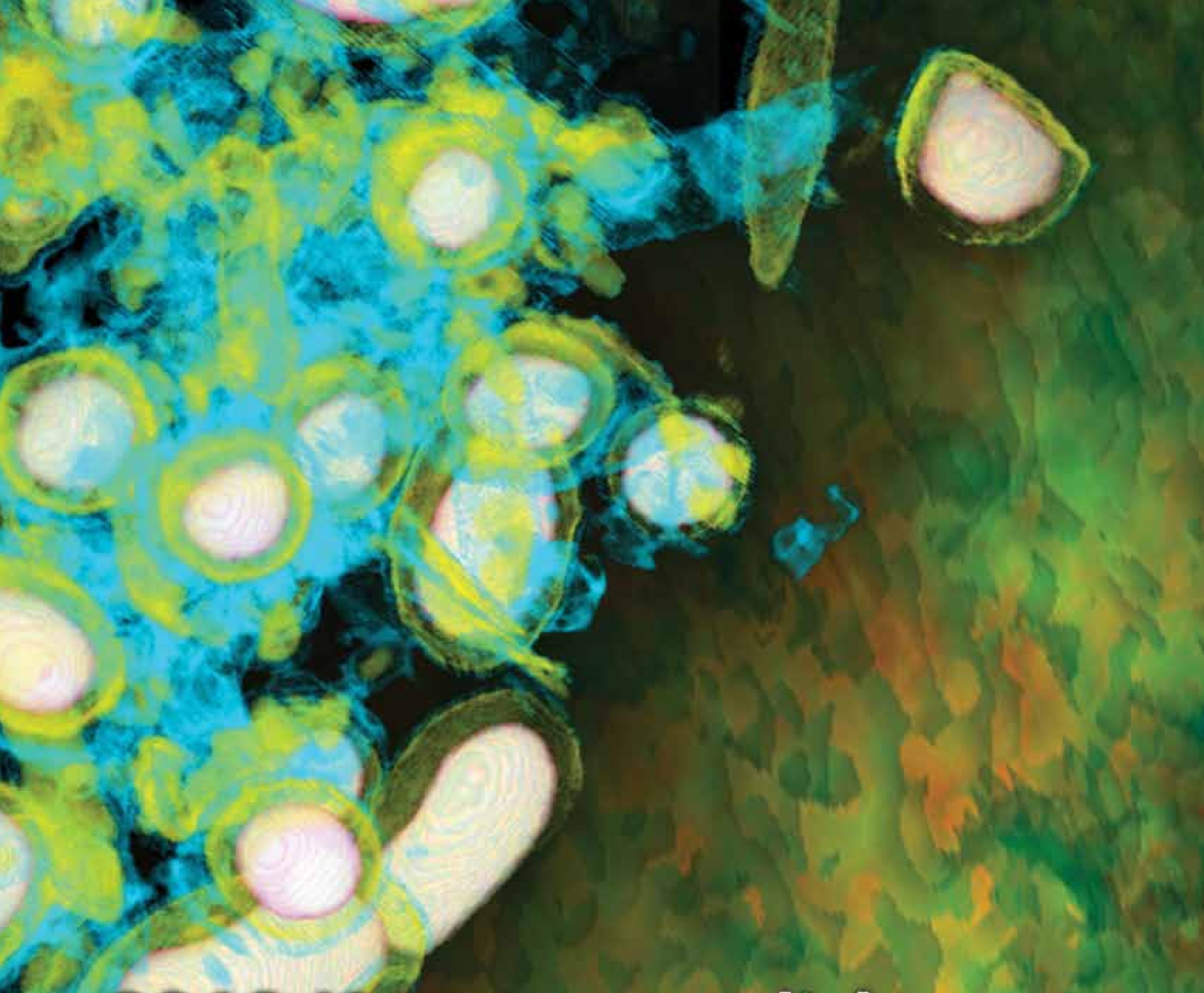


2012 Key Accomplishments

FUNDAMENTAL & COMPUTATIONAL SCIENCES

Pacific Northwest
NATIONAL LABORATORY

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

Cover image: Soft x-ray microtomography images showing high-resolution reconstructed biofilm cells grown at Pacific Northwest National Laboratory. Characterizing the chemical and physical interactions of biofilms will provide insight to how microorganisms influence larger, pore-scale biogeochemical processes.

