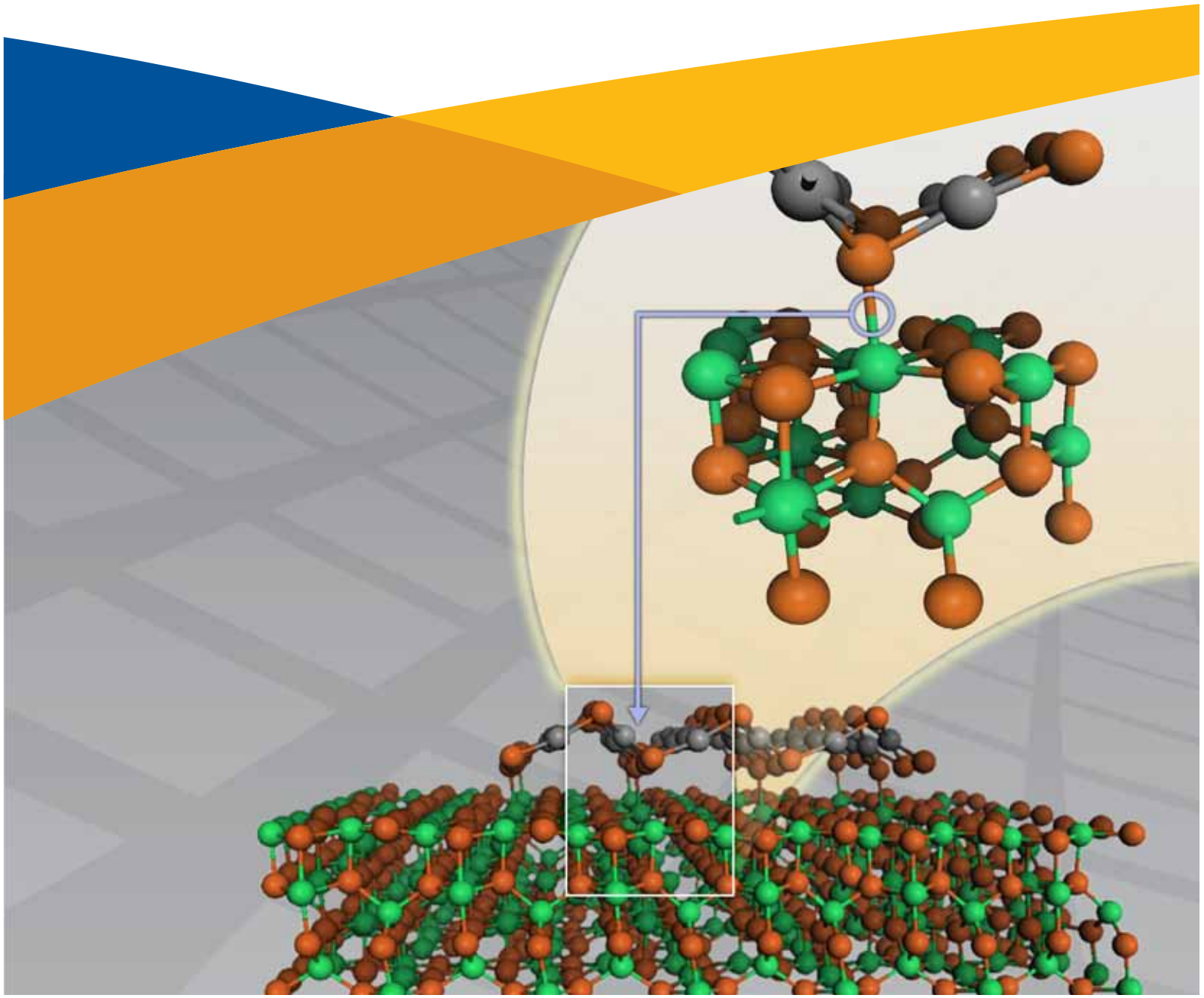
Pacific Northwest
NATIONAL LABORATORY

Proudly Operated by Battelle *Since 1965*

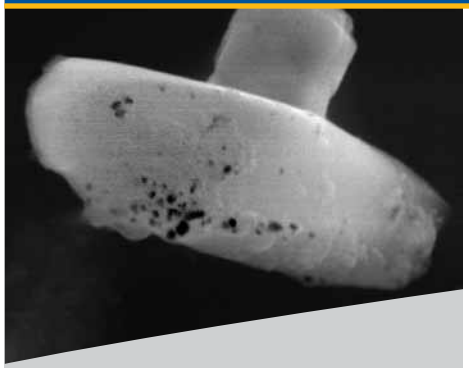
FY 2009

KEY ACCOMPLISHMENTS

Fundamental & Computational Sciences Directorate



Atmospheric Sciences & Global Change



Lead shows as black dots in a scanning electron image of ice-crystal residual particles from clouds collected in the Swiss Alps. Lead from human activities may influence climate through cloud formation.

LEAD in Clouds: A Bad News/Good News Scenario

By sampling clouds and making their own, an international team led by Pacific Northwest National Laboratory has shown for the first time that lead from human activities is changing the properties of clouds and, therefore, the way the sun's energy affects the atmosphere.

The study's results suggest a bad news/good news scenario. The bad news is lead causes clouds to form at warmer temperatures and with less water. This could change rainfall patterns and reduce snowpack, impacting everything from salmon runs to hydropower output. The good news is lead-laden clouds send more heat from the Earth back into space, cooling the world slightly and possibly lessening global warming by greenhouse gases.

Knowing more about the effects of atmospheric lead is important for understanding the total picture of climate change. The influence of aerosol particles from human sources, particularly the use of fossil fuels, is less understood than the contributions from greenhouse gases.

Cziczo DJ, O Stetzer, A Worringen, M Ebert, S Weinbruch, M Kamphus, SJ Gallavardin, J Curtius, S Borrmann, KD Froyd, S Mertes, O Möhler, and U Lohmann. 2009. "Inadvertent Climate Modification Due to Anthropogenic Lead." *Nature Geoscience* 2:333-336. DOI: 10.1038/NGEO499.

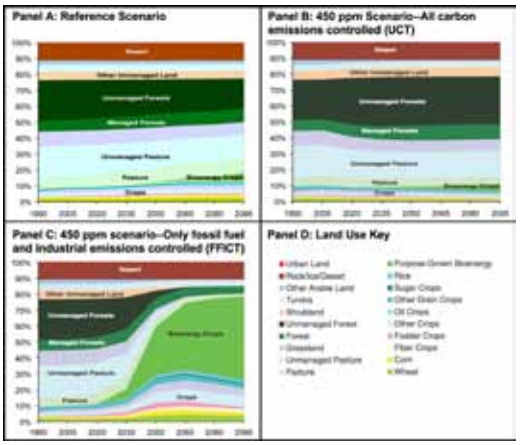
Sponsors: Atmospheric Composition Change: A European Network, ETH Zurich, the German Research Foundation, and PNNL's Aerosol Climate Initiative

TERRESTRIAL CO_2 Economically Important in Greenhouse Gas Control

Failing to include land-use changes in policies to stabilize greenhouse gases in the atmosphere could lead to massive deforestation and higher costs for limiting carbon emissions, according to a study by the Joint Global Change Research Institute, a collaboration between the University of Maryland and the Pacific Northwest National Laboratory. The study results also suggest improved agricultural technology will be as important as new energy technology in a carbon-limited future.

We typically think of carbon dioxide emissions as coming from industrial or fossil fuel sources. But another source is from the earth itself: from land-use practices such as deforestation. Oddly, steps being taken to decrease emissions from the first two sources could increase terrestrial carbon emissions globally.

Why? Because policies that promote the use of dedicated biomass crops divert land that would otherwise be left for food and fiber crops, forests, and unmanaged ecosystems. This land-use shift releases excess CO_2 into the air just as industrial activities and the burning of fossil fuels do.



Without a universal carbon tax, there's more incentive to use land for bioenergy crops (panel C) than for food and fiber crops (panels A and B).

Wise MA, KV Calvin, AM Thomson, LE Clarke, RD Sands, SJ Smith, AC Janetos, and JA Edmonds. 2009. "Implications of Limiting CO_2 Concentrations for Land Use and Energy." *Science* 324(5931):1183-1186. DOI: 10.1126/science.1168475.

Sponsors: Department of Energy's Office of Science and the Electric Power Research Institute

THE SKY Is Not Falling: Pollution in Eastern China Cuts Light, Useful Rainfall

New research shows that air pollution in eastern China has reduced the amount of light rainfall over the past 50 years and decreased by 23 percent the number of days of light rain in the eastern half of the country. The results suggest that bad air quality might be affecting the country's ability to raise crops as well as contributing to health and environmental problems.

Led by atmospheric scientist Dr. Yun Qian at Pacific Northwest National Laboratory, the study links for the first time high levels of pollutants in the air with conditions that prevent the light kind of rainfall critical for agriculture.

"People have long wondered if there was a connection, but this is the first time we've observed it from long-term data," said Qian. "Besides the health effects, acid rain, and other problems that pollution creates, this work suggests that reducing air pollution might help ease the drought in north China."

Qian Y, D Gong, J Fan, LR Leung, R Bennartz, D Chen, and W Wang. 2009. "Heavy Pollution Suppresses Light Rain In China: Observations and Modeling." *Journal of Geophysical Research-Atmospheres* 114:D00K02. DOI: 10.1029/2008JD011575.

Sponsor: Office of Biological and Environmental Research within the DOE Office of Science under a bilateral agreement on regional climate research with the China Ministry of Science and Technology

THIN Is In

A team from the Pacific Northwest National Laboratory gathered direct measurements from thin, low-lying clouds as part of a field campaign in Oklahoma from January to June 2009. The results of this campaign will ultimately lead to more accurate climate change predictions. The campaign is part of the Department of Energy's Atmospheric Radiation Measurement Program, a multi-laboratory effort that has been making important contributions to global climate change research for two decades. The field campaign, known as RACORO, is the first long-term aircraft campaign to conduct systematic sampling of cloud properties from the air.

Sponsor: DOE funds the ARM Program and this campaign

The Twin Otter takes off to test the on-board instruments for the RACORO field campaign that began in January 2009. Researchers gathered data on the properties of certain low-level clouds. The data will be used to make climate model predictions more accurate.

Climate Researchers Say "Hola" to Chile for Six-Week **FIELD STUDY**

As part of an international field study, researchers from Pacific Northwest National Laboratory traveled to the Chilean coast. The purpose of the Variability of the American Monsoon Systems Ocean-Cloud-Atmosphere-Land Study, or VAMOS, was to better understand the interactions among the ocean, clouds, air, and land in the Southeastern Pacific. PNNL is among 40 institutions from 8 nations that have 150 scientists contributing to this field study.

Sponsor: Department of Energy's Atmospheric Sciences Program

Most Comprehensive, Authoritative Report on **GLOBAL CLIMATE CHANGE IMPACTS**

In a 200-page report released by the White House Office of Science and Technology, authors such as Dr. Tony Janetos of Pacific Northwest National Laboratory summarized current climate change science projects as well as the regional and national consequences of the changing environment. The report also discusses actions society can take to respond to the climate challenge.

"The most important thing in this report is that the impacts of climate change are not something your children might theoretically see 50 years from now," said Janetos at the White House news conference. "The thing that concerns me the most is that we have a whole host of impacts that we now observe in the natural world that are occurring sooner and more rapidly and that appear to be larger than we might have expected 10 years ago."

Karl TR, JM Melillo, and TC Peterson (eds.). 2009. *Global Climate Change Impacts in the United States*. Cambridge University Press, New York.

Sponsor: Janetos' work was funded by the Department of Energy's Biological and Environmental Research, as part of the Global Change Research Program

CLOUDING the Issue

Over time scales spanning at least a decade, the amount of sunlight that reaches the Earth's surface has varied. These variations affect the total amount of incoming and outgoing energy in the Earth system, which, in turn, affects climate. These variations are called global dimming and brightening. Scientists had attributed much of these variations to changes in the amounts of atmospheric aerosols. Analysis of new climate data shows the answer is not so simple.

A multidisciplinary team led by Pacific Northwest National Laboratory found that, at least in the continental United States, changes in clouds and cloudiness have a greater influence on brightening than any decrease in aerosol amounts alone. The team further discovered that the magnitudes of dimming and brightening are regional, rather than global, phenomena. Researchers expect that adequately capturing the dimming and brightening phenomena will challenge every aspect of global climate models.

Long CN, EG Dutton, JA Augustine, W Wiscombe, M Wild, SA McFarlane, and CJ Flynn. 2009. "Significant Decadal Brightening of Downwelling Shortwave in the Continental United States." *Journal of Geophysical Research-Atmospheres* 114:D00D06. DOI: 10.1029/2008JD011263.

Sponsors: Department of Energy Office of Biological and Environmental Research's Atmospheric Radiation Measurement Program; National Oceanic and Atmospheric Administration Climate Goal; National Aeronautics and Space Administration Radiation Projects Office; and Swiss National Centre for Competence in Climate Research

Although brightening occurred throughout the continental United States from 1995 to 2007, more precise measurements revealed regional differences that may significantly test the abilities of climate models.

Biological Sciences

For years, radiation biologists thought that human DNA was the primary target for energy deposition after exposure to ionizing radiation—such as that from X-rays and gamma rays. However, the discovery of non-targeted responses to radiation, such as the bystander response, has called this paradigm into question.

Are Radiation-induced **BYSTANDER EFFECTS** a Universal Phenomenon?

When radiation strikes cells, those cells nearby suffer *sometimes*, but not always, according to a recent study. The study showed the damage to nearby cells, known as the bystander effect, is not a universal phenomenon. The damage is dependent on the type of radiation used as well as the specific pattern of energy deposition produced by radiation as it interacts with the cell or tissue. In addition, many confounding factors may influence bystander responses reported in the literature.

The research was done by scientists from the Pacific Northwest National Laboratory, the University of Maryland, the University of Medicine and Dentistry of New Jersey, and the University of Virginia.

Sowa MB, W Goetz, JE Baulch, DN Pyles, J Dziegielewski, S Yovino, AR Snyder, SM de Toledo, EI Azzam, and WF Morgan. 2009. "Lack of Evidence for Low-LET Radiation Induced Bystander Response in Human Fibroblast and Colon Carcinoma Cells." *International Journal of Radiation Biology*. In Press.

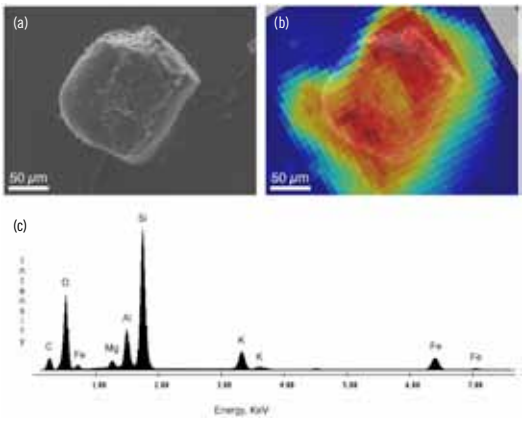
Sponsors: Department of Energy's Biological and Environmental Research, the National Aeronautical and Space Administration, and the National Cancer Institute

Iron Minerals in Subsurface Sediment **REDUCE TECHNETIUM MOBILITY**

New insights into the reactive phases and processes occurring within radioactively contaminated subsurface sediments will pay off for current and future studies of how technetium moves at Department of Energy sites. The results from a recent study by scientists at Pacific Northwest National Laboratory will help resolve questions about the movement of subsurface contaminants and develop effective site remediation strategies.

Previous studies at PNNL have demonstrated that the contaminant technetium-99 can be reduced from its most mobile state to tetravalent technetium, which can form a solid and remain associated with the sediment. This reaction occurs when pertechnetate loses electrons, either by direct interaction with microbes or by interacting with certain forms of iron that exist naturally in the sediment.

The scientists have also shown that reduced iron created by microbe-mediated reactions can be very efficient at converting technetium to the less mobile form, but this reaction depends on the form of iron in the subsurface, and the form dictates the reaction rates and end products.



Characterization of a technetium-containing particle isolated from oxidized sediment: (a) backscattered electron micrograph, (b) electron microprobe energy dispersive X-ray analysis, and (c) results from the X-ray microprobe.

Further, the scientists investigated the fate of immobilized technetium after it was exposed to air. In one sample, the reduced technetium was oxidized rapidly and became mobile again. In the other sample, it did not. The researchers found the reason for the different behaviors was because the technetium's reactivity depends on its association with the iron in the sediment.

Fredrickson JK, JM Zachara, AE Plymale, SM Heald, JP McKinley, DW Kennedy, CX Liu, and P Nachimuthu. 2009. "Oxidative Dissolution Potential of Biogenic and Abiogenic TcO_2 in Subsurface Sediments." *Geochimica et Cosmochimica Acta* 73:2299-2313.

Sponsor: DOE's Biological and Environmental Research

New Strategy Better **CHARACTERIZES PROTEIN MODIFICATIONS**

A novel strategy that allows scientists to identify proteins that have been modified by cells is adding knowledge to studies of heart disease, cancer, and essentially any other area of biology. At Pacific Northwest National Laboratory, scientists developed this novel strategy, which can be used to probe post-translational modifications of proteins.

Protein modifications may alter a protein's physical and chemical properties and, consequently, function. Modifications often play a key role in protein signaling, controlling many important cellular processes. But, these alterations also can lead to disease.

The novel approach will enable scientists to identify proteins and their modifications with more certainty and lower false discovery rates. They can discover protein post-translational modifications, including complex multiple unknown/unexpected modifications on a single protein sequence, and discover sequence mutations and genome-predicted database sequence errors.

The cover of the October 15, 2008, issue depicts procedures used to determine protein post-translational modifications. *Copyright 2008. American Chemical Society*

Shen Y, N Tolic, KK Hixson, SO Purvine, GA Anderson, and RD Smith. 2008. "De Novo Sequencing of Unique Sequence Tags for Discovery of Post-Translational Modifications of Proteins." *Analytical Chemistry* 80(6):7742-7754.

Sponsors: Environmental Molecular Sciences Laboratory, Department of Energy's Biological and Environmental Research, and the National Institutes of Health's National Center for Research Resources

NEW MONITORING METHOD for Microbial Activity Validated at Colorado Site

Scientists performed the first field demonstration of a minimally invasive monitoring approach for tracking subsurface biogeochemical changes accompanying the remediation of a uranium-contaminated aquifer. Their results showed that the approach, called surface spectral-induced polarization or SSIP, is feasible and practical for remote monitoring of microbial activity stimulated during bioremediation.

The SSIP approach enables scientists to track geochemical and mineralogical changes accompanying the addition of electron donors, such as acetate, which is similar to diluted vinegar. These donors stimulate subsurface microbial activity. The new approach may also be used to spatially extend geochemical data from a limited number of boreholes, providing data for assessing remediation efficacy over large areas—in essence, requiring less monitoring but still providing a high level of assurance that the remedial process is working as intended.

The team: SSIP was developed by scientists from Lawrence Berkeley National Laboratory; Pacific Northwest National Laboratory; the University of Bonn in Germany; and the University of California, Berkeley. The field demonstration took place at a former uranium mill tailings site near Rifle, Colorado.

Why it matters: Groundwater contamination by industrial sources and nuclear weapons programs has spurred research into the use of microbes to facilitate remediation by sequestering aqueous metals and radionuclides

Dr. Kenneth H. Williams (LBNL) and graduate student Adrian Flores Orozco (University of Bonn) collecting surface spectral induced polarization data at the Rifle site to detect and delineate regions of naturally elevated subsurface microbial activity.

in insoluble forms. Much of the research has focused on microorganisms capable of either iron or sulfate reduction. Such organisms have also been shown to immobilize contaminants, such as uranium, following the introduction of organic carbon compounds, such as acetate, lactate, and ethanol.

But understanding how microorganisms alter their physical and chemical environment during bioremediation is hindered by the inability to adequately assess subsurface microbial activity over field-relevant dimensions, which can encompass lateral and vertical distances of tens to hundreds of meters. However, the SSIP monitoring approach makes it possible to monitor the subsurface with very high spatial resolution—areas as small as 0.3 m—and without the need for groundwater wells.

Williams KH, A Kemna, MJ Wilkins, J Druhan, E Arntzen, AL N'Guessan, PE Long, SS Hubbard, and JF Banfield. 2009. "Geophysical Monitoring of Coupled Microbial and Geochemical Processes During Stimulated Subsurface Bioremediation." *Environmental Science & Technology* 43(17):6717-6723.

Sponsor: Department of Energy's Biological and Environmental Research

On the Light Path to BIOENERGY

Pollutant-free fuel cells require a cheap, abundant source of hydrogen fuel. Plants, algae, and blue-green bacteria produce hydrogen—by harvesting sunlight and using the energy to split water. This reaction is done by a large protein complex that slowly degrades and must be regenerated. A study by scientists from the Pacific Northwest National Laboratory and Washington University in St. Louis shed new light on how this protein complex, called Photosystem II, regenerates.

The team found a novel cluster of genes that encode six proteins. These six proteins help put Photosystem II back together.

"This can lead to a better understanding of how these proteins work, which could alter how we view this entire process," said PNNL's Jon Jacobs.

Wegener KM, EA Welsh, LE Thornton, NS Keren, JM Jacobs, KK Hixson, ME Monroe, DG Camp II, RD Smith, and HB Pakrasi. 2008. "High Sensitivity Proteomics Assisted Discovery of a Novel Operon Involved in the Assembly of Photosystem II, a Membrane Protein Complex." *Journal of Biological Chemistry* 283(41):27829-27837.

Sponsors: Environmental Molecular Sciences Laboratory and National Science Foundation

Discovery Fleshes out METABOLISM of Key Bacteria

An international team of researchers discovered a new enzyme in a species of bacteria with potential roles in energy and environmental cleanup. This is the first multi-protein enzyme of its kind. It's called L-lactate dehydrogenase.

Although many microbes use a single-protein version to consume a certain food, such as lactate, the new study suggests that dozens of bacteria use only a multi-protein version. This advance in understanding the microbe's efficient metabolism will help researchers clean up radionuclides and metals.

The research team was from Pacific Northwest National Laboratory, Burnham Institute for Medical Research in California, Russian Academy of Sciences, Chinese Academy of Sciences, Fellowship for Interpretation of Genomes in Illinois, Argonne National Laboratory in Illinois, Institut National de la Recherche Agronomique in France, and Dartmouth College in New Hampshire.

Pinchuk GE, DA Rodionov, C Yang, X Li, AL Osterman, E Dervyn, OV Geydebrekht, SB Reed, MF Romine, FR Collart, JH Scott, JK Fredrickson, and AS Beliaev. 2009. "Genomic Reconstruction of *Shewanella oneidensis* MR-1 Metabolism Reveals a Novel Machinery for Lactate Utilization." *Proceedings of the National Academy of Sciences*, USA 106(8):2874-2879.

Sponsor: Department of Energy's Biological and Environmental Research

Researchers discovered a new bacterial enzyme with potential environmental cleanup and energy roles.

Chemical & Materials Sciences

The new titanium oxide structures on carbon sheets could help the batteries hold more energy, easing several energy challenges the United States currently faces. *Copyright 2009. American Chemical Society.*

BUILDING BETTER BATTERIES Today for a Greener Tomorrow

High-capacity, safe batteries are needed for hybrid or electric cars and for storing and releasing electricity from intermittent sources. That's where an innovation by scientists at Pacific Northwest National Laboratory and Princeton University comes in. The team devised a way to build tiny titanium oxide and carbon structures that greatly improve the performance of lithium ion batteries. These batteries are a popular option, because pound for pound, they are some of the most energetic rechargeable batteries available. This new material stores twice as much electricity at high charge/discharge rates as materials used in lithium ion batteries that don't use it.

Wang D, D Choi, J Li, Z Yang, Z Nie, R Kou, D Hu, C Wang, LV Saraf, J Zhang, IA Aksay, and J Liu. 2009. "Self-Assembled TiO_2-Graphene Hybrid Nanostructures for Enhanced Li-Ion Insertion." *ACS Nano* 3(4):907-914.

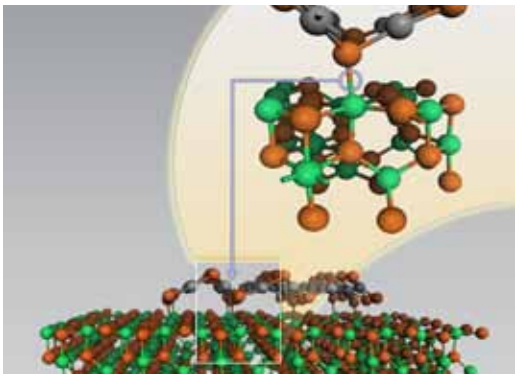
Sponsors: PNNL Laboratory-Directed Research and Development Program and Department of Energy's Basic Energy Sciences

COMMON INDUSTRIAL CATALYST Sports Rafts Made of Platinum

Research in *Science* reveals new, important details about how rafts of chemically reactive platinum form in the catalyst. The new work yields insights into how to improve an industrial catalyst for oil refining, chemical processing, and environmental uses.

The study shows that aluminum atoms in the catalyst's supporting material, thirsty for another bond, grab and anchor platinum. The anchors allow platinum atoms to group into rafts that float above the supporting surface, providing ample space for catalytic reactions.

Researchers in the Institute for Interfacial Catalysis at Pacific Northwest National Laboratory and Oak Ridge National Laboratory performed the analysis of the industrial catalyst known as aluminum oxide-supported platinum. Such precious metal and oxide combinations are the most common kinds of industrial catalysts. The new work will help engineers control the preparation of the catalyst, which will lead to better performance.



For the first time, researchers viewed the bonds that anchor platinum rafts over an aluminum oxide surface, important research for catalysts involved in energy markets.

"We've been able to specifically identify an important site for the anchoring of platinum on the aluminum oxide surface that's formed during synthesis," said PNNL chemist Dr. Chuck Peden, co-author of the study. "Although platinum rafts have been observed before, this is the first time we've had a clear molecular-level view of the processes that create them."

Kwak JH, J Hu, D Mei, CW Yi, DH Kim, CHF Peden, LF Allard, and J Szanyi. 2009. "Co-ordinatively Unsaturated Al^{3+} Centers as Binding Sites for Active Catalyst Phases on γ-Al_2O_3." *Science* 325:1670-1673.

Sponsors: Department of Energy's Basic Energy Sciences and Energy Efficiency and Renewable Energy

Seeing the World in a **COLUMN OF SAND**

By examining the behavior and characteristics of a small volume of sediment, scientists at Pacific Northwest National Laboratory created a coupled experimental and computational approach that may better predict the behavior of uranium over relatively large areas in the field. Using this approach, the team accurately scaled the chemical effects they observed in a small sample to describe the physical and chemical effects on uranium transport in a much larger system.

When and how much of this uranium from the former plutonium production complex in south-eastern Washington State reaches the nearby Columbia River is a question whose resolution could have large impacts on remediation. The Department of Energy, which manages the Site, must predict the uranium's arrival.

An accurate determination of river shore impacts will allow effective and efficient implementation of technologies to capture or stabilize the uranium before it enters the river.

Scientists developed a combined experimental and computational approach that may better predict the behavior of uranium in the field.

Liu C, JM Zachara, N Qafoku, and Z Wang. 2008. "Scale-dependent Desorption of Uranium from Contaminated Subsurface Sediments." *Water Resources Research* 44(8):W08413.

Sponsors: DOE's Biological and Environmental Research and Environmental Management

CENTER for Molecular Electrocatalysis **ESTABLISHED**

Pacific Northwest National Laboratory will be home to a new multi-million-dollar Energy Frontier Research Center. The Department of Energy plans to award $22.5 million over five years for PNNL's new Center for Molecular Electrocatalysis.

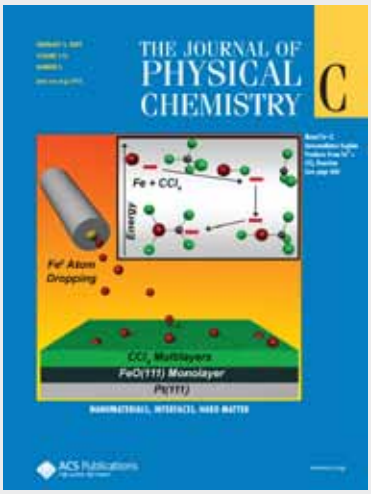
At the electrocatalysis center, researchers will study catalysts that convert electrical energy into chemical bonds and back again. Of interest are catalysts that pack energy into bonds involving hydrogen, oxygen, or nitrogen. These reactions are at the core of technologies such as solar energy and fuel cells.

Led by Dr. Morris Bullock (right), more than a dozen scientists are working to study catalysts that convert electrical energy into chemical bonds and back again.

The Center comprises more than a dozen researchers from PNNL, the University of Washington, Pennsylvania State University, and the University of Wyoming.

Iron Takes Full Ten Rounds to **DESTROY TOXIN**

Previously thought to be a simple reaction, scientists at Pacific Northwest National Laboratory found that tiny iron particles instigate a complex series of reactions to turn harmful carbon tetrachloride into harmless chemicals. The team of experimental scientists and theoreticians uncovered 10 molecules that may be created during the reactions, including an iron-carbon-chloride molecule that energetically reacts with iron.



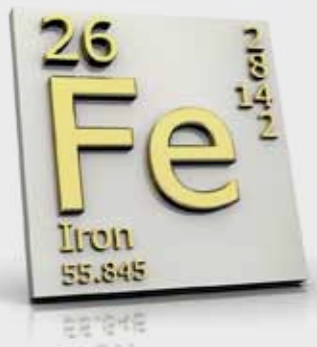
Experimental scientists and theoreticians uncover complex reactions as metal turns toxic carbon tetrachloride to harmless chemicals. *Copyright 2009. American Chemical Society.*

"What was thought to be a simple reaction proved to be far harder when working with nanoparticles and tiny clusters," said Dr. Donald Camaioni, a theoretical chemist at PNNL.

Soil at hundreds of sites across the country is contaminated with carbon tetrachloride. These sites range from dry cleaners to plutonium processors. Particulate iron is one technology considered to treat carbon tetrachloride spills on the soil.

"The problem, of course, was that no one understood what actual reactions were happening," said Dr. Scott Smith, an experimental chemist on the project. "You could see the carbon tetrachloride going away, but you didn't know exactly how."

So, the PNNL team decided to find out what was happening. With insights about the effectiveness of different sizes of iron particles and concentrations, researchers may more effectively turn carbon tetrachloride lodged deep underground into benign compounds.



Parkinson GS, Z Dohnalek, RS Smith, and BD Kay. 2009. "Reactivity of FeO Atoms, Clusters, and Nanoparticles with CCl_4 Multilayers on FeO(111)." *Journal of Physical Chemistry C* 113:1818.

Camaioni DM, B Ginovska, and M Dupuis. 2009. "Modeling the Reaction of Fe Atoms with CCl_4." *Journal of Physical Chemistry C* 113:1830.

Sponsors: Department of Energy's Basic Energy Sciences and Biological and Environmental Research

IONS Disturb Water's Structure in Unexpected Ways

When a symmetrical ion settles onto the asymmetrical surface of water, it does not disturb the surface evenly. But according to scientists at Pacific Northwest National Laboratory and Louisiana Tech University, the same thing occurs when a symmetrical ion settles onto a symmetrical water environment. The ion pushes unevenly on the surrounding water molecules. The ions form a small bubble on one side.

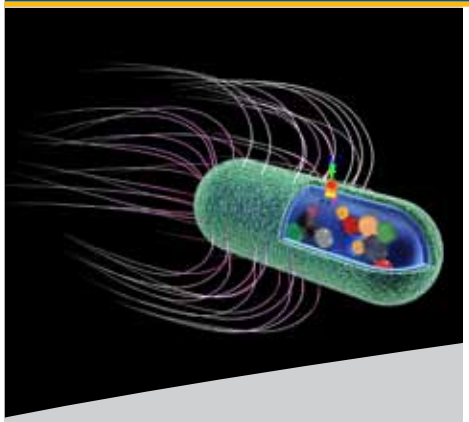
Understanding the structure of a volume of water or bulk water and the way it is perturbed by accommodating various ions and solutes is of paramount importance to understanding key chemical and biological processes. For example, ions take part in acid-base reactions that determine the formation and transport of environmental pollutants. Also, ions are pumped across cell membranes by proteins, creating necessary energy reservoirs for the cell.

Wick CD and SS Xantheas. 2009. "Computational Investigation of the First Solvation Shell Structure of Interfacial and Bulk Aqueous Chloride and Iodide Ions." *Journal of Physical Chemistry B* 113(13):4141-4146.

Sponsors: Department of Energy's Basic Energy Sciences and Louisiana Board of Regents

Researchers found that symmetrical ions perturb bulk water asymmetrically. *Copyright 2009. American Chemical Society.*

Computational Sciences & Mathematics



An idealized illustration of *Salmonella typhimurium*, with a type III secretion system and gears, represents a systems biology approach to studying this and other pathogens. Research to elucidate how these pathogens function could lead to improved antibiotics or therapeutics. In other words, we are trying to identify the best place to "throw a wrench into the works." Credit: Ken Auberry.

COMPUTATIONAL SCIENCE To Take on Infectious Diseases

Two five-year research programs, funded for over $30 million, are collaboratively using a systems biology approach to understand the process involved in developing infections caused by the influenza and SARS viruses and the pathogenic bacteria *Yersinia* and *Salmonella*.

Scientists at Pacific Northwest National Laboratory will provide modeling and analysis of the generated high-throughput data. The goal is to determine the mechanisms by which these pathogens adapt to and manipulate the cellular environment after infecting their host targets. The discoveries from the research could lead to more precise drug therapies and control strategies for a wide range of viral and bacterial pathogens.

Sponsor: National Institutes of Health's National Institute of Allergy and Infectious Diseases

HIGH-PERFORMANCE COMPUTING Aids in Study of Power Grid Failures

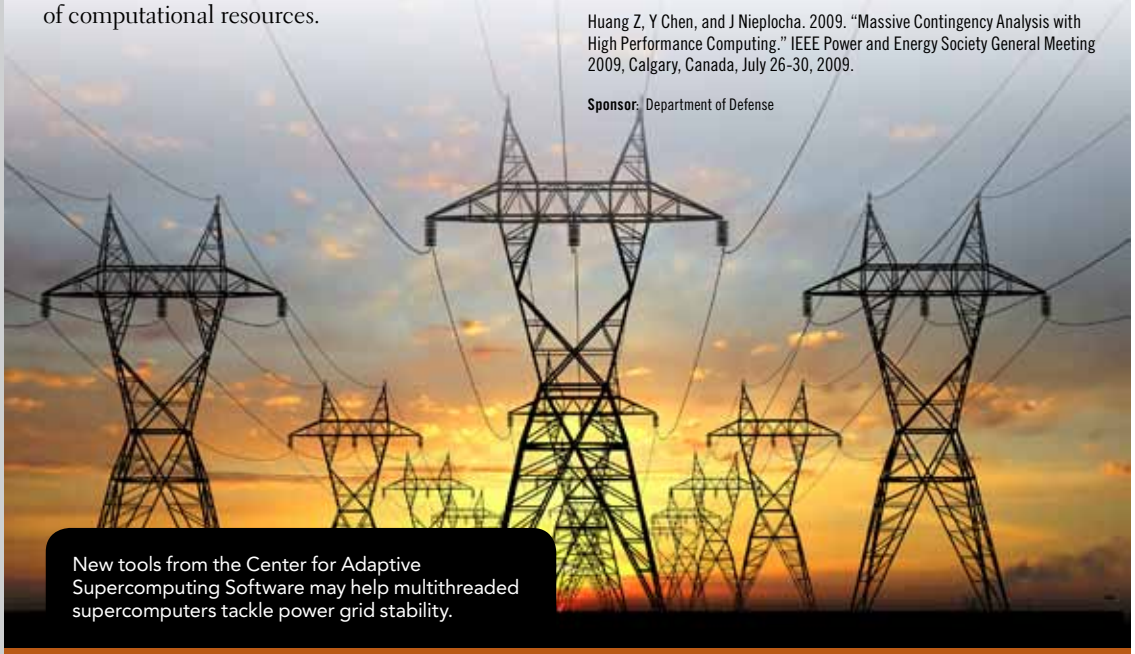
Research at Pacific Northwest National Laboratory to gain a greater understanding of electric grid failures is producing promising results. Using PNNL's Cray XMT machine, researchers are conducting advanced power grid contingency analysis, a valuable tool to help determine the impact of potential component failures. Early results from the research show superior performance in selecting critical contingency cases from a large candidate set of possibilities. Detailed contingency analysis can then be performed for selected cases only. Without contingency selection, the number of contingency cases would be so large as to exceed the capability of computational resources.

As electricity demand continues to grow and renewable energy increases its penetration in the power grid, the personnel operating and managing the power grid are facing some fundamental challenges. Contingency analysis evolves from previous "N-1" analysis (i.e., failures of any one component) to "N-x" analysis (i.e., failures of multiple components). The combinatorial number of contingency cases increases exponentially as "x" becomes larger. This results in many more cases to analyze and much more data from the analysis to present to operators.

To address these challenges, researchers at PNNL are exploring the use of graph theory to select contingency cases and advanced visualization techniques to analyze and present the information to operators in a meaningful way, allowing for faster responses to adverse power grid situations.

Huang Z, Y Chen, and J Nieplocha. 2009. "Massive Contingency Analysis with High Performance Computing." IEEE Power and Energy Society General Meeting 2009, Calgary, Canada, July 26-30, 2009.

Sponsor: Department of Defense

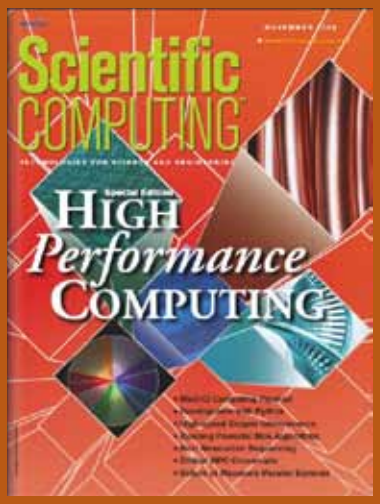


New tools from the Center for Adaptive Supercomputing Software may help multithreaded supercomputers tackle power grid stability.

MeDICi Highlighted in Special Issue of SCIENTIFIC JOURNAL

Developed at Pacific Northwest National Laboratory, MeDICi was featured in the November 2008 special digital edition of *Scientific Computing*. MeDICi is a middleware platform that makes it easy to integrate separate codes into complex applications that operate as a data analysis pipeline. The MeDICi framework is the first step in an evolving development project to create an underlying architecture for high-performance analytical applications.

Gorton I, CS Oehmen, and JE McDermott. 2008. "It Takes Glue to Tango." *Scientific Computing* November 2008:17-20.



CREATING TOOLS AT EXTREME SCALE for Subsurface Flow and Transport

To better understand the physicochemical processes that govern subsurface flow and transport and improve scientific predictive capability, a multidisciplinary team of researchers developed PFLOTRAN, a massively parallel, multiphase, and multi-component reactive flow and transport code.

PFLOTRAN is capable of simulating subsurface flow and transport at the petascale on the world's largest open science supercomputer, Jaguar. To our knowledge, there is no other subsurface flow and transport simulator capable of running at PFLOTRAN's computational scales; that is, numbers of degrees of freedom and numbers of processor cores. This code has executed simulations on up to 131,072 processor cores on problems composed of up to 2 billion degrees of freedom.

The superior accuracy enabled by massively parallel, leadership-class computing was demonstrated for simulating flow and multicomponent geochemical transport and calculating uranium fluxes to the Columbia River from a nearby former uranium fuel production complex.

The team responsible for PFLOTRAN is from Pacific Northwest National Laboratory, other national laboratories, and the University of Illinois.

Hammond GE, PC Lichtner, RT Mills, and C Lu. 2008. "Towards Petascale Computing in Geosciences: Application to the Hanford 300 Area." *Journal of Physics: Conference Series* 125, 012051. DOI: 10.1088/1742-6596/125/1/012051.

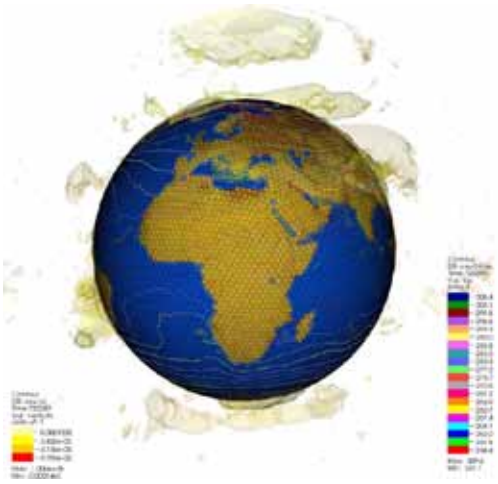
Sponsor: Department of Energy under the Scientific Discovery through Advanced Computing Program

INCREASE IO BANDWIDTH to Better Understand Climate Change

An important milestone for modeling and understanding the role of clouds in global climate change was met when researchers achieved an effective aggregate input/output (IO) bandwidth of 5 Gigabytes/sec for writing output from a global atmospheric model to shared files.

This bandwidth number represents the minimum value required to write data fast enough that IO does not slow running of the Global Cloud-Resolving Model.

The increase in IO bandwidth will allow researchers to run models at higher resolution, and therefore achieve higher accuracy, and will also enable simulations representing longer periods of time. Both are crucial to understanding future climate change.



The team was from Pacific Northwest National Laboratory, National Energy Research Scientific Computing Center, Argonne National Laboratory, and Cray.

Sponsor: Department of Energy's Scientific Discovery through Advanced Computing Program

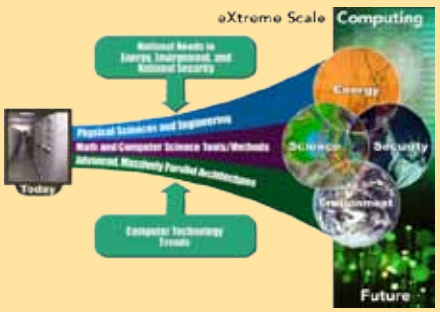
GO BIG or Go Home: eXtreme-Scale Computing Initiative

This new initiative, launched by Pacific Northwest National Laboratory in October 2008, develops next-generation, extreme-scale modeling and simulation capabilities. These capabilities will enable scientific advancements and breakthroughs in energy technologies, environmental impact, and climate change prediction.

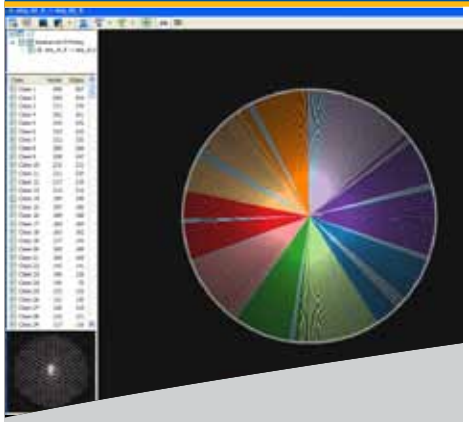
The initiative, known as XSCI, is enhancing and developing scalable methods, algorithms, and software for use in computers orders-of-magnitude faster than any available today. The initiative's scientists are advancing existing and emerging codes in application areas where PNNL holds a leadership position to be able to use next-generation massively parallel hardware.

The XSCI has three research and development thrust areas:

- **Scalable Domain Science Applications** focuses on subsurface and molecular sciences, where PNNL has substantial modeling and simulation capabilities.
- **Applied Computational Mathematics** focuses on the development, evaluation, and scalable implementation of solvers and other numerical methods.
- **High-Performance Computer Science** focuses on the development of tools and libraries and validating their effectiveness on massively parallel hardware, and on building performance models for extrapolation to peta- and exascale systems.



Awards & Honors



This graphical cluster compares 42,000 unknown proteins from 10 species of *Shewanella* against a single known protein at the center of the pie. The user has zoomed in on this cluster from the panoply of clusters presented.

RESEARCHERS Earned Top Honors at Supercomputing Conference

Led by Christopher Oehmen, Lee Ann McCue, Bobbie-Jo Webb-Robertson, Scott Dowson, Justin Almquist, Jason McDermott, and Chandrika Sivaramakrishnan captured "Best Overall" for their entry at the Supercomputing 2008 High-Performance Computing Analytics Challenge. Their entry demonstrated that high-performance computing can be integrated into an iterative workflow, which is the way biologists really work.

JASON TOMLINSON Leads National Research Aircraft Committee

Government agencies use research aircraft for everything from hunting hurricanes to measuring Arctic sea ice shrinkage. Since 1997, the Interagency Coordinating Committee for Airborne Geosciences Research and Application has been making it easier to combine and share these resources. Tomlinson was appointed the new leader for this group.

JEAN FUTRELL Receives Chemistry Honor

Futrell, Ph.D., was selected for the first class of American Chemical Society Fellows. This prominent honor, given to only 0.1 percent of the society's more than 150,000 members, reflects Futrell's achievements and contributions to the research community.

JANOS SZANYI Wins Fellowship to Conduct Catalytic Research Abroad

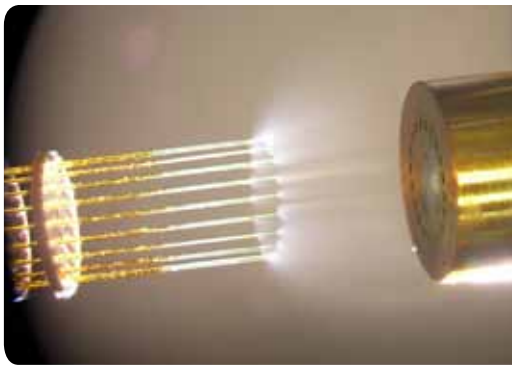
Szanyi, Ph.D., received a Fulbright Fellowship to spend five months in Hungary studying catalysts that may reduce nitrogen oxide emissions from cars and trucks. The fellowship, sponsored by the State Department, provides opportunities for American scientists to conduct research and exchange ideas with international colleagues.

BEAT SCHMID Receives Dual Honors from DOE Office of Science

Schmid, Ph.D., was honored with two awards recognizing his contributions to the Atmospheric Radiation Measurement Program, a Department of Energy multi-laboratory, interagency program for global climate change research. The awards honored his three-year terms as a member of the ARM Climate Research Facility Science Board and as leader of the ARM Program's Aerosol Working Group.

ULTRASENSITIVE ESI-MS Source and Interface Wins R&D 100 Award

When characterizing small, hard-to-acquire samples, scientists need sensitive instruments that can provide highly accurate data. By integrating a combination of inventions and approaches, Drs. Richard D. Smith, Ryan Kelly, Jason Page, and Keqi Tang developed the Ultrasensitive ESI-MS Source & Interface. This instrument enables a 40-fold increase in the sensitivity of mass spectrometry instrumentation. And, the scientists gained a 2009 R&D 100 Award for their efforts. The awards are given annually by *R&D Magazine* to recognize the most technologically significant products of the year.



The Ultrasensitive ESI-MS Source Interface integrates four technologies to enable a 40-fold increase in the sensitivity of mass spectrometry instrumentation while requiring smaller samples.

ALEXANDRE TARTAKOVSKY
Wins Presidential Award

Tartakovsky, Ph.D., won a Presidential Early Career Award for Scientists and Engineers. The award honors his work on subsurface flow that addresses energy needs, such as storing carbon dioxide from fossil fuels underground. Tartakovsky is an acknowledged leader in the field of computational mathematics for subsurface flow and transport in heterogeneous media.

SOTIRIS XANTHEAS Receives Award to Collaborate in Germany

Xantheas, Ph.D., was selected for an Alexander von Humboldt Foundation award to study the ubiquitous solvent: water. The award will cover Xantheas' travel to the Technical University of Munich at Garching and local expenses during his stay in Germany.

BRUCE GARRETT Fellow at Royal Society of Chemistry

Garrett, Ph.D., was appointed a Fellow of the Royal Society of Chemistry, UK. The honor is given to researchers who have made outstanding contributions to the advancement of chemical science.

TIM SCHEIBE
Distinguished Lecturer

Scheibe, Ph.D., was selected as the 2010 Henry Darcy Distinguished Lecturer in Ground Water Science. He was invited by the National Ground Water Research and Educational Foundation to spend a year lecturing at colleges and universities to educate and create interest in groundwater science and technology.

BILL MORGAN Serves as Scientific Director at NASA School

Morgan, Ph.D., was selected as Scientific Director of the 2009 NASA Space Radiation Summer School. The school offers graduate students, postdoctoral fellows, and junior faculty the opportunity to learn about the unique characteristics of space radiation and how to perform experiments exposing targets to high-energy, high-charge particles.

JULIA LASKIN in Russian, U.S. Journals

Laskin, Ph.D., was honored in the *Journal of the American Society of Mass Spectrometry* and *Mass-Spectrometria*, a prestigious Russian mass spectrometry journal. The tributes in these journals honored Laskin's 2008 Biemann Medal given for outstanding achievement in mass spectrometry by a young scientist.

THREE JOINED
Ranks of AAAS Fellow

Three members of the Fundamental & Computational Sciences Directorate were elected Fellows of the American Association for the Advancement of Science. They were recognized at the AAAS national meeting in Chicago in February 2009:

Michel Dupuis– *"distinguished contributions to the fields of computational and theoretical chemistry, particularly for the development of electronic structure methods and computer codes for the simulation of molecular properties and reactivity."*

Ruby Leung– *"outstanding contributions to the development and application of regional climate models."*

Chuck Peden– *"distinguished contributions to the fundamental understanding of catalyst materials and processes for vehicle emission control that have enabled the implementation of new technologies."*

The LAST WORD

In these pages you saw some of the most significant accomplishments in the biological, chemical, computational, environmental, and materials sciences by **Fundamental & Computational Sciences Directorate** scientists in fiscal year 2009. I am proud of their potential to transform our ability to understand and control chemical, physical, and biological processes and to impact the most important challenges in energy, national and homeland security, and environmental sustainability.

Please don't hesitate to contact me or one of the individuals listed at right for more information or to discuss potential collaborations.

Douglas Ray, Ph.D.
Associate Laboratory Director
Fundamental & Computational Sciences Directorate

ABOUT Pacific Northwest National Laboratory

Pacific Northwest National Laboratory is a Department of Energy Office of Science national laboratory where interdisciplinary teams deliver on America's most intractable problems in science, energy, national security, and the environment. PNNL employs 4,250 staff, has a $918 million annual budget, and has been managed by Ohio-based Battelle since the lab's inception in 1965.

For more information about the Fundamental & Computational Sciences Directorate, contact:

Douglas Ray, Ph.D.
Pacific Northwest National Laboratory
P.O. Box 999, MSIN K9-80
Richland, WA 99352
509-375-2500
doug.ray@pnl.gov

Charlette A. Geffen, Ph.D.
Director Atmospheric Sciences & Global Change Division
509-375-3646
ca.geffen@pnl.gov

Harvey Bolton, Jr., Ph.D.
Director Biological Sciences Division
509-371-6958
harvey.bolton@pnl.gov

Bruce C. Garrett, Ph.D.
Director Chemical & Materials Sciences Division
509-372-6344
bruce.garrett@pnl.gov

Moe Khaleel, Ph.D.
Director Computational Sciences & Mathematics Division
509-375-2438
moe.khaleel@pnl.gov

▶ **www.pnl.gov/science**

About the Cover: *For the first time, scientists viewed the bonds that anchor platinum rafts over an aluminum oxide surface, vital knowledge for oil refining and chemical processing.*

PNNL-SA-68598 | September 2009

Pacific Northwest NATIONAL LABORATORY

U.S. DEPARTMENT OF ENERGY

Proudly Operated by **Battelle** *Since 1965*