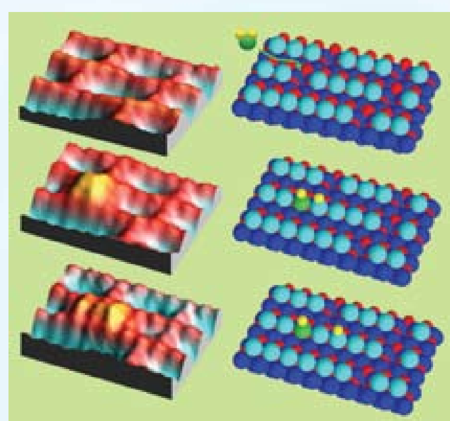
Hopping hydrogen

The behavior of individual hydrogen atoms on titanium oxide surface reveals intriguing details about a popular oxide catalyst

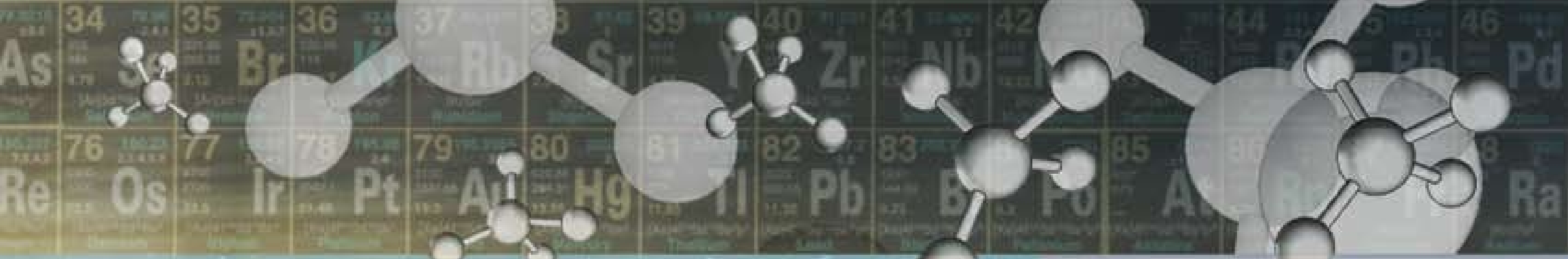
Researchers at Pacific Northwest National Laboratory and the University of Texas at Austin discovered that a single hydrogen atom just can't keep still after it splits from a water molecule on the surface of the catalyst rutile titanium oxide. The hydrogen atom hopscotches across the oxygen atoms that stud the surface of the catalyst, while the hydrogen on what is left from water remains fixed, suggesting that the electronic structure of this popular catalyst is not entirely as it seems.

By understanding how water's atoms behave on the catalyst surface, scientists and engineers may be able to develop technologies that use abundant, free sunlight to split water to generate hydrogen gas, a possible alternative fuel for everything from heating homes to powering automobiles.

The researchers plan to study the titanium oxide material at higher temperatures to see how fast the hydrogen atoms move. They are also working on developing a detailed understanding of the underlying mechanisms and involved intermediate species.



Scanning tunneling images (left, from top) show atoms on the titanium oxide catalyst surface before and after water adsorption and after hydrogen hopping. Light blue oxygen atoms appear as depressions, red titanium atoms as protrusions. Yellow indicates hydrogen atoms from the water molecule. On the right is a model showing water splitting.



Cytochrome studies provide biofuel cell potential

Electrical charge measurements may point way to miniature biofuel cell development

Researchers from Pacific Northwest National Laboratory and collaborators have purified the protein called outer membrane cytochrome A (OmcA) from *Shewanella oneidensis*, a bacterium with promise for bioremediation of contaminants and the design of microbial fuel cells. They have measured its ability to bind and transfer electrons to mineral hematite, a solid ferric oxide. The team has shown that purified OmcA can directly reduce solid metals and that purified proteins are a next step in biofuel cell development. The work appeared in the November 1, 2006, issue of the *Journal of the American Chemical Society*.