In these pages you will find some of the noteworthy achievements made by Pacific Northwest National Laboratory (PNNL) scientists in 2012. I am proud of their potential to advance scientific frontiers and to unravel some of the most important challenges in energy, national security, and environmental sustainability.

In 2012, we significantly enhanced our capabilities in materials characterization, including adding new scientific talent and bringing several new state-of-the-art transmission electron microscopes online. In addition, we have significantly expanded our utilization of the nation's x-ray light sources. With these and other new capabilities in chemical imaging, we are accelerating scientific discovery and innovation.

If you are interested in collaborating with us, please don't hesitate to contact me or one of the individuals listed on the back of this booklet for more information.

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

A novel, cutting-edge custom light enclosure for photobioreactors blocks ambient light from entering a bioreactor while providing red and blue light using energy-efficient LEDs. This photobioreactor is used to optimize hydrogen and biofuel production from photosynthetic microbes, such as *Cyanothece*. Its large volume and continuous culture capability enable mass-production of biomass for biofuels and alternative fuel research.

Biological systems science encompasses the ability to measure, predict, design, and ultimately control multicellular biological systems and bioinspired solutions for energy, environment, and health. It involves fundamental research and technology development of natural and engineered biological systems in the laboratory and in the field using systems and synthetic biology approaches. PNNL is recognized internationally for our biological systems science capabilities, including leadership in proteomics and other 'omic technologies, environmental microbiology, systems toxicology, and biotechnology. Our expertise includes cell biology and biochemistry, radiation biology, computational biology, and bioinformatics. The biological systems science performed here contributes to advances in bioenergy, biogeochemistry of inorganic contaminants and carbon, human health, and national security.

Genome-Scale Model of Cyanobacterium Developed

In an important step toward engineering bacteria to produce biofuel, scientists at PNNL, University of Wisconsin-Madison, and Burnham Institute for Medical Research developed one of the first global models for the cyanobacterium *Cyanothece* sp. ATCC 51142. Cyanobacteria have potential for producing biofuel because they photosynthesize, have relatively rapid growth rates and tolerance to extreme environments, and can accumulate high amounts of intracellular compounds. But only a few models have been developed for investigating them because they are so complex. This genome-scale metabolic reconstruction and simulation model describes *Cyanothece's* complete metabolism, not just isolated pathways, and how carbon and energy are distributed throughout the cell for photosynthesis and respiration. It will aid in developing similar models for other cyanobacteria and serve as an engineering tool for manipulating photosynthetic microorganisms to improve biofuel production.

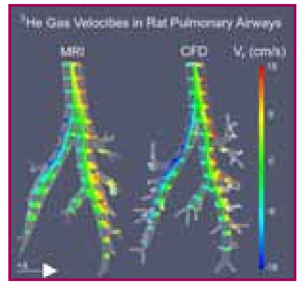
TT Vu, SM Stolyar, GE Pinchuk, EA Hill, LA Kucek, RN Brown, MS Lipton, AL Osterman, JK Fredrickson, AE Konopka, AS Beliaev, and JL Reed. 2012. "Genome-Scale Modeling of Light-Driven Reductant Partitioning and Carbon Fluxes in Diazotrophic Unicellular Cyanobacterium *Cyanothece* sp. ATCC 51142." *PLoS Computational Biology* 8(4):e1002460. DOI: 10.1371/journal.pcbi.1002460.

Sponsor: Department of Energy Office of Biological and Environmental Research

"Developing this model brings us closer to a systems-level understanding of the metabolism of photoautrophs such as *Cyanothece*, putting metabolic engineering of these organisms within reach."

— Dr. Alex Beliaev, PNNL

Lung Imaging Research Gets Second Wind



Patterns of helium-3 gas velocity measured with magnetic resonance imaging are compared to numerical predictions formulated using computational fluid dynamics.

Scientists use computational fluid dynamics (CFD) as a quantitative basis for predicting airflow patterns that carry inhaled materials inside the body. This not only helps establish safer exposure limits to airborne pollutants but also can improve targeted drug delivery in patients with pulmonary disease. But simulated predictions must be thoroughly tested in a living organism, where respiratory airflows not only depend on airway shape and curvature but also local lung mechanics and differences between health and disease. Until recently, this level of testing was not possible, but researchers at PNNL took an important step by making the first-ever comparison between CFD-predicted and measured airflow patterns in a live rat. Their findings highlight the practical use of magnetic resonance imaging for developing and assessing predicted airflow patterns within the breathing lung and for testing the mass-transfer models that are fundamental to gas mixing in respiratory physiology.

