ADVANCING FRONTIERS IN SCIENCE

Pacific Northwest
NATIONAL LABORATORY

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

Society's advances are built on scientific discoveries, many of which transformed our understanding of the world.

In the late 1600s, Anton van Leeuwenhoek discovered tiny creatures in plaque. The microbes he discovered have changed how we see everything from disease to environmental cleanup.

In the 1700s, Isaac Newton determined the three laws of motion, which explain how objects in the universe move.

In the late 1700s, Antoine Lavoisier published a list of elements, substances that could not be broken down further by any chemical process. Today, these elements are manipulated to build materials for the International Space Station and studied to determine the formation of clouds.

In the 1800s, scientists such as Alessandro Volta figured out how to make electricity flow. In addition to the practical applications, electricity's flow led to discoveries that changed our understanding of the physical world.

In the 1900s, Francis Crick and James Watson discovered the structure of DNA. Today, scientists study DNA in cells as well as a host of other chemicals to understand how to turn biomass into fuels.

In the 2000s, new discoveries will be made. How will they change the world?

On the cover: Researchers at PNNL are leading a multimillion-dollar effort to control chemical transformations for energy applications.

THE NEED FOR TRANSFORMATIONAL SCIENCE

Many people see science as a selfish pursuit; researchers conduct expensive experiments with no application to today's problems, but this view misses the raison d'être for fundamental science—our prosperity and security rely on our understanding the world around us.

For example, discovering how electrons flow across and through a newly designed material could provide insights necessary to design batteries that can ease reliance on fossil fuels. But, without first understanding how the electrons move, nothing more can happen.

This knowledge of our world is not static. It must change and evolve with new information, new viewpoints, and new ideas. New materials, new processes, and new questions continue to arise.

At the Department of Energy's Pacific Northwest National Laboratory, our scientists are pushing the frontiers of that knowledge, from the behavior of subatomic particles to shifts in the global climate patterns.

The problems of *today*.

Fundamental research plays a vital role in solving immediate challenges and creating new knowledge and transformational tools for continued prosperity and security in the 21st century. At PNNL, our research provides knowledge to solve near-term problems for our primary DOE client and others. This new knowledge often generates compelling insights for regulators, legislators, and other decision-makers. In 2007, more than 20 PNNL researchers contributed to the global efforts of the

Scientists at PNNL are designing new tools, such as SPLAT II, that are transforming how we see the particles that lead to the creation of clouds and other climate-influencing factors.

Intergovernmental Panel on Climate Change, which received the Nobel Peace Prize in equal part with former Vice President Al Gore.

Discovery. We also take the longer view to research. Discoveries throughout the ages, such as the laws of motion or the formation of clouds, have transformed how we think, act, and live. Yet, these discoveries were not made to design solar power stations or clean the groundwater. They were made because smart people wanted to know why.

To understand why, our experts collaborate, working on in-house teams as well as with others around the world. Gone are the days of lone scientists slaving away for years in ivory towers. Rather, teams work closely to quickly gain knowledge from multiple angles, bringing together different ideas from a host of scientific disciplines.

These discoveries require developing and deploying new tools and techniques. Further, these tools must be integrated with existing instruments. New computational tools are also needed to conduct the extreme-scale simulations and peta-scale data analytics needed to turn data into discoveries.

Understanding unknowns. While collaborations and instruments can speed discoveries, transformations take time and dedication. At PNNL, we've been leading fundamental science for more than 40 years. Our scientists have made numerous breakthroughs and are continuing to answer that fundamental question about our world: why?

At the Energy Smart Data Center at Pacific Northwest National Laboratory, computer scientists are leading efforts to study data centers' power generation, conversion, and distribution as well as cooling challenges.

PNNL's work in low-dose radiation is helping to determine the mechanistic basis for the interaction of low doses of radiation with biological systems.

PREDICTING CLIMATE CHANGE AND ITS IMPACTS

Climate change is one of the most urgent and far-reaching problems facing our world. Nations are grappling with how to stabilize greenhouse gas concentrations while meeting growing energy demands and maintaining robust economies. Legislators, business leaders, and resource managers need a strong scientific foundation to make informed, climate-related decisions about energy and natural resources.