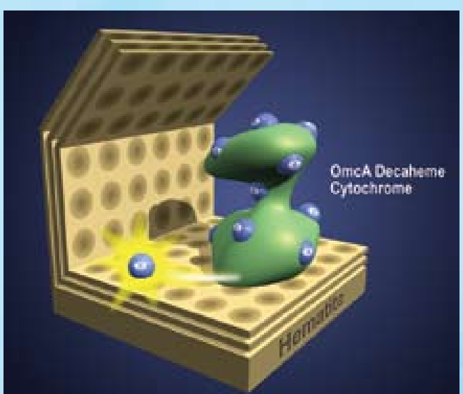
"We showed that you can directly transfer electrons to a mineral using a purified protein, and I don't think anyone had shown that before," said Thomas Squier, PNNL senior author and Laboratory Fellow. The feat is the bacterial equivalent of removing lungs and coaxing the disembodied tissue to breathe.

Bio-cells use enzymes to oxidize reduced materials in the cells and release electrons. An optimal enzyme system would directly transfer electrons captured from a chemical reaction to an electrode surface—ideally, to use enzymes immobilized on the surface of an electrode. Lack of a membrane permits miniaturization for use in biomedicine or other remote applications where self-sustaining systems are needed.

PNNL staff scientist Liang Shi devised a new protein expression system that enabled the team to isolate sufficient amounts of protein. The researchers used techniques including fluorescent correlation spectroscopy and confocal microscopy to measure protein-mineral binding. These measurements yielded a "fluorescence intensity trace" whose brightness depended entirely on whether hematite was available to bind with OmcA in solution. No hematite, dim; hematite, bright. In addition to binding, they also detected direct electron transfer from OmcA to the hematite.

Using pure protein opens up the possibility of shrinking biofuel cells to power small electronic devices, according to Squier. Whole-organism biofuel cells require engineers to design a space-adding membrane that prevents unwanted reactions between fuel, the charge-transporting agent and the electron-accepting metal that carries electricity to the device. In purified protein fuel cells, the seal made by the protein coating on the electrode acts in place of the membrane.

The work was performed at the Environmental Molecular Sciences Laboratory as part of the Department of Energy's Genomics: GTL and Biogeochemistry Grand Challenge programs.



Artist's depiction of purified, electrified bacterial cell outer membrane protein binding with and passing electrons to the iron-rich mineral hematite. In this purified-protein fuel cell, the seal made by the protein coating on the electrode effectively acts in place of a membrane necessary in whole-organism biofuel cells. Eliminating the membrane could aid the design of bioreactors to power small electronic devices.

In Niamey, Niger, the ARM Mobile Facility collected atmospheric data from January through December 2006.

Dust in the wind

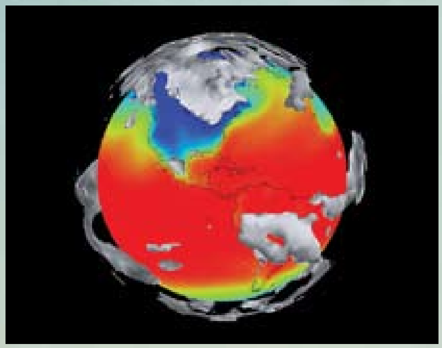
In March 2006, a major dust storm occurred in Niamey, Niger. Although a common occurrence, this was the first time both satellite- and ground-based instruments were used simultaneously to assess the impact of airborne Saharan dust on incoming and outgoing solar radiation. Pacific Northwest National Laboratory scientists involved in the study are members of the science team for the Department of Energy's Atmospheric Radiation Measurement (ARM) Program. For this study, the researchers gathered data obtained from satellite observations and from the ARM Mobile Facility (AMF), a portable atmospheric research facility, temporarily deployed to Niamey. They entered these measurements into climate models to see how well the models would simulate the impact of the dust on the solar radiation balance. Using a broader data set from the AMF deployment, PNNL researchers will calculate the long-term warming and cooling effects of Saharan dust and the warming and cooling effects of aerosols in climate models.

Aerosol particles and cloud droplets—microscopic modulators of climate

Scientists around the world use sophisticated computer models to simulate future scenarios of all types—including global climate. Researchers at Pacific Northwest National Laboratory are playing a key role in the improvement of these models by providing new information about the role of aerosols in the atmosphere.