KR Minard, AP Kuprat, S Kabilan, RE Jacob, DR Einstein, JP Carson, and RA Corley. 2012 "Phase-Contrast MRI and CFD Modeling of Apparent ^{3}He Gas Flow in Rat Pulmonary Airways." *Journal of Magnetic Resonance* 221:129-138. DOI: http://dx.doi.org/10.1016/j.jmr.2012.05.007.

Sponsor: National Heart, Lung, and Blood Institute

Annotating Plague with Proteogenomics

Strains of bacteria from the genus *Yersinia* cause maladies such as intestinal distress and plague. To better understand and potentially design ways to mitigate *Yersinia's* effects on human health, researchers from PNNL, the J. Craig Venter Institute, and University of Texas Medical Branch refined the genome maps of three *Yersinia* strains. The team used *Yersinia's* proteome and transcriptome to discover new information about the genome. They confirmed the validity of nearly 40 percent of the computationally predicted genes and discovered 28 novel proteins expressed under infection-relevant conditions. They also showed that 68 previously identified protein-coding sequences were invalid. These refined annotations provide essential information needed to better understand how *Yersinia* functions, may provide new targets for therapeutics, and should speed characterization of other pathogenic bacteria.

AC Rutledge, MB Jones, S Chauhan, SO Purvine, J Sanford, ME Monroe, HM Brewer, SH Payne, C Ansong, BC Frank, RD Smith, S Peterson, VL Motin, and JN Adkins. 2012. "Comparative Omics-Driven Genome Annotation Refinement: Application Across *Yersiniae*." *PLoS One* 7(3):e33903. DOI: 10.1371/journal.pone.0033903.

Sponsor: National Institute of Allergy and Infectious Diseases

BIOLOGICAL SYSTEMS SCIENCE

Bacteria Tend Leafcutter Ants' Gardens

Known for carrying leaves through tropical forests, leafcutter ants also cultivate underground gardens of fungi and bacteria. PNNL research about the roles bacteria play in those gardens could eventually help scientists turn plants into biofuel. *Photo courtesy of Alejandro Soffia Vega.*

Leafcutter ants, tiny red dots that carry green leaves through tropical forests, are also talented farmers that cultivate gardens of fungi and bacteria. Ants eat fungi from the fungal gardens, but the bacteria's role has been unclear until now. Scientists at PNNL and the University of Wisconsin-Madison showed that the bacteria help decompose the leaves and play a major role in turning the leaves into nutrients of importance to both ants and fungi. Metagenomics and proteomics studies of the community's genes and proteins provided some of the first tangible details about the symbiotic relationship between ants, fungi, and bacteria. Such understanding could help improve plant deconstruction needed before biofuel production.

FO Aylward, KE Burnum, JJ Scott, G Suen, SG Tringe, SM Adams, KW Barry, CD Nicora, PD Piehowski, SO Purvine, GJ Starrett, LA Goodwin, RD Smith, MS Lipton, and CR Currie. "Metagenomic and Metaproteomic Insights into Bacterial Communities in Leaf-Cutter Ant Fungus Gardens." *The ISME Journal* 6(9):1688-1701. DOI: 10.1038/ISMEJ.2012.10.

Sponsor: Department of Energy Office of Biological and Environmental Research

Human Skin Model Shows Low Dose Exposure Effects

In studies on a human skin tissue model, researchers at PNNL showed that an ionizing radiation dose mimicking that received during a CT scan is sufficient to alter genes in two cell layers. They found 428 genes altered in the epidermis, the outer skin layer, and 1452 genes altered in the dermis underneath. Altered genes in the two layers showed little overlap, but their affected signaling pathways were similar. These results agreed with human subject data, suggesting that the 3D human skin tissue model is a faithful representation of intact tissue. The low exposure mimics the dose limit for a full-body spiral CT and other radiotherapy procedures and will help establish correct estimates of the risk of developing radiation-induced health problems in the low-dose region.

C von Neubeck, H Shankaran, NJ Karin, PM Kauer, WB Chrisler, X Wang, RJ Robinson, KM Waters, SC Tilton, and MB Sowa. 2012. "Cell Type-Dependent Gene Transcription Profile in a Three-Dimensional Human Skin Tissue Model Exposed to Low Doses of Ionizing Radiation: Implications for Medical Exposures." *Environmental and Molecular Mutagenesis* 53(4):247-259. DOI: 10.1002/em.21682.