At PNNL, our fundamental research is helping transform the nation's ability to predict climate change and its impacts. The science community is using our climate models to evaluate the long-term impacts of human activities on climate and natural resources. Decision-makers are using our insights to help shape risk-management and energy strategies.

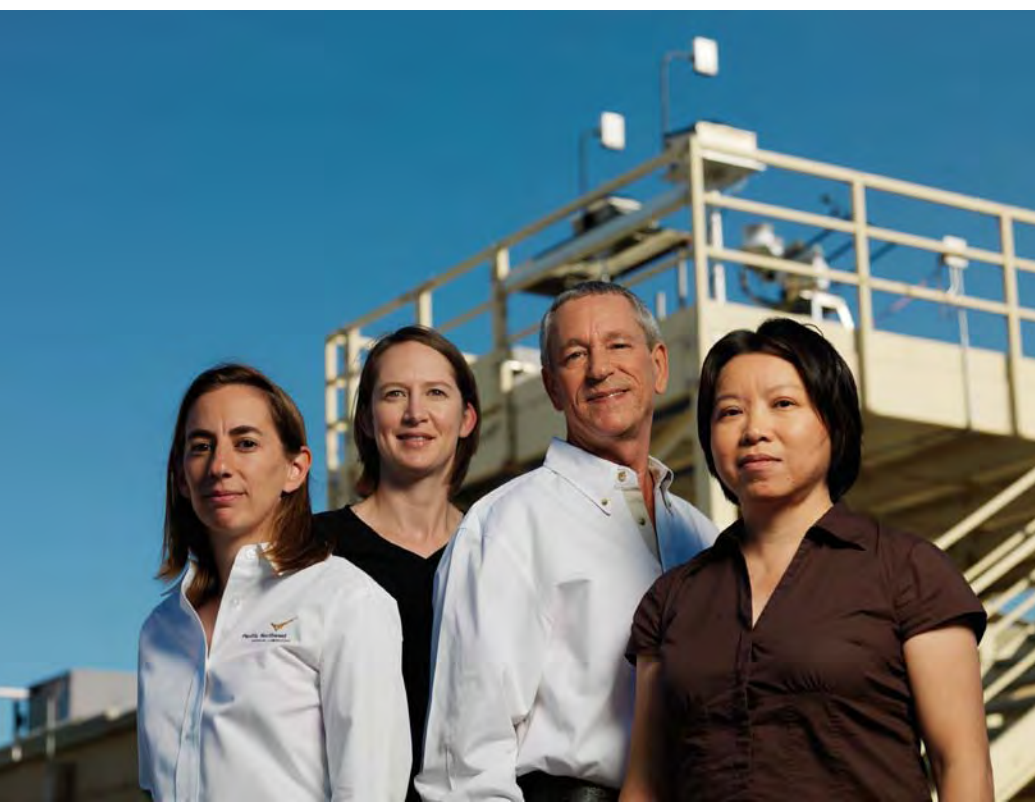
Measurements. Much of the uncertainty in climate predictions is because of the complexity of environmental interactions—such as clouds and aerosols—and the challenges of measuring them. At PNNL, we develop and use sophisticated instruments in the laboratory, on the ground, and in the air to measure these complex interactions. These measurements provide the detail necessary for high-resolution climate models and simulations.

In addition, through our stewardship of the DOE national user facility known as the Atmospheric Radiation Measurement Climate Research Facility, scientists are obtaining continuous field measurements at sites worldwide to make climate predictions as realistic as possible.