Aerosols are tiny particles that are continually present in Earth's atmosphere as the result of either natural or manmade processes. Whether in solid (smoke, dust) or liquid (sea salt, sulfuric acid) form, aerosols affect Earth's climate in two ways: directly, through scattering and absorption of solar and infrared radiation, and indirectly, by influencing the creation of cloud droplets. More cloud droplets leads to increased surface area, in turn increasing the amount of energy reflected from the clouds and back into space. The degree to which these different aerosol effects impact the Earth's energy balance is a critical element in climate simulations.

In spring 2006, a technique for aerosol treatment developed by PNNL researchers was implemented in the Community Climate System Model (CCSM), one of the world's leading global climate models. Prior to that time, the model did not take into account the indirect effect of aerosols, which is considered a major contributor to the energy feedbacks that modulate Earth's climate.



Scientists use the Community Climate System Model to increase their understanding of the world's climate patterns and learn how they may affect regions around the globe.

Steve Ghan, a PNNL staff scientist who developed the new aerosol treatment, worked with researchers at the National Center for Atmospheric Research, where the CCSM is maintained, to analyze the results from the new simulations.

"As expected, there are significant differences from the previous version of the model," said Ghan. "The new version is sensitive to treatment of aerosols, and that's what we're concentrating on now."

Ghan and his PNNL colleagues are implementing a new scheme for aerosol treatment in the CCSM that includes aerosol particles within cloud droplets. They expect this to improve the simulation of cloud-aerosol interactions by allowing for a more realistic treatment of cloud effects on aerosols, as well as aerosol effects on clouds.

On thin ice

Thin clouds high in the upper troposphere, like cirrus clouds, may have a significant influence on Earth's climate and enhance the "greenhouse effect" by absorbing more of the sun's radiation than they take in. Unknown is how ice crystals in these clouds absorb and reflect radiant energy and enhance the amount of radiant energy emitted toward the earth's surface.

Pacific Northwest National Laboratory scientists who are part of a science team supported by the Department of Energy's Atmospheric Radiation Measurement Program have found that upper tropospheric clouds cannot be detected by most remote sensors. This is unfortunate because these clouds, which are found 9 miles above sea level, may contribute significantly to the radiative heating of the upper troposphere.

To better understand the properties of these clouds, the scientists need to know the size, shape, density and microphysical properties of the ice crystals within the cloud. Upper tropospheric clouds are difficult to measure because they are continuously changing and their size distribution and habit are not well characterized.

To understand these types of clouds, scientists rely on a variety of complex mathematical formulas—called retrieval algorithms—to estimate the microphysical properties of clouds. The ground-based algorithms are compared with in situ measurements made by airborne sensors and satellite-based algorithms. Accurate retrievals are important for understanding the radiative feedback of high clouds and parameterization development for global climate models. Scientists will use these results to help develop combined retrievals that choose the best algorithm based on atmospheric conditions.

PNNL manages two DOE field research sites for studying contaminant transport

New program enables multidisciplinary research, data sharing

Two Department of Energy sites contaminated by uranium are now field sites where research results will lead to cleanup strategies. Pacific Northwest National Laboratory manages the sites as part of the new Integrated Field-Scale Subsurface Research Challenge sponsored by DOE's Environmental Remediation Sciences Division. Site studies will enable large interdisciplinary teams to understand and simulate processes affecting contaminant transport.

The sites also provide capabilities to other ERSD investigators to collect, permit and ship environmental samples and gives access to others to test subsurface contaminant fate and transport concepts or techniques.

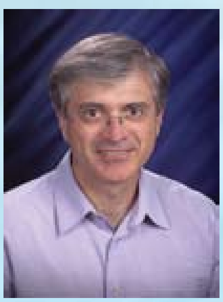
In the 300 Area at DOE's Hanford Site, a multidisciplinary team will evaluate hypotheses related to a uranium plume that resulted from nuclear fuel fabrication from 1943 to 1975. The team will use an innovative monitoring array for experiments on contamination in the vadose zone—the area from the top of the ground surface to the water table, through aquifers, to final discharge to the Columbia River.

The second field study is at a uranium mill tailings site in Rifle, Colorado. A diverse team of researchers is examining the stimulation of subsurface microorganisms to reduce and immobilize uranium in place. They hope to understand the microbial factors and associated geochemistry controlling uranium movement.

Photo: Bob Peterson

Approximate location of Washington State test site.