Sponsor: Department of Energy Office of Biological and Environmental Research, National Aeronautics and Space Administration

The geothermal systems in Yellowstone National Park are field laboratories for scientists seeking to understand the origin and evolution of metabolic processes necessary for life in extreme environments, particularly in the microbial mats found in hot springs.

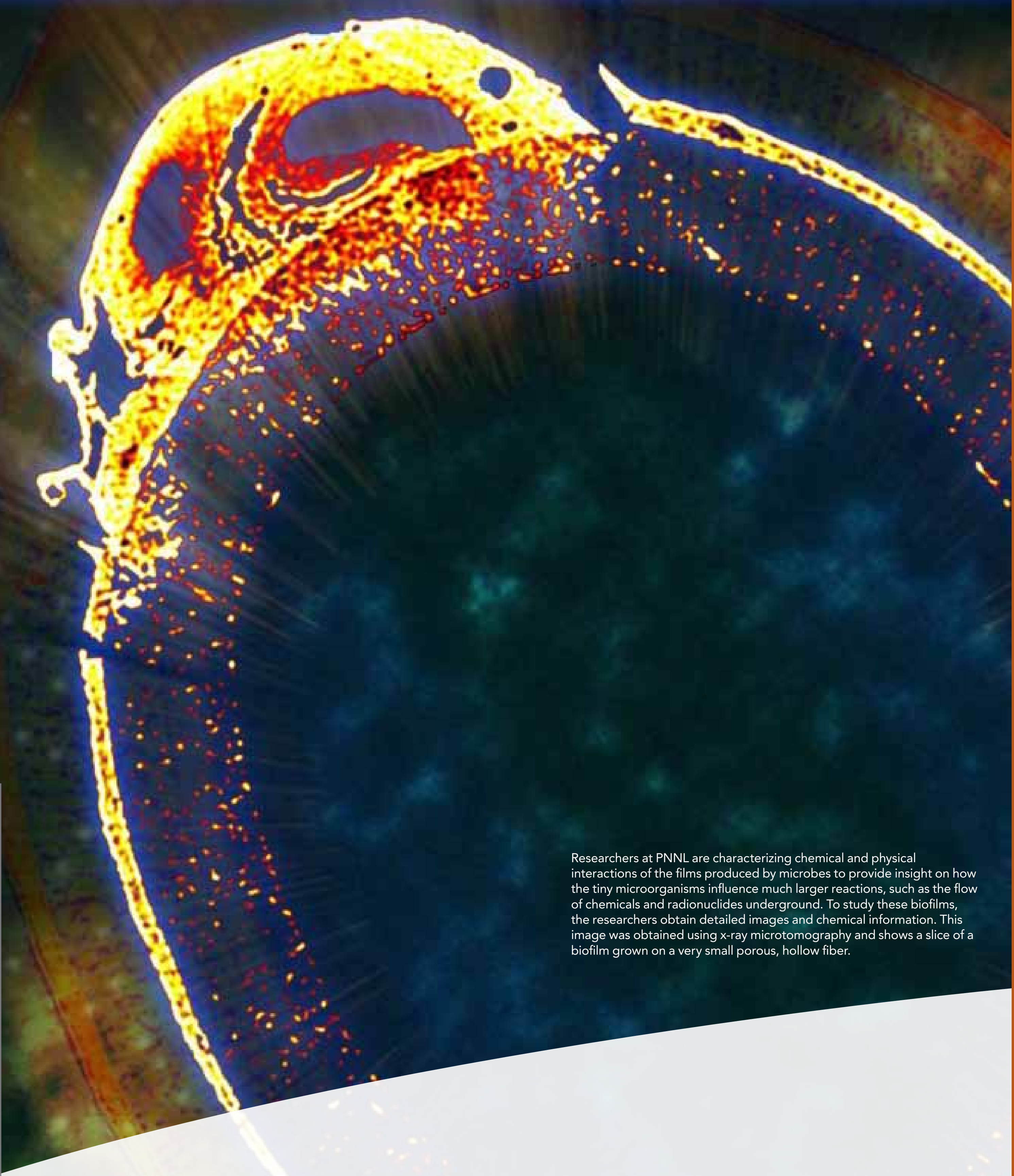
Novel Archaea Found in Yellowstone National Park Hot Springs

Hot springs in our oldest national park harbor microbial communities that can convert CO_2 into organic compounds while oxidizing inorganic compounds for energy to fuel the process. Detailed analyses of four metagenome sequence assemblies from Yellowstone National Park microbial mats by scientists at PNNL, Montana State University, Indiana University, and the Joint Genome Institute revealed a proposed new archaeal phylum, Geoarchaeota, the sixth named to date. Geoarchaeota bridges gaps between other phyla within the domain Archaea, a group of single-celled microorganisms with no cell nucleus. The discovery is part of ongoing research to discover key microbial interactions enabling formation of stable microbial communities where the primary influx of carbon is mediated by CO_2 fixation using reduced chemical or light as energy.