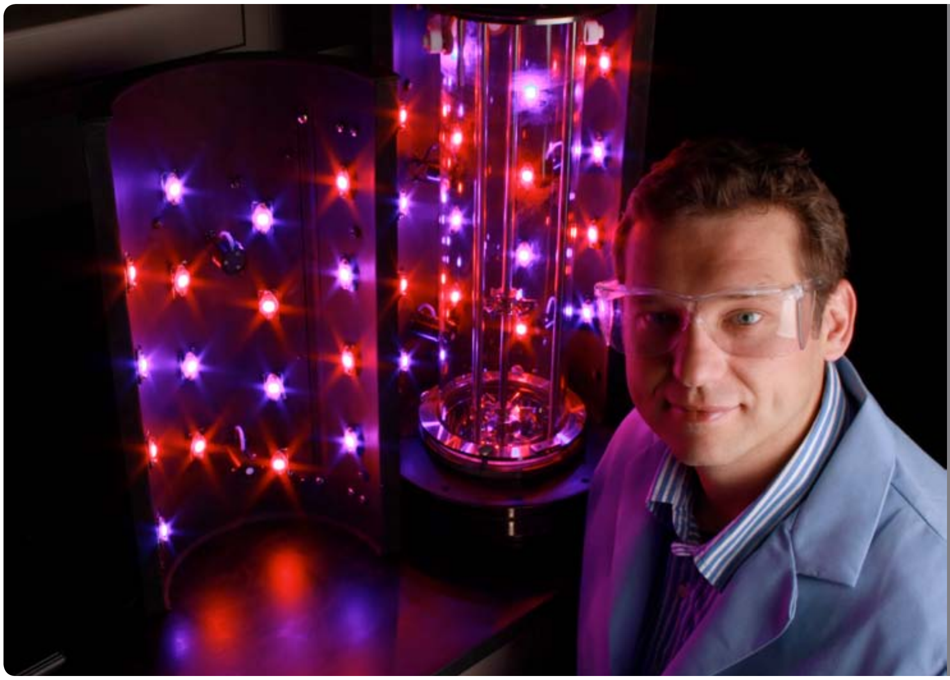
Models. We develop and improve community climate models, both regional and global. The models simulate and predict potential climate changes, including extreme events. Our regional climate models are based on atmospheric processes, weather, and physical features of a particular geographic area. The models are widely used to investigate ways climate features may affect regional systems such as water and agriculture.

Integration. To provide a complete picture of climate change consequences, models must link physical earth processes with human systems, such as energy use, land and water use, policy, and economics. Our research teams create and use the integrated models necessary to understand the dynamics of climate change, its consequences, and the effects of adopting strategies ranging from energy efficiency and biofuels to carbon capture and sequestration.

For a carbon-constrained world, PNNL's climate science is delivering a better understanding of the magnitude of climate change—and the scientific foundation for practical solutions.



At Pacific Northwest National Laboratory, our teams measure and model climate drivers such as cloud properties and aerosol effects. We integrate these with human elements to provide a holistic view of climate change, its consequences, and ways to cope with it.



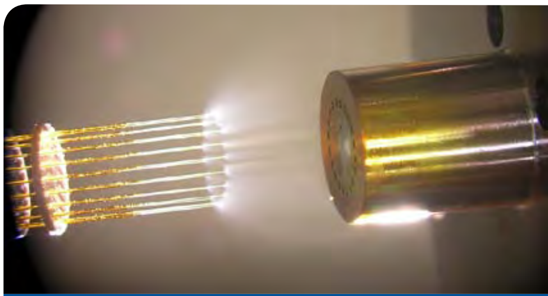
Researchers at Pacific Northwest National Laboratory designed a novel, cutting-edge light enclosure for a photobioreactor that blocks ambient light while providing red and blue light using energy-efficient LEDs. This photobioreactor is aiding in optimizing hydrogen and biofuel production from photosynthetic microbes.

OBTAINING A PREDICTIVE UNDERSTANDING OF MULTI-CELLULAR SYSTEMS

To paraphrase John Donne: no cell is an island. Whether it is a bacterium such as *E. coli* or part of a plant, animal, or fungi, each cell has a specific role for which it was created. But a cell doesn't act alone. Cells are part of multi-cellular biological systems—from microbial communitites to humans. The environment, neighboring cells, and other processes all impact a cell's behavior and function.

Limited information is available about how communities of cells and organisms respond and adjust to environmental stress or changes as multi-cellular systems. PNNL is developing and applying technologies for measuring biological, chemical, and physical properties at relative spatial and time scales. We are also developing the computational framework that links this information to cell communities and environmental interfaces.

Because of the ever-increasing volume of cell information, today's instruments can't easily analyze and interpret the data. So, scientists at PNNL are creating first-of-a-kind tools and techniques that can provide high-throughput data and quickly analyze these large data sets with unprecedented resolution. By combining experimental data with theoretical studies and computational resources, we are pushing the state of the science and learning how living systems composed of different types of cells will respond and adjust to change. By doing so, we can also find ways to understand and predict how cells perform in ways that will benefit us by providing new energy sources, cleaning up our environment, influencing carbon sequestration, and impacting human health.



Integrating experimental data from award-winning tools such as the ESI-MS Source & Interface with theoretical studies and computational models, biologists at Pacific Northwest National Laboratory are pushing the state of science regarding proteins and other cellular molecules.

CHANGING HOW SCIENTIFIC COMPUTING IS DONE

Global climate experts, energy security analysts, and others are seeking previously unseen patterns and unknown consequences from complex, massive data sets. For example, higher resolution climate models will produce terabytes of data in a single day of run time, a 1,000-fold increase in the amount of data. To turn these extreme data sets into discoveries requires new computational capabilities.

Fast, fault-free *software*. The need for new capabilities includes programs that take advantage of the power of supercomputers. Many models, simulations, and analysis programs take exponentially more resources to run on larger computer systems than on smaller ones. Many of these programs are also fault-sensitive, crashing when they encounter a faulty component, such as a bad disk. Often scientists must re-run the program—sometimes waiting months to do so, because the computers are so highly subscribed. With the large number of components in supercomputers, hardware faults occur far too often.

Our researchers are creating techniques to improve fault resiliency. We are working on different approaches and performing tests on the Chinook supercomputer in the Environmental Molecular Sciences Laboratory.

Memory *bottlenecks*. As supercomputers grow larger and more powerful, performance is still determined mainly by the speed at which the memory can deliver information to the processor. For activities in which the data is arranged in an unpredictable manner, such as grid analysis, the processor is idle 80 to 90 percent of the time while waiting for data from memory.

To overcome this bottleneck, our scientists are collaborating with their peers on a different approach: the multithreaded supercomputer. The multithreaded system enables multiple, simultaneous processing, compared to the linear approach of other systems. Through the Center for Adaptive

Our scientists are devising applications to run on multithreaded supercomputers configured for data discovery and analysis.

Supercomputing—Multithreaded Architectures at PNNL, we are designing applications for this new high-performance computing approach and testing them on our Cray XMT.

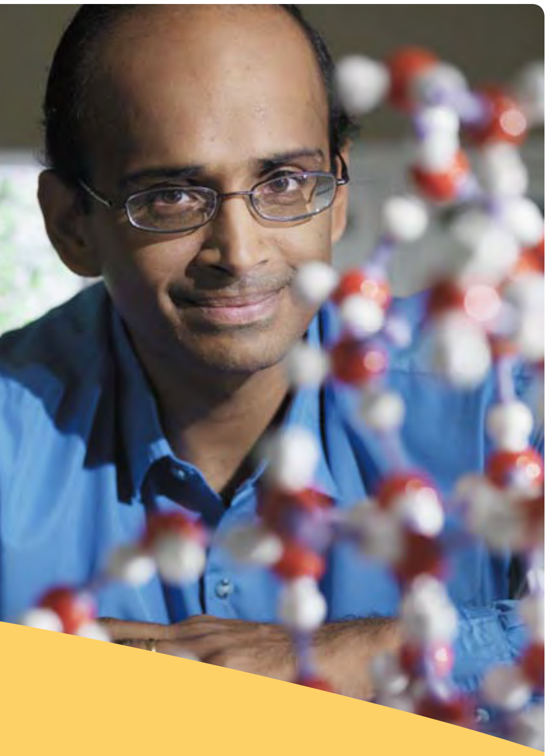
Team approach. Scientific computing is undergoing a rapid transformation as high-resolution models, high-throughput instruments, and highly sensitive sensors provide extreme levels of data. At PNNL, we are working with biologists, physicists, and others to help solve the computing challenges necessary for new discoveries.

WORLD-CLASS SCIENTIFIC USER FACILITY

Scientific advancements cannot be made without similar advances in the tools used to make discoveries. At the Department of Energy's Environmental Molecular Sciences Laboratory, a national scientific user facility at PNNL, scientists and engineers are developing, integrating, and deploying new tools that will enable researchers to change how they view chemical and biological systems: from single molecules to communities of species, from static to dynamic processes, from *ex situ* systems to *in situ* observation. Further, these new tools and techniques will enable the type of discoveries that truly change the face of science.

A transmission electron microscope with capabilities for cryo-stage and tomography is one of the many cutting-edge instruments available at the Environmental Molecular Sciences Laboratory.

EMSL



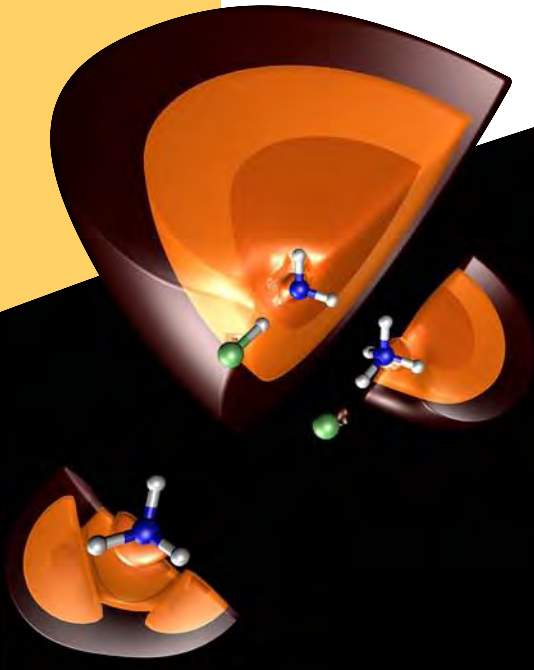
UNDERSTANDING AND CONTROLLING CHEMICAL AND PHYSICAL PROCESSES IN COMPLEX ENVIRONMENTS

Photosynthesis. Burning coal. Refining oil. For hundreds of years, scientists have examined these and other processes to understand how reactions work in the real world. Understanding is key to controlling. However, much of our knowledge is limited to simpler gas-phase systems. How atoms, molecules, and microbes behave in liquid water and other condensed phases as well as at interfaces presents a host of mysteries. At PNNL, our scientists are solving these mysteries.

Our experts combine experimental, theoretical, and computational approaches to shed light on processes and reactions, such as the movement of charges through water, in next-generation fuel cells.

***Working* on the small scale.** Through new methods and technologies, scientists are learning how atoms, molecules, and ions interact with photons and electrons, and how to make and break chemical bonds. This understanding is transforming how we view the interaction of minerals, microbes, and other subsurface reactions. Further, understanding reactions from electrons to molecules is key to building new materials. At PNNL, scientists are learning to build, atom by atom, materials that control charge transport in sensors, batteries, and fuel cells.

***Leading* on the world stage.** In the United States, China, and other countries, catalyzing reactions efficiently is key to mitigating the impacts of energy use and manufacturing. In looking to solve near-term issues, scientists at the Laboratory's Institute for Interfacial Catalysis conduct world-leading research to convert biomass and coal to cleaner energy sources. Taking a more fundamental discovery approach, scientists at the newly formed Center for Molecular Electrocatalysis are delving into molecular systems that convert electrical energy into chemical bonds and back again.



This depiction of electrons helping to spur the chemical reaction between an acid and a base was featured on the cover of *Science*.

Credit: Maciej Haranczyk.

UNDERSTANDING ENERGY AND MATERIALS TRANSFER IN THE SUBSURFACE FROM MOLECULAR TO FIELD SCALES

The Earth's subsurface is of intense interest to scientists, whether it's being mined for coal, providing water free from contaminants, or capturing carbon to help prevent global climate change.

As demands rise for energy and clean water, so does the demand to understand the subsurface from the molecular to the field scale.

Integrated research at multiple scales from molecule to field is required to understand energy and material transfer in the subsurface. Microenvironments and transition zones are key areas that can exert a disproportionate influence on the subsurface. Within these areas, microbial, geochemical, and other processes work together at accelerated rates, changing the dynamics underground. To characterize and control these processes, scientists at PNNL are integrating laboratory, field, and computational modeling studies of coupled processes.

By understanding these coupled interactions and processes that take place in the subsurface on a small scale, scientists can then create models that will predict behavior on a large scale. Having this knowledge will lead to informed decisions about environmental remediation and carbon sequestration, as just two examples.

Our scientists conduct complex experiments and computer simulations to provide insights into microbes' impact on subsurface reactions.

Researchers interrogate a well field near the Columbia River to understand processes controlling the fate and transport of subsurface uranium.

SCIENTIFIC LEADERSHIP

At the Pacific Northwest National Laboratory, our leaders influence national and international direction of scientific discovery.

Jean H. Futrell, Ph.D.

Battelle Fellow

Recognized for pioneering research in mass spectrometry fundamentals

Fellow of the American Chemical Society, the American Physical Society, the American Society for Advancement of Science, and the World Innovation Foundation

Bruce Garrett, Ph.D.

Laboratory Fellow

Director, Chemical & Materials Sciences Division

Recognized for advances in theoretical physical chemistry, especially reaction rate theory

Fellow, Royal Society of Chemistry, UK; American Physical Society; and the American Association for the Advancement of Science

Mohammad (Moe) A. Khaleel, Ph.D.

Laboratory Fellow

Director, Computational Sciences & Mathematics Division

Recognized for research in superplasticity of aluminum alloys and computational mechanics

Fellow, American Society of Mechanical Engineers and the American Association for the Advancement of Science

James K. Fredrickson, Ph.D.

Laboratory Fellow

Chief Scientist, Biology

Recognized for pioneering research in microbial ecology and environmental microbiology of geologically diverse subsurface environments

Leader of the U.S. Department of Energy's *Shewanella* Federation

Fellow, American Association for the Advancement of Science

Philip Rasch, Ph.D.

Laboratory Fellow

Chief Scientist, Climate Change

Recognized internationally for climate modeling and atmospheric chemistry

American Chair and Steering Committee, National Science Foundation Science and Technology Center for International Global Atmospheric Chemistry

Steering Committee, Community Climate System Model Program and Chair, Atmospheric Model Working Group

Richard D. Smith, Ph.D.

Battelle Fellow

Chief Scientist, Proteomics

Internationally recognized for advanced analytical methods for quantitatively probing the entire array of proteins expressed by a cell, tissue, or organism

Eight R&D 100 Awards for innovation, 2003 American Chemical Society Award for Analytical Chemistry, Council of the Human Proteome Organisation Member

Fellow, American Association for the Advancement of Science

Lou Terminello, Ph.D.

Chief Scientist, Fundamental & Computational Sciences

Recognized for leadership of science and technology program development, and materials characterization using synchrotron radiation

Fellow, American Physical Society

John Zachara, Ph.D.

Laboratory Fellow

Chief Scientist, Biogeochemistry

Recognized for research on the geochemical interaction of organic, metal, and radionuclide contaminants with organic materials, mineral matter, and subsurface materials

E.O. Lawrence Award, 2007

Fellow, American Association for the Advancement of Science

Laboratory Fellows – Advancing Fundamental Science

Donald Baer – surface analysis methods to examine corrosion processes and the reactive properties of oxide and mineral surfaces

R. Morris Bullock – factors governing the rates and mechanisms of metal-hydrogen bond cleavage

Scott Chambers – synthesis and properties of novel oxide films and surfaces

Richard Corley – pharmacokinetic modeling to improve health risk assessments

Michel Dupuis – theoretical and computational chemistry to the characterization of the electronic structure and reactivity of molecules, solids, and interfaces in chemical processes

Jae Edmonds – one of the founders of the field of integrated assessment modeling for climate change

Paul Ellis – large-molecule characterization techniques using unique magnetic resonance and mass spectrometry

Andy Felmy – measurement and modeling of the aqueous thermodynamics and solid-phase equilibria in high ionic strength electrolytes

James Franz – kinetics and theory of reactions of organic and organometallic free radicals

Jay Grate – interdisciplinary research in chemically selective materials, chemical microsensors, and analytical fluidics

Michael Henderson – physical and chemical properties of complex oxide surface phenomena

R. César Izaurralde – soil carbon sequestration and greenhouse gas emissions in agriculture

Bruce Kay – chemical kinetics and molecular dynamics to gain a detailed physical understanding of the microscopic molecular-level interactions

David L. King – catalysis, fuel chemistry

Allan Konopka – population and community ecology of aquatic and soil microorganisms and investigations of microbiological influences on contaminant fate and transport

David Koppenaal – development of atomic mass spectrometry for inorganic and isotopic characterization, and demonstration of new analysis techniques

Ruby Leung – regional climate models that couple climate and hydrologic processes in regions with complex orography

Yuehe Lin – nanomaterial-based chemical sensors and biosensors

Jun Liu – pioneering research in self-assembled nanoscale materials

Charles Peden – heterogeneous catalytic chemistry of metals and oxides (reaction mechanisms, materials)

Karin Rodland – signal transduction pathways that regulate proliferation in normal and malignant cells

Gregory K. Schenter – theoretical chemistry

Thomas Squier – calcium homeostasis and transport in biological systems

T.P. Straatsma – advanced modeling and simulation methods as key scientific tools in the computational study of chemical and biological systems

Yong Wang – structural and functional relationship of metal oxide catalysts

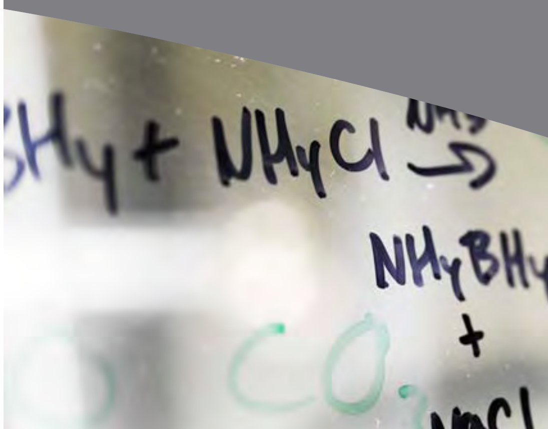
William Weber – radiation-solid interactions, radiation effects, and defects and defect processes in ceramics

Steven Wiley – mechanisms of cell communication and signaling using the epidermal growth factor receptor system

Sotiris Xantheas – use of *ab-initio* electronic structure calculations to elucidate structural and spectral features of intermolecular interactions in aqueous ionic clusters

Pacific Northwest National Laboratory's science agenda

- Achieve a predictive understanding of multi-cellular biological systems
- Understand energy and materials transfer in the subsurface from molecular to ecosystem scales
- Develop tools and understanding required to control chemical and physical processes in complex multiphase environments
- Create new computational capabilities to solve problems using extreme-scale simulation and peta-scale data analytics
- Transform the nation's ability to predict climate change and its impacts
- Develop, integrate, and deploy transformational tools in the Environmental Molecular Sciences Laboratory that accelerate scientific discovery and innovation



ABOUT PACIFIC NORTHWEST NATIONAL LABORATORY

PNNL is one of DOE's national laboratories, managed by the Department's Office of Science. Researchers at PNNL perform work for other DOE offices as well as government agencies, universities, and industry to deliver breakthrough science and technology to meet today's key national needs. Our Laboratory

- provides the facilities, unique scientific equipment, and world-renowned scientists/engineers to strengthen U.S. scientific foundations for fundamental research and innovation
- prevents and counters acts of terrorism through applied research in information analysis, cyber security, and the non-proliferation of weapons of mass destruction
- increases U.S. energy capacity and reduces dependence on imported oil through research of hydrogen and biomass-based fuels
- reduces the effects of energy generation and use on the environment

PNNL has approximately 4,250 staff members and a business volume of $918 million. PNNL operates a marine research facility in Sequim, and has satellite offices in Seattle and Tacoma, Washington; Portland, Oregon; College Park, Maryland; and Washington, D.C.

Battelle has operated PNNL for DOE and its predecessors since 1965.

Scientists at Pacific Northwest National Laboratory conduct research in laboratories and in the field around the world.

For more information, contact

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U.S. DEPARTMENT OF ENERGY

Sept. 2009 | PNNL-SA-68037