Climate change beginning to show in the environment, experts say



Tony Janetos

"We shouldn't leave this world worse off than when we came into it," said Tony Janetos when explaining why he helped co-author a newly released assessment of climate change impacts and adaptations from the Intergovernmental Panel on Climate Change. "There are only one or two environmental issues that will affect us 100 years or more into the future, and we have an obligation to tell people what it will take to adapt technologically and economically," he concluded.

While the April 2007 IPCC report, *Working Group II, Impacts, Adaptation and Vulnerability*, does not make policy recommendations, it does recount the current impacts of climate change on natural resources with more certitude. "The last time Working Group II issued a report on impacts and adaptations, you couldn't make a claim (of natural resource impacts) as clearly as we can today," Janetos said.

The chapter Janetos helped to write is a first for the IPCC, which has issued three sets of climate change reports for the United Nations Environment Programme and World Meteorological Organization since 1990. The chapter, "Perspectives on Climate Change and Sustainability," examines the options for coping with climate change and its effect on sustainable development in poor nations. Janetos and his co-authors found that climate change will present serious potential challenges to the goal of sustainable development and make it more difficult to produce nutritious food, clean water and livable conditions in these countries.

But does Janetos think that we have lost the climate change battle? No. He counts himself a pragmatist, principally because of his work as director of the Joint Global Change Research Institute. "We are beginning to understand what it would take, both technologically and economically, to reduce or limit changes from greenhouse gas emissions." At JGCRI, a partnership between Pacific Northwest National Laboratory and the University of Maryland, scientists model interactions between the environment and human activities to better understand technology strategies for limiting the scope of climate change and perform vulnerability and adaptation studies for adapting to these changes.

"These reports are meant to inform, not set policy," Janetos firmly replied when asked about recommendations. "They help people who have a lot of crucial decisions staring them in the face to make better decisions because they contain the latest information from the scientific community."

Iron nanoparticles could lead to more effective carbon tetrachloride cleanup

Researchers at Pacific Northwest National Laboratory, the University of Minnesota and Oregon Health and Science University discovered that not all iron nanoparticles are created equal. Some, in fact, may be especially useful for cleaning up groundwater contaminated with carbon tetrachloride.

In the past, carbon tetrachloride was used for various purposes by industry and government. Today, it is found in the soil and groundwater at sites around the country. Exposure to high levels of this chemical can damage the liver, kidneys and nervous system.

"Nanoparticles could find use in remediating deep inaccessible groundwater plumes, where other remediation technologies cannot be used cost-effectively," said James Amonette, PNNL senior research scientist.

When carbon tetrachloride reacts with iron particles, the carbon tetrachloride breaks apart. Some of the products that can be produced are harmful, such as chloroform. Others are completely benign, such as water. The researchers' challenge was to figure out how to tip the balance of this reaction to the safest possible products.

The research team characterized iron nanoparticles from a wide variety of sources. They discovered that one type of iron nanoparticle in particular produced much less chloroform than the other particles.

Then, the team determined the specific properties of this type of nanoparticle to understand why carbon tetrachloride followed the more benign reaction path. The team characterized the particles using x-ray diffraction and x-ray photoelectron spectroscopy in DOE's Environmental Molecular Sciences Laboratory. At OHSU, the researchers performed electrochemical studies using an electrode designed especially for nanoparticles.

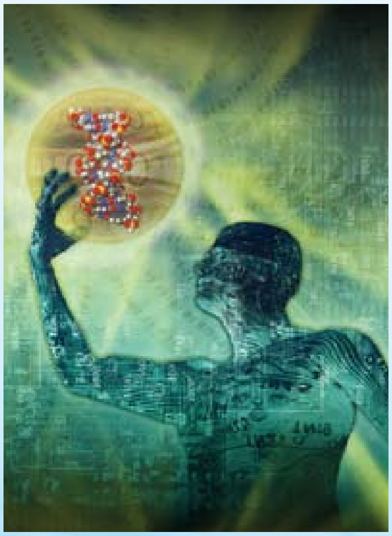
Based on the results of this fundamental research, the team believes they have identified the key contributors to chloroform formation. This new information could be used to help select and design iron nanoparticles for future carbon tetrachloride remediation efforts.

Discovering the details of dissolution

New combination of technologies gives insights into one of the most fundamental chemical reactions

Ions in a liquid are like celebrities at a movie opening—surrounded by fans who jostle each other to get as close as the velvet ropes around the red carpet will allow. So it is with ions in water or other liquids or solvents. At Pacific Northwest National Laboratory and Argonne National Laboratory, researchers brought together an unusual combination of theoretical and experimental approaches to determine the number, relative positions and motions of the liquid molecules surrounding ions. This is an initial step in developing fundamental principles that explain how ions move in complex systems.

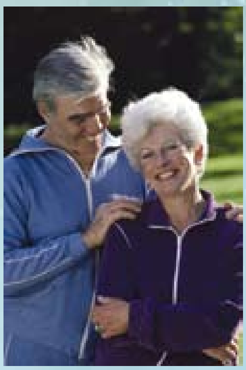
By combining two techniques that are not commonly used together, the team created simulations, or short video clips, that show the location of the ions and the water molecules. The first technique, known as extended x-ray absorption fine structure spectroscopy, uses x-rays to probe the relative positions of atoms in a solution. The second technique uses advanced calculations and molecular modeling to simulate the structure and motion of relevant systems. The team showed the model's accuracy by comparing it to laboratory measurements.



Researchers brought together theoretical and experimental approaches to learn more about the liquid molecules surrounding ions. The knowledge of the structure formed by the ion and the first layer of surrounding solvent molecules has broad applications, from understanding how pollutants move in the soil to how neurotransmitters work in the brain.

This research was funded by the Department of Energy Office of Basic Energy Sciences.

Brain 3D mapping to combat neurodegenerative disease



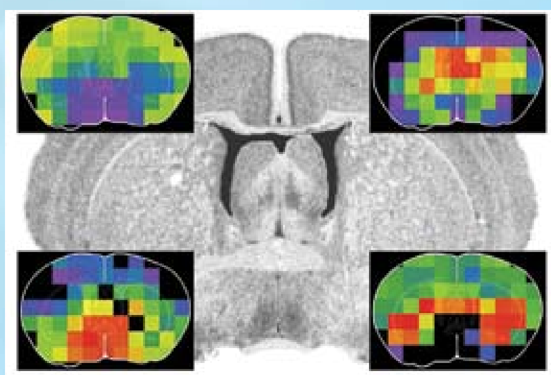
Wanda felt a jolt of frustration run through her when her husband forgot to meet her at the clubhouse after their round of golf. How many times had this happened lately? It was becoming an embarrassment. Later that evening, Wanda noticed that Robert seemed to be staring at the TV rather than watching it. She was becoming concerned. He had been a bit moody lately in addition to his increasing forgetfulness. Were these symptoms of something serious, she wondered?

Neither Robert nor Wanda was prepared for the devastating news that Robert had Alzheimer's disease, a progressive brain disorder that gradually destroys a person's memory and ability to learn, reason, make judgments, remember specific words and even carry out daily activities. As Alzheimer's progresses, individuals may also experience changes in personality and behavior. Today, more than 5 million people in the United States are living with Alzheimer's disease. The cost of caring for people with the disorder is $100 billion per year in the United States alone.

Although currently no cure for Alzheimer's exists, new treatments are on the horizon as a result of increasing insight into the biology of the brain. Research now being performed at DOE's Environmental Molecular Sciences Laboratory may accelerate the development of a cure for Robert and others with neurodegenerative disorders such as Alzheimer's, Parkinson's or multiple sclerosis through advanced 3D mapping of brains.

As part of their research, scientists at Pacific Northwest National Laboratory have demonstrated a technological platform for spatial mapping of mouse brain proteins. The protein map is "the first to apply quantitative proteomics to imaging," says Richard D. Smith, Battelle Fellow at PNNL.

A key challenge in neuroscience derives from the molecular complexity of the brain; about one-third of the mammalian genome appears to be dedicated exclusively to brain function. Armed with information such as the types and locations of biomolecules within the mammalian brain—the organ with the most complicated 3D structure—scientists can begin to understand the origin and progression of brain diseases.



Brain proteomics in 3D: Abundance profiles of four different proteins (of more than 1,000 proteins) compiled from 1-millimeter cubes (voxels) in a mouse brain. The boxes correspond to the locations of the voxels in the brain, and the colors represent their relative abundance in each region (from high, red, to low, violet).

Current imaging techniques provide only limited protein identification—typically, only one or a few proteins at a time—in spite of good spatial resolution technology. For the first time ever, scientists have been able to detect over 1,000 different proteins in a single experiment and map them to the brain structures. "Proteins are the lead actors, the most important part of the picture," PNNL's Smith says. "They are the molecules that do the work of the cells."

To produce the map, the team of scientists characterized brain pieces in scores of small 1-millimeter cubes, or voxels, to see where proteins appear in the brain and where they vary in abundance. By labeling all proteins from another mouse brain, they developed reference points to compare the amounts of protein in the different parts of the brain and from one mouse to another. Their research represents a step toward the complete characterization of the detailed spatial abundance patterns of the brain proteome and provides a methodological basis for future studies. The integrated methodology includes tissue voxelation, automated microscale sample processing, use of reference samples for quantification, high-throughput analysis and a strategy for identifying proteins based on precisely measured masses of the molecules using advanced mass spectrometers.

The next steps for this team of researchers are to use their methodology to develop a 3D visualization of an entire mouse brain and then compare proteome maps for healthy brains with others whose protein portraits look different. Because contrasts in location and abundance of proteins may display the earliest detectable stages of neurological diseases, scientists hope neurodegenerative diseases such as Alzheimer's might be curbed if caught and treated early enough, giving patients and their families a new hope.

Surplus electricity could "fill up" plug-in vehicles

Plug in your car. Unplug foreign oil, greenhouse gases and other emissions that contribute to urban smog.

A new study by Pacific Northwest National Laboratory has found that off-peak electricity production and transmission capacity could fuel 70 percent of the 220 million cars, light trucks, SUVs and vans on the road today—if they were plug-in hybrid electrics.

The study, performed for the Department of Energy, also suggests that replacing gasoline-powered vehicles with vehicles powered by off-peak electricity could improve urban air quality and potentially reduce expected increases in electricity rates by using the current infrastructure more effectively without building new power plants and power lines.

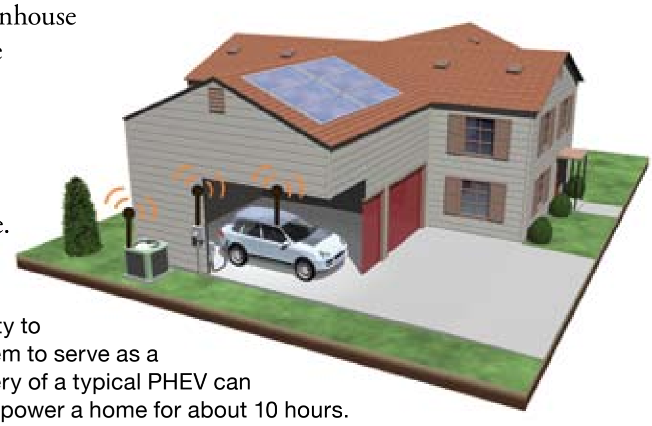
Batteries for plug-in hybrid electric vehicles, or PHEVs, will easily store enough energy for the national average commute, about 33 miles a day. Researchers found that if drivers charged up overnight when demand for electricity is low, most regions of the country would have plenty of off-peak generation, transmission and distribution capacity to provide for that region's PHEVs.

The impact on national security could be significant. "Since gasoline consumption accounts for 73 percent of imported oil, it is intriguing to think of the national security benefits if our vehicles switched from oil to electrons," said PNNL energy researcher Rob Pratt.

The extra electricity needed to power PHEVs would come from coal-fired and natural gas-fired plants. Even though these power plants emit greenhouse gases, overall levels would be reduced because it is more efficient to move a car one mile using electricity than producing gasoline and burning it in the car's engine.

Another long-term benefit is that the steady demand for electricity is likely to spur investments in cleaner coal-fired power plants.

"PHEVs would increase residential consumption of electricity by about 30-40 percent depending on how many PHEVs we will own. The increased generation could lead to replacing aging coal-fired plants sooner with newer, more environmentally friendly versions," said PNNL scientist Michael Kintner-Meyer.



An added benefit of plug-in hybrid vehicles is their capacity to store energy, which allows them to serve as a back-up power unit. The battery of a typical PHEV can produce enough electricity to power a home for about 10 hours. So, while the vehicle is parked in the garage or at work, its energy reserves could be used by utilities for a fee.

Pacific Northwest National Laboratory

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