M Kozubal, MF Romine, RdeM Jennings, ZJ Jay, SG Tringe, DB Rusch, JP Beam, LA McCue, and WP Inskeep. 2012. "Geoarchaeota: A New Candidate Phylum in the Archaea from High-Temperature Acidic Iron Mats in Yellowstone National Park." Submitted to *The ISME Journal*.

Sponsor: Department of Energy Office of Biological and Environmental Research, National Science Foundation, Montana Agricultural Experiment Station

CHEMICAL IMAGING



Researchers at PNNL are characterizing chemical and physical interactions of the films produced by microbes to provide insight on how the tiny microorganisms influence much larger reactions, such as the flow of chemicals and radionuclides underground. To study these biofilms, the researchers obtain detailed images and chemical information. This image was obtained using x-ray microtomography and shows a slice of a biofilm grown on a very small porous, hollow fiber.

Scientists have long wanted to "see" chemical, material, and biochemical processes, in time and space, with enough detail to determine what is happening at the molecular level. This level of detail will allow them to move from observing processes to controlling them. But today's tools cannot reach the needed level of clarity. In collaboration with U.S. and U.K. universities, scientists at PNNL are inventing the tools and techniques to generate in situ, or in-place, images at the nanometer and near-nanometer scales. They are also building the computational tools to analyze the massive data quantities generated.

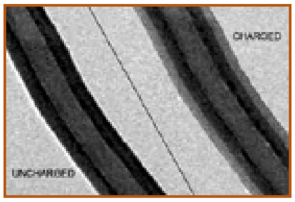
Getting a More Realistic View of Nanoparticle Toxicity

Everyday products from sunscreens to paints use nanoparticles because of their unique features. The particles' small diameter allows them to penetrate deep into the lungs, and the effect these tiny particles can have on the cells that line the lungs is unknown. According to scientists at PNNL and the University of Oregon, how zinc oxide nanoparticles damage lung cells depends on whether the material is intact or dissolved. Conventional toxicity studies of nanoparticles use cells submerged in liquid nutrients. But human lung cells aren't immersed in growth media. The team wanted to know if closely mimicking real-world conditions, specifically cells' exposure to air, changed the results. Using microscopy and other imaging techniques, they found that zinc oxide nanoparticles are just as toxic, but the path the particles used to damage the cells was different. This study and others shed new light on the underlying reactions that govern whether the cells ignore or become stressed by the particles.

Y Xie, NG Williams, A Tolic, WB Chrisler, JG Teeguarden, BL Maddux, JG Pounds, A Laskin, and G Orr. 2012. "Aerosolized ZnO Nanoparticles Induce Toxicity in Alveolar Type II Epithelial Cells at the Air-Liquid Interface." *Toxicological Sciences* 125(2):450-461. DOI: 10.1093/toxsci/kfr251.

Sponsors: National Institute of Environmental Health Sciences, Air Force Research Laboratory/Oregon Nanoscience and Microtechnologies Institute/Safer Nanomaterials & Nanomanufacturing Initiative

Silicon-Carbon Electrodes Snap, Swell, Don't Pop



This composite image shows a silicon-carbon nanofiber electrode before (left) and after (right) being charged with lithium ions.

Scientists at PNNL, Oak Ridge National Laboratory, Applied Sciences, Inc., and General Motors examined a new type of silicon-carbon nanocomposite electrode and revealed details of how they function and how repeated use could wear them down. With an electrical capacity five times higher than conventional lithium-ion battery electrodes, silicon-carbon nanocomposite electrodes could lead to longer-lasting, cheaper rechargeable batteries for electric vehicles.

CM Wang, X Li, Z Wang, W Xu, J Liu, F Gao, L Kovarik, JG Zhang, J Howe, DJ Burton, Z Liu, X Xiao, S Thevuthasan, and DR Baer. 2012. "In Situ TEM Investigation of Congruent Phase Transition and Structural Evolution of Nanostructured Silicon/Carbon Anode for Lithium Ion Batteries." *Nano Letters* 12(3):1624-1632. DOI: 10.1021/nl204559u.

Sponsors: PNNL Laboratory Directed Research and Development, Department of Energy Office of Energy Efficiency and Renewable Energy

NanoDESI takes samples from a microbial colony, such as this one, for transfer to a mass spectrometer.

Listening to Life

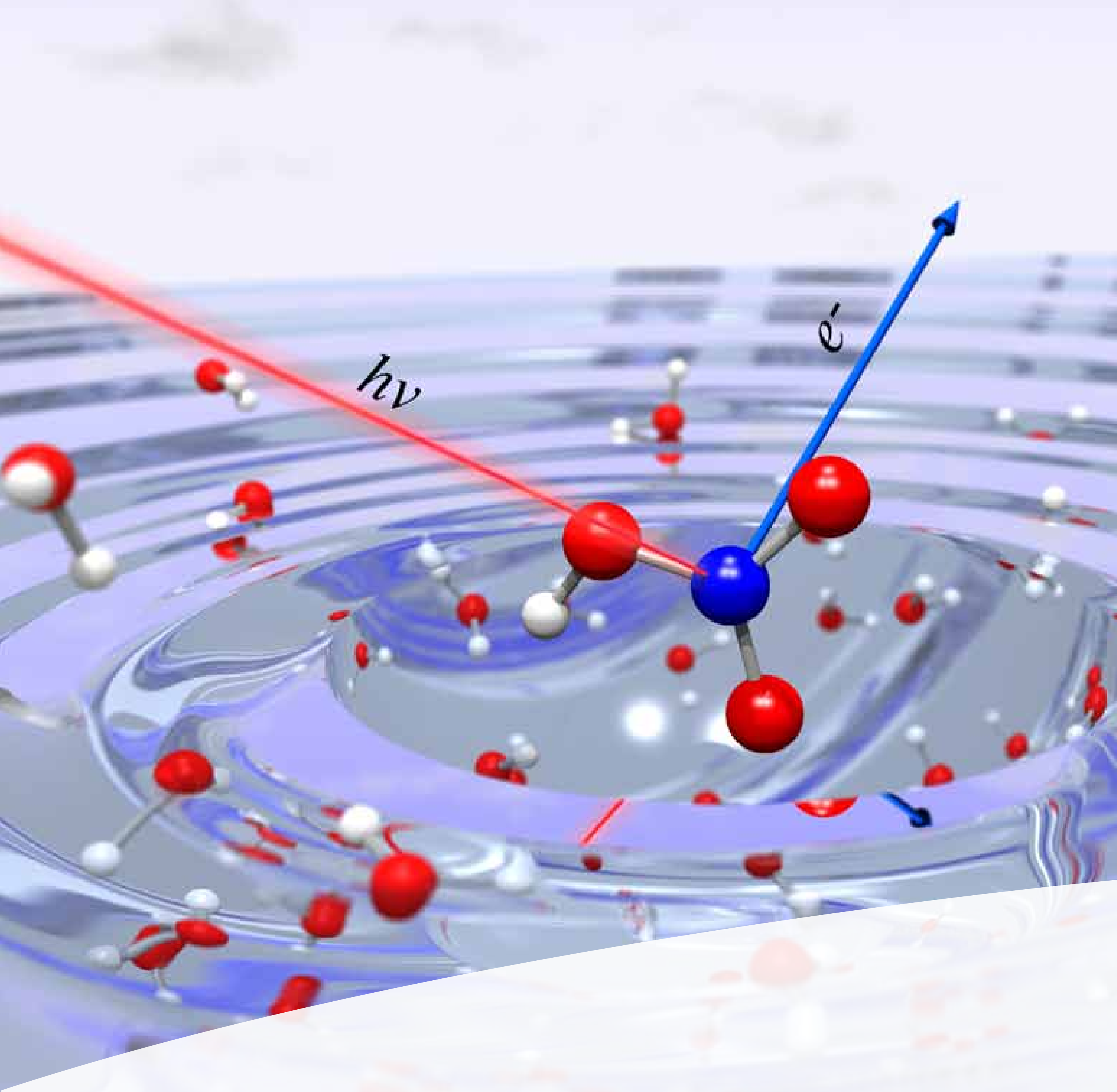
Once impossible, scientists can now eavesdrop on microbes, thanks to a new technique from scientists at PNNL and three universities. Microbes converse by releasing molecules called metabolites. The metabolites interact with and alter their environment and nearby cells. To listen in, the team combined nanospray desorption electrospray ionization mass spectrometry, or nanoDESI, and a new bioinformatics technique. This approach allows scientists to identify and quantify, in time and space, the metabolites around living bacterial colonies.

NanoDESI uses liquid drops to gently draw samples from the microbial colony and transfer them to a mass spectrometer. The mass spectrometer provides structural information about the thousands of molecules detected. The data is analyzed, organized, and visualized using molecular networking. Understanding the timing and distribution of metabolite exchanges will help interpret and potentially manipulate microbial communities, whether those communities are involved in breaking down biomass into fuel or gaining insights into how microbes make mobile uranium stationary.

J Watrous, P Roach, T Alexandrov, BS Heath, JY Yang, RD Kersten, M van der Voort, K Pogliano, H Gross, JM Raaijmaker, BS Moore, J Laskin, N Bandeira, and PC Dorrestein. 2012. "Mass Spectral Molecular Networking of Living Microbial Colonies." *Proceedings of the National Academy of Sciences* 109(26):E1743-E1752. DOI: 10.1073/pnas.1203689109.

Sponsors: PNNL Laboratory Directed Research and Development, National Institutes of Health, Johnson & Johnson, the German Research Foundation, Dutch Science Organization Ecology Regarding Gene-Modified Organisms, Netherlands Genomics Initiative ECOLINC and PreSeed, PNNL Science Undergraduate Laboratory Internship program

Combining experiment and theory, researchers discovered that nitric acid dissociates less in water than previously thought because it gains structure by building more connections at higher concentrations. Reprinted with permission from T Lewis; B Winter; AC Stern; MD Baer; CJ Mundy; DJ Tobias; JC Hemminger, 2011. *The Journal of Physical Chemistry C*, 115:21183-21190. © 2011 American Chemical Society.



CHEMICAL SCIENCES

Whether studying ions' behavior in water or catalysts' performance in exhaust systems, basic and applied chemical research is vital to understanding and controlling complex interactions that can solve energy, environmental, and security issues. At PNNL, scientists conduct research in catalysis, computational chemistry, condensed-phase and interfacial chemical physics, separations, and detection. They synthesize unique and routine samples, analyze the samples, and model the results. Our teams form around the disciplines needed to solve the problem, allowing us to bring different scientific perspectives to our clients. We also bring in collaborators from academia, other national labs, and industry.

Studying the Chemistry as It Happens

Catalysts are involved in ~90 percent of all commercially produced fuels and chemical products. To improve existing catalysts and processes and invent new ones, scientists need data about the steps that occur during the reaction. To clarify these steps, scientists at PNNL built a new probe. With it, scientists can flow a gaseous reaction mixture through a solid catalyst and determine the final products and the molecules created along the way. The data are generated by a nuclear magnetic resonance (NMR) spectrometer. The probe also allows use of large catalyst samples for enhanced sensitivity.

JZ Hu, JA Sears, HS Mehta, JJ Ford, JH Kwak, K Zhu, Y Wang, J Liu, DW Hoyt, and CHF Peden. 2012. "A Large Sample Volume Magic Angle Spinning Nuclear Magnetic Resonance Probe for In Situ Investigations with Constant Flow of Reactants." *Physical Chemistry Chemical Physics* 14:2137-2143. DOI: 10.1039/c1cp22692d.

Sponsor: Department of Energy Office of Basic Energy Sciences

"NMR is a powerful technique. Being able to apply it to catalytic reactions while they are occurring has been a really tough problem. This new in situ NMR probe lets us perform experiments we couldn't do before."

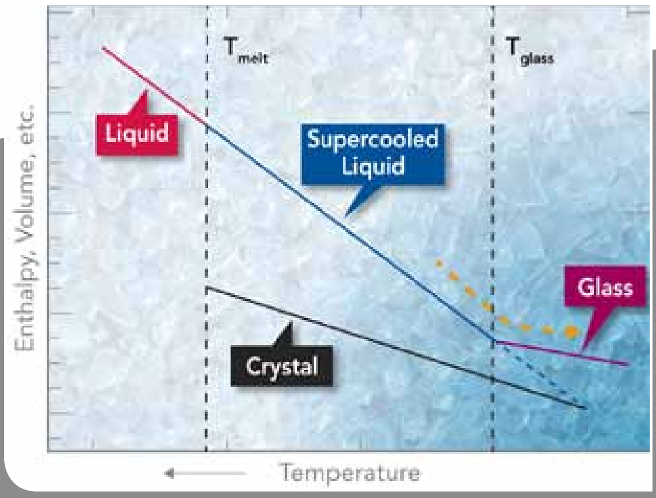
— Dr. Jian Zhi Hu, PNNL

Ionic Liquid Improves Speed, Efficiency of Hydrogen-Producing Catalyst

Researchers at PNNL have found a condition that creates hydrogen faster without a loss in efficiency. The results provide insights into making better materials for energy production. In an important step in the transformation of lab results into useable technology, the scientists combined an acidic ionic liquid and water with an efficient but slow hydrogen-producing catalyst, making it produce up to 53,000 hydrogen molecules per second. The results also provide molecular details into how the catalytic material converts electrical energy into the chemical bonds between hydrogen atoms. This information will help researchers build better catalysts that can be made with the common metal nickel instead of expensive platinum.

DH Pool, MP Stewart, M O'Hagan, WJ Shaw, JAS Roberts, RM Bullock, and DL DuBois. 2012. "An Acidic Ionic Liquid/Water Solution as Both Medium and Proton Source for Electrocatalytic H_2 Evolution by $[Ni(P_2N_2)_2]^{2+}$ Complexes." *Proceedings of the National Academy of Sciences USA* Early Edition online the week of June 8. DOI: 10.1073/pnas.1120208109.

Sponsor: Department of Energy Office of Basic Energy Sciences



As liquids cool, they can take on different states depending on various conditions. A liquid can cool to become a supercooled liquid and then a glass, given the right conditions. The more common route is for the liquid to cool into a crystalline solid.

Watching Molecules in Slow Motion

As a liquid cools, it can become a glass, given the right conditions. The more common route is for the liquid to cool into a crystalline solid. The location of exceedingly slow-moving molecules in glasses can now be quickly and efficiently measured, thanks to a new technique designed at PNNL that uses vapor and extreme cold to drop the molecules' speed a trillion times. The technique meets the long-standing challenge to supercool a liquid without getting the crystal form by supercooling vapor molecules, which turns them into a glassy film. Then, the film is heated just enough to get the molecules moving at the desired speed to study. Before the liquid molecules can rearrange themselves into crystals, the scientists can apply different analytical techniques, resulting in precise data that will answer basic questions about the properties of glass and one day may guide transformations into key industries.

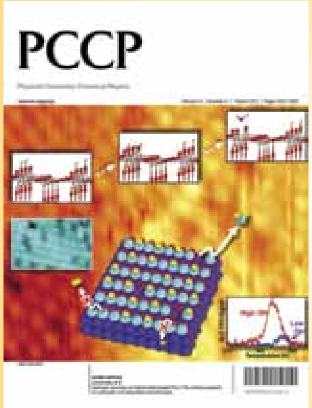
RS Smith and BD Kay. 2012. "Breaking Through the Glass Ceiling: Recent Experimental Approaches to Probe the Properties of Supercooled Liquids near the Glass Transition." *The Journal of Physical Chemistry Letters* 3(6):725-730. DOI: 10.1021/jz201710z.

Sponsor: Department of Energy Office of Basic Energy Sciences

CHEMICAL SCIENCES

Getting Your Catalyst What It Needs

To do its job, the popular catalyst titanium dioxide often needs an even layer of hydroxyl groups across its surface. A new method developed by scientists at PNNL now provides it. A hydroxyl group is a hydrogen atom bonded to an oxygen atom. In a catalyst, the oxygen is part of the material structure. It just needs a hydrogen atom. The new method covers about half of the surface with hydroxyl groups. In addition, the hydrogen atoms on the surface do not migrate inside the material when the catalyst is heated, but combine with the catalyst's lattice oxygen to create water. The titanium-based catalysts use light to split water into oxygen and hydrogen, to synthesize or degrade various organic molecules, and for other applications, including fuel cells and solar cells.



Artwork from this catalysis research appeared on the cover of *Physical Chemistry Chemical Physics*. Image reproduced by permission of Dr. Igor Lyubinetsky and the PCCP Owner Societies from PCCP. 2012.

Y Du, NG Petrik, NA Deskins, