Pacific Northwest National Laboratory

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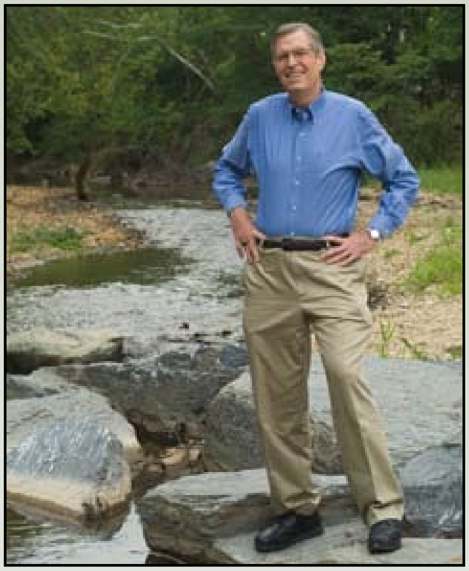
FY 2007

Key Accomplishments

FUNDAMENTAL SCIENCE DIRECTORATE

Atmospheric Science & Global Change

PNNL Scientists, Computer Model Make Key Contributions to Major Climate Report



Laboratory Fellow Jae Edmonds leads the Global Energy Technology Strategy Program at PNNL with active collaborations in more than a dozen institutions. He is well known for his contributions to the integrated assessment of climate change and the examination of interactions among energy, technology, policy and the environment. He has frequently testified before Congress and briefed the Executive Branch of the U.S. Government.

What forces will shape the 21st century's global energy and economic systems? A new report released by the U.S. Climate Change Science Program strives to answer that question and more. The report provides a long-term, global reference for greenhouse gas stabilization scenarios and an evaluation of the process by which scenarios are developed and used. The report shows that stabilizing the concentration of carbon dioxide—the most important greenhouse gas released by human activities—requires global emissions to peak in the 21st century and then decline indefinitely thereafter. Pacific Northwest National Laboratory's integrated assessment model, MiniCAM, was one of three models used to analyze emissions scenarios.

"This report is the first major assessment of the energy, economic and land-use implications of stabilizing global change," said PNNL scientist Jae Edmonds, a co-author for the report. He added that the report is also the first major assessment since the *Special Report on Emissions Scenarios,* published in 2000 by the Intergovernmental Panel on Climate Change.

Along with Edmonds, Leon Clarke and Hugh Pitcher, all PNNL scientists at the Joint Global Change Research Institute, co-authored sections of the report. In addition, Clarke was the leader for the overall study.

Edmonds and colleagues at the Joint Global Change Research Institute originally developed and continue to refine the MiniCAM. It was chosen as one of three "integrated assessment" models used to develop the scenarios evaluated in Part A of the report. Integrated assessment models are analysis tools that combine information pertaining to economic, energy and climate variables across various scientific disciplines, time and spatial scales.

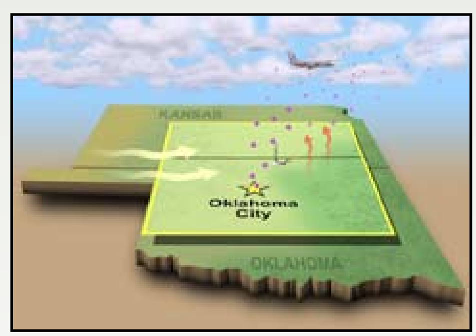
Clarke, L, J Edmonds, J Jacoby, H Pitcher, J Reilly, R Richels, E Parson, V Burkett, K Fisher-Vanden, D Keith, L Mearns, C Rosenzweig, and M Webster. 2007. *Scenarios of Greenhouse Gas Emissions and Atmospheric Concentrations (Part A) and Review of Integrated Scenario Development and Application (Part B). A Report by the U.S. Climate Change Science Program and the Subcommittee on Global Change Research.* U.S. Department of Energy, Office of Biological & Environmental Research, Washington, D.C., 260 pp.

Researchers Combine Atmospheric Science with Heartland Farming

Two major scientific field studies were conducted in Oklahoma to investigate major uncertainties in climate models: aerosols and clouds. The $5.5 million multi-partner effort was coordinated by PNNL and sponsored by the U.S. Department of Energy. It included nine scientific aircraft and dozens of ground-based instrument platforms. These capabilities allowed researchers to obtain data during a key season in the region, the winter wheat harvest, which coincides with fields of fair-weather clouds throughout the Midwest.

The Cloud and Land Surface Interaction Campaign, or CLASIC, explored how changes in land use affect clouds through changes to surface heating and associated dynamics. It focused on the Southern Great Plains site in Oklahoma, managed by the Atmospheric Radiation Measurement Program's Climate Research Facility. The second campaign, called the Cumulus Humilis Aerosol Processing Study, or CHAPS, investigated the interactions of aerosols on clouds and of clouds on aerosols from Oklahoma City.

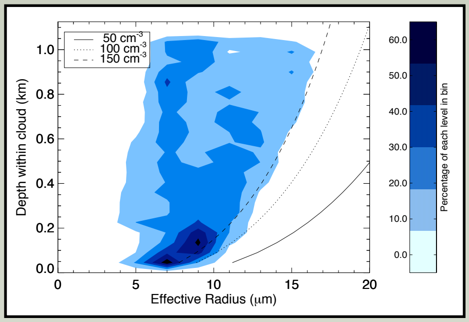
These campaigns represent the culmination of nearly two years of preparation and coordination among the participating organizations, including the National Oceanic and Atmospheric Administration, National Aeronautics and Space Administration, U.S. Department of Agriculture, numerous national laboratories, DOE user facilities and universities.



The primary goal of the CHAPS campaign was to characterize and contrast freshly emitted aerosols above, within and below fields of fair-weather cumulus clouds. These observations will be used to examine the aerosol optical properties and cloud nucleating properties from below, in and above clouds, and how they differ downwind of a mid-size city relative to similar aerosols in air less affected by emissions.

Shallow Clouds Make the Case for Remote Sensing Instrumentation

Findings from a recent study on cloud formation by PNNL and its collaborators show that thin, low-lying cumulus clouds are significantly diluted by mixing with surrounding dry air. The study also shows that mean cloud droplet size varies significantly relative to a droplet's height and position within the cloud. This level of detail is important for accurately representing cloud properties in climate models. The study also illustrates the utility of using remote sensing data to validate models of cloud microphysical processes—such as water condensation, evaporation and conversion of cloud water to rain—which typically are used in studies concerning these shallow cumulus clouds.



Lines indicate theoretical calculations of cloud droplet size for clouds with various droplet concentrations in which no mixing occurs. The cloud droplet size shows significant variability with height.

Properties of shallow clouds, such as those examined by this study, play an important role in the Earth's energy balance. The effects of aerosols on clouds, particularly the influence of aerosols on cloud droplet size and distribution, are major sources of uncertainty in climate models. Modeling these effects requires assumptions about how clouds and their properties might be impacted by the mixing of dry and cloudy air. To constrain models, observations of the relationship between mixing and cloud droplet size are needed.

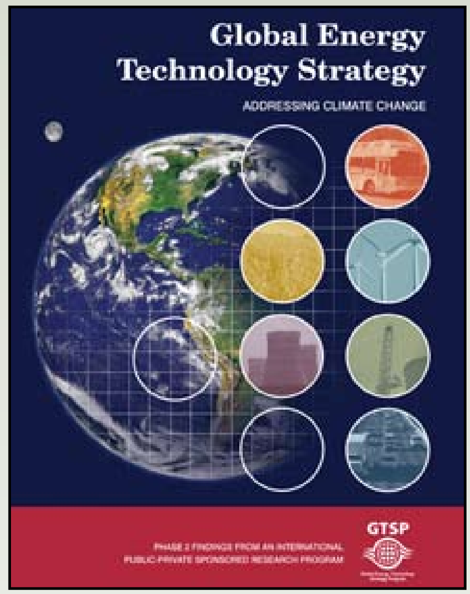
McFarlane, SA, and WW Grabowski. 2007. "Optical Properties of Shallow Tropical Cumuli Derived from ARM Ground-Based Remote Sensing." *Geophysical Research Letters* 34:L06808.

Landmark Report Documents Role of Technology in Addressing Climate Change

The cost of stabilizing atmospheric concentrations of greenhouse gases can be reduced by trillions of dollars in this century if current energy technologies are improved and emerging ones are developed and deployed, according to a report from the Global Energy Technology Strategy Program.

The May 2007 report, *Global Energy Technology Strategy,* summarizes nearly a decade of research on the role technology will play in addressing climate change. The report examines the potential relative contributions and costs of six energy technology classes used in combination to reduce greenhouse gases. The analysis is the first to delve deeply into the economics of the potential solutions, helping decision-makers balance the costs of energy technology development against other societal priorities. The report also outlines the research and development needed for each technology area and the benefits of including greenhouse gases other than carbon dioxide in the technology strategies.

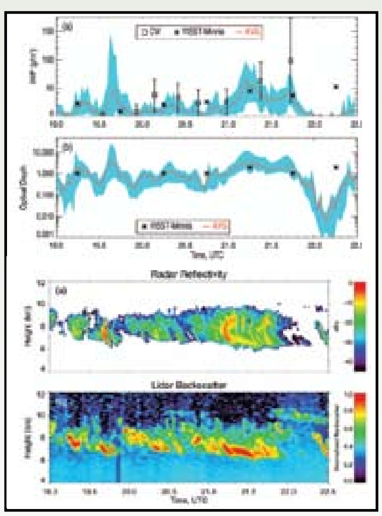
Edmonds, JA, MA Wise, JJ Dooley, SH Kim, SJ Smith, PJ Punci, LE Clarke, EL Malone, and GM Stokes. 2007. *Global Energy Technology Strategy Addressing Climate Change: Phase 2 Findings from an International Public-Private Sponsored Research Program.* Battelle, Columbus, Ohio. Online at http://www.pnl.gov/gtsp.



Retrieval Algorithms for Ice Clouds Remain Slippery

As part of a science team supported by DOE's Atmospheric Radiation Measurement Program, PNNL researchers specializing in ice cloud properties found that thin clouds (optical depth less then 0.3) are often below the detection level of most remote sensors. Yet, these clouds may play a significant role in the radiative heating in the upper troposphere, particularly in tropical regions where cirrus clouds persist at extremely cold temperatures. This data gap represents one of the key uncertainties in climate model simulations—how ice crystals in cirrus clouds absorb and reflect radiant energy, and in some cases, enhance the amount of radiant energy emitted towards the Earth's surface.

Like cirrus clouds, upper tropospheric clouds are found at altitudes of about 9 miles above sea level. An important aspect of understanding the radiative feedbacks of upper tropospheric clouds is being able to measure the size, shape, density and other microphysical properties of the ice crystals within the cloud. The microphysical properties of cirrus clouds are difficult to measure and model because they are highly variable in nature and their ice crystal size distribution and habit are not well characterized. However, these clouds are important modulators of the Earth's energy balance and climate because they reflect less incoming solar radiation and absorb more infrared radiation than water clouds, in essence enhancing the "greenhouse effect."



Radar reflectivity and lidar backscatter of cirrus clouds demonstrate the optical depth range of cirrus clouds.

Comstock, JM, R d'Entremont, D DeSlover, GG Mace, SY Matrosov, SA McFarlane, P Minnis, D Mitchell, K Sassen, MD Shupe, DD Turner, and Z Wang. 2007. "An Intercomparison of Microphysical Retrieval Algorithms for Upper-Tropospheric Ice Clouds." *Bulletin of the American Meteorological Society* 88:191-204.

Biological Sciences

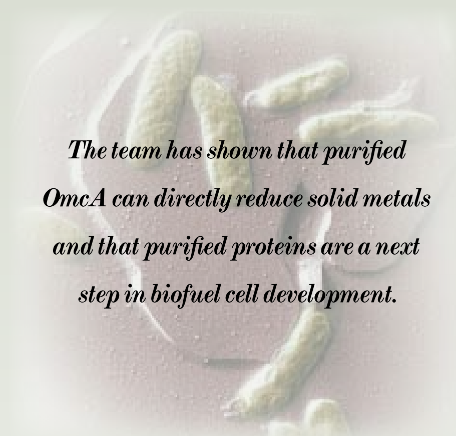
Cytochrome Studies Provide Biofuel Cell Potential

Laboratory Fellow Tom Squier, a key contributor on the cytochrome study, is well known for his biological research in calcium homeostasis and transport as well as his work in cellular adaptation methods. Squier strongly believes in giving back to the scientific community, mentoring both graduate students and staff at PNNL.

Researchers from Pacific Northwest National Laboratory and collaborators from the U.S. Department of Energy's Biogeochemistry Grand Challenge have purified the protein called "outer membrane cytochrome A or OmcA" from *Shewanella oneidensis,* a bacterium with promise for bioremediation of contaminants and the design of microbial fuel cells. The researchers have measured the microbe's 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.

Purified proteins could funnel the electrons right into a surface of a conductor, providing the first step to building a biofuel cell—using proteins only, not live cells. 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.

Xiong, Y, L Shi, B Chen, MU Mayer, BH Lower, Y Londer, S Bose, MF Hochella, JK Fredrickson, and TC Squier. 2006. "High-Affinity Binding and Direct Electron Transfer to Solid Metals by the *Shewanella oneidensis* MR-1 Outer Membrane C-Type Cytochrome OmcA." *Journal of the American Chemical Society* 128(43):13978-13979.

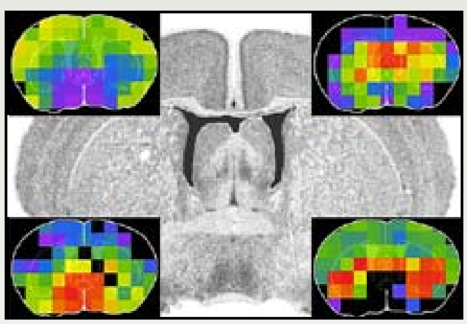


The team has shown that purified OmcA can directly reduce solid metals and that purified proteins are a next step in biofuel cell development.

3D Brain Mapping to Combat Neurodegenerative Disease

Through advanced 3D mapping of brains, PNNL scientists may accelerate the development of a cure for neurodegenerative disorders such as Alzheimer's, Parkinson's or multiple sclerosis. As part of their research at the Environmental Molecular Sciences Laboratory, the scientists have demonstrated a technological platform for spatial mapping of mouse brain proteins. EMSL is a DOE national scientific user facility located 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.



Abundance profiles of four different proteins compiled from 1-millimeter cubes (voxels) in a mouse brain. The boxes correspond to the locations of the voxels in the brain; the colors represent their relative abundance in each region (from high, red, to low, violet).

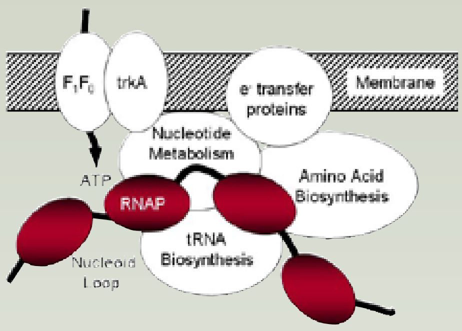
Current imaging techniques provide limited protein identification, in spite of good spatial resolution technology. For the first time ever, scientists have been able to detect over 1,000 different proteins in a single experiment and map them to the brain structures. "Proteins are the lead actors, the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

To produce the map, the 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.

Petyuk, VA, WJ Qian, MH Chin, HX Wang, EA Livesay, ME Monroe, JN Adkins, N Jaitly, DJ Anderson, DG Camp II, DJ Smith, and RD Smith. 2007. "Spatial Mapping of Protein Abundances in the Mouse Brain by Voxelation Integrated with High-Throughput Liquid Chromatography-Mass Spectrometry." *Genome Research* 17(3):328-336.

Changes in Environmental Conditions Impact Cell Function

Scientists at PNNL have found the first evidence that, when environmental conditions are right, cells "reprogram" to create faster and more efficient cellular machinery. Their study explained changes in the assembly of a large supramolecular protein complex involving RNA polymerase.



Suggested organization of RNA polymerase in complex with metabolic enzymes.

RNA polymerase is an enzyme responsible for making RNA from a DNA template (the transcription process) in all cells. The results suggest that the coupling between RNA polymerase and identified metabolic enzymes takes place at the membrane, enabling faster enzyme growth.

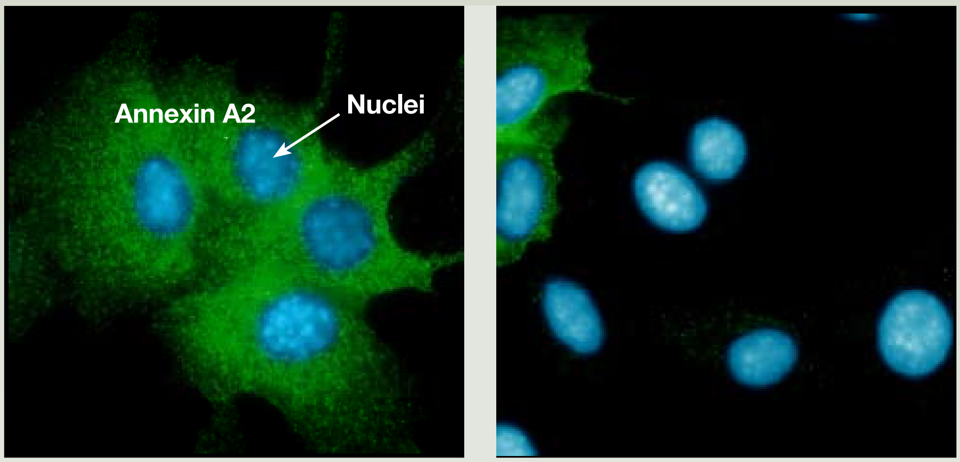
Verma, S, Y Xiong, MU Mayer, and TC Squier. 2007 "Remodeling of Bacterial RNA Polymerase Supramolecular Complex in Response to Environmental Conditions." *Biochemistry* 46(11):3023-3035.

Protein Found for Modeling Radiation Effects on Mammalian Cells

A research team at PNNL has identified a candidate target for modeling the response of mammalian cells to low doses of radiation received by neighboring cells. Led by PNNL biologist Tom Weber, the scientists have identified a membrane-binding protein—annexin A2—as a candidate molecular target for modeling these pathways.

Scientists know that different biological mechanisms can work at high versus low doses for a variety of toxicants including radiation; however, they know little about the pathways that specifically mediate the biological effects of low doses of radiation. Identifying these pathways is a necessary first step to determine whether radiation will impact them in adverse, beneficial or benign ways.

In ongoing research for DOE's Low Dose program, the PNNL scientists found that silencing annexin A2 expression using small hairpin RNA markedly reduces the growth response of the bystander cells to low-dose x-ray radiation. The new understanding gained about the biological function of annexin A2 will contribute to opportunities to mitigate potential risks to human health from radiation exposure.



The protein annexin A2 is shown in green at left before the addition of small hairpin RNA. The shRNA "silences" the protein's expression, as shown at right. This gives scientists insight into the protein's behavior, which in turn will help in understanding how cells respond to low doses of radiation.

PNNL Managing Two DOE Field Research Sites for Studying Contaminant Transport

PNNL is managing two field research sites being established by DOE to investigate contaminant transport. The awards for these sites provide funding to enable large interdisciplinary teams to advance the understanding and simulation of subsurface processes affecting transport of uranium and other contaminants.

The sites are part of the Integrated Field-Scale Subsurface Research Challenge, a program sponsored by DOE's Environmental Remediation Sciences Division. The sites, in Washington State and Colorado, are home to contaminant research previously sponsored by the ERSD; the program takes it up to a new level by providing support for multi-investigator teams to perform large, benchmark-type experiments focused on pressing field-scale science issues.

The field sites are providing researchers the opportunity to collect, permit and ship environmental samples of different types to other ERSD investigators and provide site access to those interested in testing specific concepts or technologies/techniques relevant to the study of subsurface contaminant fate and transport.

The Hanford Site hosts a field experiment where research results will lead to new cleanup strategies. A multidisciplinary team is evaluating 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.

Chemical & Materials Sciences

Behavior of Hydrogen Atoms on Surface Reveals Intriguing Details about Popular Catalyst

Zdenek Dohnalek, Zhenrong Zhang and their colleagues discovered that a single hydrogen atom from a water molecule hops across the surface of the catalyst rutile titanium oxide. Dohnalek's work has opened new doors for technologies that use sunlight to split water to generate hydrogen, a possible alternative fuel.

Researchers at Pacific Northwest National Laboratory and the University of Texas at Austin discovered that a single hydrogen atom cannot 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 what remains of the water molecule stays 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.

Using a scanning tunneling microscope and other resources in the U.S. Department of Energy's Environmental Molecular Sciences Laboratory, a national scientific user facility, the researchers examined the atoms on the surface of the catalyst before and after water adsorption. The researchers found the surface looks like a rutted dirt road with ridges and valleys repeating indefinitely. Here the ridges are rows of oxygen atoms and the valleys are rows of titaniums. When an oxygen atom is removed from one of the ridges, it exposes a titanium atom underneath and creates the reactive pocket on the catalyst.

When water reaches the surface of the catalyst, at room temperature, the water molecule discards one of its two hydrogen atoms. What remains of the water molecule, an oxygen bonded to a hydrogen, settles into one of the reactive pockets, and the discarded hydrogen binds to the nearest oxygen.

Then, the discarded hydrogen begins to hop down the row of oxygen atoms. This hydrogen is roughly 10 times more likely to move than the other hydrogen from the same water molecule. This research points to an underlying difference in the atomic structure near the catalyst's active sites.

Zhang, Z, O Bondarchuk, BD Kay, JM White, and Z Dohnalek. 2006. "Imaging Water Dissociation on TiO_2(110): Evidence for Inequivalent Geminate OH Groups." *Journal of Physical Chemistry, Part B* 110:21840-21845.

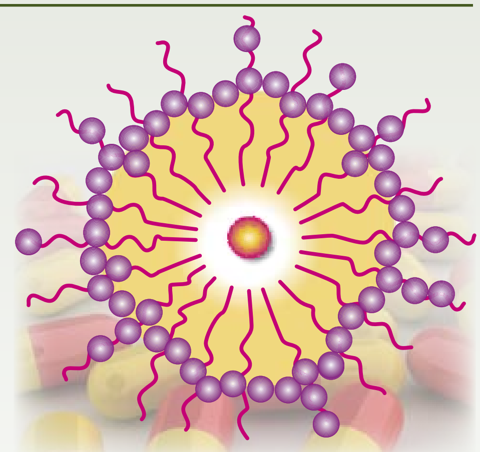
Wrapping Up Sensitive Molecules in Nanoparticles

Like a tough protective bubble, a new class of tiny particles can envelop and carry certain drugs past an array of hazards to their destination inside the human body. Developed by PNNL's researchers and their collaborators at the University of New Mexico and Sandia National Laboratories, these nanoparticles could provide an inexpensive way to administer certain medications that have a notoriously hard time reaching their target.

Called core-shell nanoparticles, these particles break apart slowly, gradually releasing the drugs, which is preferred for certain treatments. In addition, the nanoparticles are easy to store. While some delivery systems are very sensitive to temperature changes and require expensive storage systems, these do not.

The research team created the particles from long-chain molecules. On one end of each molecule is a chemical group that clusters tightly together around the drug molecule. This action positions the long molecules so the other end, which contains a chemical group that is designed to mix well in water or other aqueous solutions, forms the outer shell. To strengthen the structure, silica particles on the long molecules are crosslinked or "polymerized."

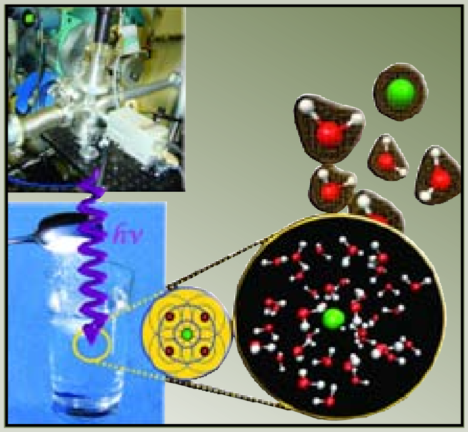
Because the chemical groups that form the particle's center are attracted to each other, as are the groups that form the outer shell, the molecules assemble on their own under the right conditions. This simple process can be tailored to develop particles with different properties.



Like a tough protective bubble, a new class of nanoparticles can envelop and carry sensitive molecules past an array of hazards to their destination.

Huo, Q, J Liu, LQ Wang, Y Jiang, TN Lambert, and E Fang. 2006. "A New Class of Silica Cross-Linked Micellar Core-Shell Nanoparticles." *Journal of American Chemical Society* 128(19):6447-6453.

Discovering the Details of Dissolution



Combining theoretical and experimental approaches, researchers determined the number, relative positions and motions of the liquid molecules surrounding ions. This research provides valuable information with broad applications, from understanding how pollutants flow through the ground to how chemicals flow through the human brain.

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 solvents. At PNNL 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 not commonly used together, the team created simulations 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.

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.

Dang, LX, GK Schenter, VA Glezakou, and JL Fulton. 2006. "Molecular Simulation Analysis and X-Ray Absorption Measurement of Ca^{2+}, K^{+} and Cl^{-} Ions in Solution." *Journal of Physical Chemistry, Part B* 110(47):23644.

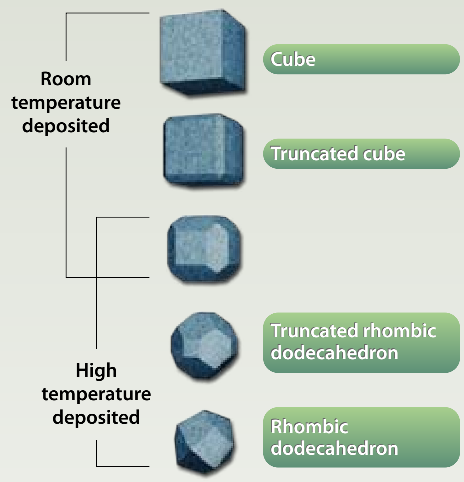
Nanoparticles Shape Up

At PNNL and the University of Idaho, scientists created metallic-iron nanoparticles with three different shapes. This was done by creating the particles at room temperature, instead of the traditional high-temperature method. In EMSL, a DOE national scientific user facility at PNNL, researchers analyzed the particles using transmission electron microscopy, electron diffraction and Wulff shape construction.

These room-temperature-deposited nanoparticles had three distinct structures. The first was a simple six-sided cube, a shape not seen in high-temperature formations. The second was a truncated cube, which looks like a cube with each of the edges shaved off. The third was a rounded shape composed of 12 hexagons and 6 squares, a shape researchers have seen when particles are formed at higher temperatures.

The shape and size of the particle affects its chemical and magnetic properties, which scientists are looking to control for potential applications, such as medical imaging, drug delivery, information storage and groundwater remediation. This research adds an important tool for tailoring iron nanoparticles' shape and hence their properties.

Wang, CM, DR Baer, JE Amonette, MH Engelhard, Y Qiang, and J Antony. 2007. "Morphology and Oxide Shell Structure of Iron Nanoparticles Grown by Sputter-Gas-Aggregation." *Nanotechnology* 18:255603-255609.



At PNNL and the University of Idaho, scientists created metallic-iron nanoparticles at room temperature. The particles have different shapes than those created in the traditional, high-temperature process.

The shape and size of the particle affects its chemical and magnetic properties, which scientists are looking to control for potential applications, such as medical imaging, drug delivery, information storage and groundwater remediation.

Radiation Degrades Materials Containing Nuclear Waste Faster than Expected

Minerals intended to entrap nuclear waste for hundreds of thousands of years may be susceptible to structural breakdown within 1,400 years, a team from the University of Cambridge and the PNNL reported in *Nature.* Researchers sponsored by the Environmental Molecular Sciences Laboratory used nuclear magnetic resonance spectroscopy to show that radiation from plutonium incorporated into the mineral zircon rapidly degrades the mineral's crystal structure. EMSL is a DOE national scientific user facility located at PNNL.

"When the samples were made in the 1980s, NMR was not in the thinking. NMR has enabled us to quantify and look at changes in the crystal structure as the radiation damage progresses," PNNL scientist and NMR expert Herman Cho, who co-wrote the report, said.

Tests developed by the research team would enable scientists to screen different mineral and synthetic forms for resistance to radiation damage. As well as making waste storage safer, new storage methods guided by the NMR technique could offer significant savings for nations facing disposal of large amounts of radioactive material.

Farnan, I, H Cho, and WJ Weber. 2007. "Quantification of Actinide-Radiation Damage in Minerals and Ceramics." *Nature* 445:190-193 (11 January).

Collaborations

Shaping Understanding of Global Climate Change

Ruby Leung – one of the contributors

Through their contributions to the Fourth Intergovernmental Panel on Climate Change 2007 Assessment Report, Pacific Northwest National Laboratory researchers are helping shape how the world views climate change. The IPCC, which was established by the United Nations and the World Meteorological Organization to provide information relevant to climate change, periodically issues reports to provide a comprehensive and up-to-date assessment of the current state of knowledge on climate change.

Since January 2007, IPCC's three Working Groups have issued summaries for policy makers. Writing these summaries is a collaborative affair, with researchers from PNNL working with experts from entities around the world, such as the Norwegian Meteorological Institute, Universidade de São Paulo in Brazil, Laboratoire des Sciences du Climat et de l'Environnement in France and China Meteorological Administration.

For Working Group I, "The Physical Science Basis," PNNL's Ruby Leung was one of the contributing authors. For Working Group II, "Impacts, Adaptation and Vulnerability," PNNL's Mike Scott and Tony Janetos served as lead authors. Liz Malone and Antionette Brenkert, also from PNNL, served as contributing authors. For Working Group III, "Mitigation of Climate Change," Jae Edmonds was the lead author, with Hugh Pitcher and Leon Clarke working as contributing authors and Liz Malone as a review editor.

The depth and breadth of contribution demonstrates PNNL staff members' standing as world-class expertise and the Laboratory's influence on the scientific, technical and socio-economic understanding of climate change.

Comprehensive Whole-Proteome Analysis Available to Scientific Community

Researchers from the University of California-San Diego, the Burnham Institute for Medical Research and PNNL recently demonstrated the capability to rapidly and efficiently improve a proteome annotation. Their work highlights the potential for using mass spectrometry-based proteomics to complement genome sequencing and improve both genome and proteome annotations. The results appeared in *Genome Research,* September 2007.

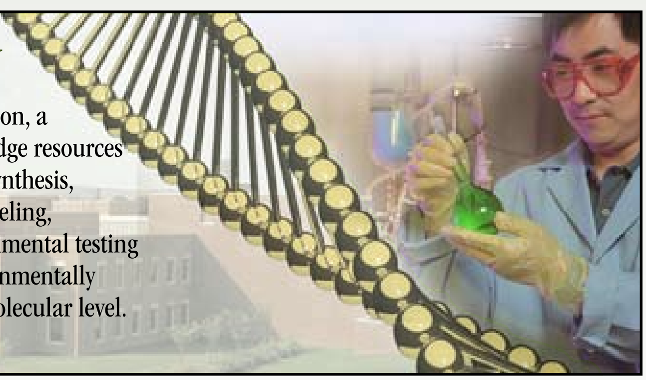
The researchers used liquid chromatography-coupled mass spectrometry for proteomic and genomic annotations of the bacterium *Shewanella oneidensis* MR-1. While bacterial genome annotations have improved significantly in recent years, techniques, such as post-translational chemical modifications, signal peptides and proteolytic events, are still in their infancy. At the same time, the number of sequenced bacterial genomes is rising sharply, far outpacing scientists' ability to validate the predicted genes, let alone annotate bacterial proteomes.

The work, portions of which were conducted in DOE's Environmental Molecular Sciences Laboratory, a national scientific user facility at PNNL, addressing the demand for proteomics measurements as they relate to understanding biological systems important to environmental remediation efforts. The study demonstrates that complementing every genome sequencing project by an MS/MS project would significantly improve both genome and proteome annotations.

Gupta, N, S Tanner, N Jaitly, JN Adkins, MS Lipton, R Edwards, MF Romine, A Osterman, V Bafna, RD Smith, and P Pevzner. 2007. "Whole Proteome Analysis of Post-Translational Modifications: Applications of Mass-Spectrometry for Proteogenomic Annotation." *Genome Research* 17:1362-1377.

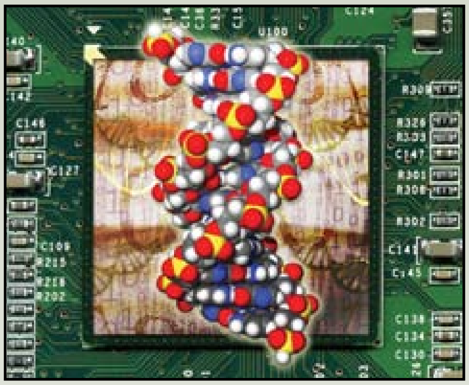
Environmental Molecular Sciences Laboratory

EMSL is a U.S. Department of Energy national scientific user facility located on the campus of PNNL in Richland, Washington. Since its inception in 1997, the 200,000-square-foot facility has hosted visiting scientists, professors and other individuals from all 50 states and 30 countries who requested use of the facility's resources through a peer-reviewed proposal process. EMSL offers, at one location, a comprehensive array of cutting-edge resources including those associated with synthesis, characterization, theory and modeling, dynamical properties and environmental testing relevant to a wide range of environmentally related issues and topics at the molecular level.



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 PNNL and Oak Ridge National Laboratory funded by DOE's Office of Advanced Scientific Computing Research.



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

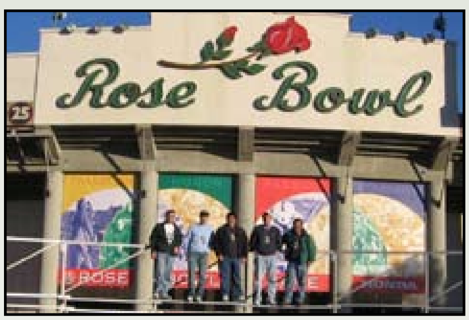
The BioPilot project is developing innovative and robust software solutions to address large-scale, data-intensive computational problems in biology and to make these new capabilities available to the biology community.

"To really understand biological systems, we must integrate complex networks and pathways for a coherent understanding of the system," said project lead TP Straatsma, a PNNL senior scientist. "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.

Time Out for Terrorists at the Rose Bowl

With refreshments in hand, Rose Bowl fans lucky enough to score tickets to the game probably never gave a second thought to their security at the event. Fortunately, someone else did. At the request of local authorities, PNNL researchers traveled to California to support the first operational deployment of the Rapidly Deployable Chemical Defense System. The system was developed to provide detection and early warning of chemicals a terrorist might use.



Posing for posterity in front of Rose Bowl stadium are members of the RDCDS deployment team.

The system consists of two main components: airborne and ground-based detection technologies, and information/communications capabilities. The airborne component consists of aircraft equipped with chemical detectors and sensors. On the ground, a network of meteorological stations track the temperature, wind speed and wind direction, while the chemical detection network monitors the air for specific chemical compounds.

Information obtained from both the airborne and ground-based sensors is fed into a central laptop computer, where the team members monitor the display. If a "hit" shows up on the screen, the weather and chemical data are fed into a computer model that generates the projected contaminant plume. This information is relayed to the event organizer or point of contact so they can see what the chemical is and what the plume will look like.

The researchers worked closely with local authorities, providing real-time information that would help them make informed decisions about evacuations and cleanup applications, if necessary.

The RDCDS team includes PNNL, Lawrence Berkeley National Laboratory, Los Alamos National Laboratory and Sandia National Laboratories.

Keeping Aerosol Research on the Straight and Narrow

In a defining document about the future of aerosol research, PNNL scientist Steve Ghan teamed with Brookhaven National Laboratory's Steve Schwartz, Chief Scientist for DOE's Atmospheric Science Program, to describe a disciplined process for successfully moving aerosol research from the observational stage to model simulations. The paper discusses the challenges faced by both the measurement and modeling communities, ways to overcome them and the resulting benefits.

"Other strategy papers related to global aerosol modeling have been published over the years, but this one focuses on how different research programs can work together to address the breadth of challenges inherent in such a complex system," said Ghan.

Aerosols are one of the greatest sources of uncertainty in climate science. Much of this uncertainty is due to the complexity of aerosols and their interactions with and impacts on cloud processes and properties, as well as the wide range of scales on which these interactions occur.

Accurate representation within global climate models of aerosol properties and the processes that influence those properties is a significant challenge facing the scientific community.

Ghan, SJ, and SE Schwartz. 2007. "Aerosol Properties and Processes: A Path from Field and Laboratory Measurements to Global Climate Models." *Bulletin of the American Meteorological Society* 88:1059-1083.

Institute for Interfacial Catalysis Industry Open House

Catalysis lies at the core of efficient and effective use of our energy sources, developing alternative energy sources, and reducing environmental impacts. To develop evolutionary and revolutionary catalysts, PNNL's Institute for Interfacial Catalysis brought together more than 50 scientists and experts from petroleum and chemical companies, such as ConocoPhillips, Chevron and Dow Chemical.

At the 2-day event, the attendees toured the IIC's laboratories, getting a chance to see analytical and experimental systems, computational resources, and combinatorial and operando tools. Much of this equipment is housed in DOE's Environmental Molecular Sciences Laboratory, a national user facility in Richland, Washington. Further, industry and government experts discussed possible collaborations and research directions.

Awards & Honors

Zachara Recipient of E.O. Lawrence Award

John Zachara

Laboratory Fellow John Zachara was one of eight scientists recognized by U.S. Department of Energy with the prestigious E.O. Lawrence Award for his work in environmental science and technology. The Lawrence Award honors scientists and engineers at mid-career for exceptional contributions in research and development that support DOE and its missions. Zachara's research has focused on chemical interactions of toxic metals and radionuclides with mineral surfaces and microbes that control the rate at which these contaminants move through soils, sediments and groundwater.

Wang Recipient of 2006 Humboldt Research Award

Lai-Sheng Wang

An Affiliate Chief Scientist at PNNL and a professor of physics at Washington State University, Lai-Sheng Wang won the Humboldt Research Award for his lifetime of achievements in nanoscience. The Alexander von Humboldt Foundation presents up to 100 of these awards annually and invites the recipients to conduct research projects of their choice in Germany for six months to a year.

Wang is a world leader in nanoclusters research. Wang and his colleagues created hollow nanoscale cages of gold atoms, the first known metallic equivalent of the buckyball. In addition, he pioneered the study of multiply charged negative ions and began the study of solution molecules in the gas phase.

Noted Radiation Biologist Named Affiliate Scientist

William Morgan

William F. Morgan was appointed Director of Radiation Biology and an Affiliate Scientist at Pacific Northwest National Laboratory on October 1, 2006. Morgan is Professor and Director of the Radiation Oncology Research Laboratory at the University of Maryland in Baltimore, where he resides. For PNNL, he is mentoring and collaborating with staff on proposals to DOE's Low Dose Radiation Research Program, the National Institutes of Health and other agencies concerned with the effects of radiation exposure to human health.

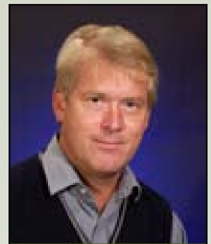
Morgan is a scientific representative for regulatory agencies such as the United Nations Scientific Committee on the Effects of Atomic Radiation, the International Commission on Radiological Protection and the National Council for Radiation Protection.

Ghan Appointed to Journal's Editorial Board

Steve Ghan

Steve Ghan was appointed to a 4-year term as editor for the Atmospheres section of the *Journal of Geophysical Research,* published by the American Geophysical Union. As editor, Ghan has the authority to accept or reject papers, as well as the responsibility for attracting new and interesting research to the journal. Along with fellow editors, Ghan will play a critical role in assuring the journal continues to be the most important in its field and serves the needs of both authors and readers.

Metting Named Chair of International Scientific Network

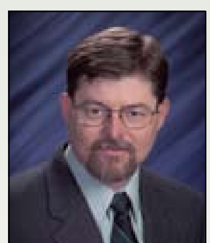


Blaine Metting

At the University of California, Berkeley, on February 16, 2007, Blaine Metting was installed as Chair of the Microalgae Biofixation Network under the auspices of the International Energy Agency Greenhouse Gas Mitigation Research & Development Programme.

The Microalgae Biofixation Network was organized based on an initiative by DOE and EniTecnologie, the research arm of the Italian oil company Eni. Its purpose is to build multi-institutional research collaborations and share scientific findings related to fundamental understanding of photosynthesis and microalgal productivity and applications to greenhouse gas abatement.

Grate Accepted Regional Industrial Innovation Award



Jay Grate

Laboratory Fellow Jay Grate accepted the American Chemical Society's Regional Industrial Innovation Award for his work in developing the patented BSP3 Polymer in June 2007. The award celebrates individuals and teams whose innovations have contributed to the good of the community and society.

An R&D 100 award winner, the BSP3 carbosiloxane compound collects and concentrates vapor molecules from the air. It can be used in detectors for organophosphorus compounds, such as chemical agents. The polymer's properties enable handheld sensor systems to detect toxic vapors quicker and at lower concentrations than was possible using previous materials.

Two Journal Articles Make ACS Most-Cited List


Stephen Callister


Mary Lipton


Dick Smith


Haixing Wang

Two articles by PNNL staff that appeared in the February 2006 issue of the *Journal of Proteome Research* are being featured as an American Chemical Society 2006 Most-Cited Article. These are articles published in ACS journals during 2006 that received the most citations in the same year, based on citation data obtained from Thomson Scientific. The two articles are:

"Normalization Approaches for Removing Systematic Biases Associated with Mass Spectrometry and Label-Free Proteomics," by Stephen Callister, Richard Barry, Josh Adkins, Ethan Johnson, Wei-Jun Qian, Bobbie-Jo Webb-Robertson, Dick Smith and Mary Lipton.

"Characterization of the Mouse Brain Proteome Using Global Proteomic Analysis Complemented with Cysteinyl-Peptide Enrichment," by Haixing Wang, Wei-Jun Qian, Mark Chin, Vladislav Petyuk, Richard Barry, Tao Liu, Marina Gritsenko, Heather Mottaz, Ron Moore, Dave Camp, Arshad Khan, Desmond Smith and Dick Smith. Several of these authors are from the University of California–Los Angeles.

A most-cited article represents critical, new research results influencing the direction of scientific discovery.

Three Named AAAS Fellow


Jim Fredrickson

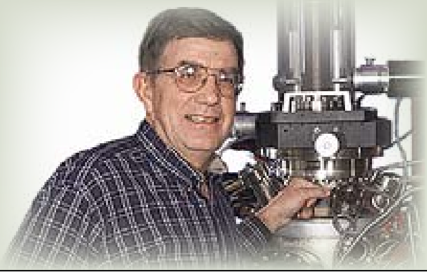

Dick Smith


William Weber

Three members of the Fundamental Science Directorate were among the PNNL staff elected Fellows of the American Association for the Advancement of Science. Jim Fredrickson, Dick Smith and William Weber were recognized at the AAAS national meeting in San Francisco in February 2007. Fredrickson was elected for his "leadership in the field of microbial ecology and environmental microbiology, with emphasis on subsurface microbiology and biogeochemistry." Smith was selected for "leadership in analytical chemistry, specifically in the deployment of advanced separation methods with high-performance mass spectrometry for high-throughput proteomics." Weber was recognized for "leadership and innovative research on defects, ion-solid interactions, and radiation effects in ceramics, particularly modeling and simulations of radiation damage processes."

Dedicated to

J. Mike White, Friend and Scholar
1938-2007

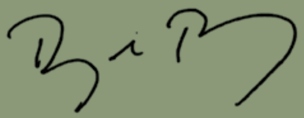


This report is dedicated to Dr. J. Mike White, 1938-2007. Mike's legacy to science and humanity reaches far beyond his position as founding director of the Institute for Interfacial Catalysis at PNNL. His passion for scientific enterprise was reflected in his own research discoveries, but found full expression in his generous personal commitment to hundreds of colleagues and students over the years. We are encouraged and inspired by his signature expression, "press on."

From the Associate Laboratory Director

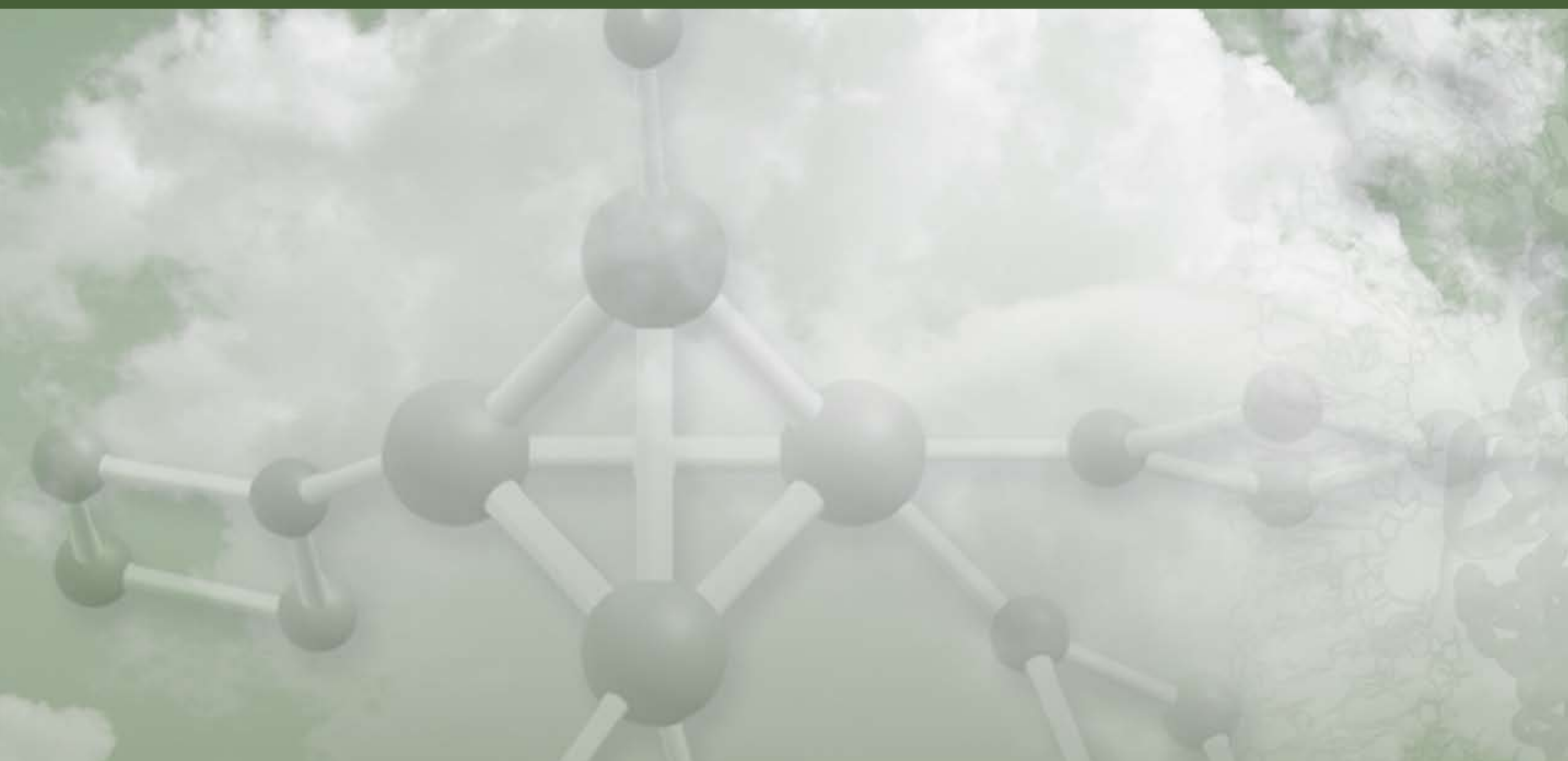
I hope you enjoyed these FY 2007 highlights. They demonstrate how the Fundamental Science Directorate staff is advancing the frontiers of science. I believe these and other discoveries will influence our nation's future—strengthening U.S. scientific foundations for innovation, increasing energy capacity and reducing dependence on imported oil, preventing and countering acts of terrorism and the proliferation of weapons of mass destruction, reducing the environmental effects of human activity and creating sustainable systems.

I also am very proud of our staff and their accomplishments and collaborations. The highlights featured showcase our best and brightest researchers and ways they are propelling science forward to make possible what is currently impossible.



Douglas Ray
Associate Laboratory Director
Fundamental Science Directorate
Pacific Northwest National Laboratory

The **Pacific Northwest National Laboratory** is a **U.S. Department of Energy** national laboratory that is advancing the fundamental understanding of complex systems to provide science-based solutions to some of the nation's most pressing challenges in national security, energy, health and environmental quality. Laboratory staff include more than 4,200 scientists, engineers, technicians and support staff. Battelle, based in Columbus, Ohio, has operated PNNL for the federal government since the Laboratory's inception in 1965.



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Pacific Northwest National Laboratory
Operated by Battelle for the U.S. Department of Energy

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PNNL-SA-58174
11/2007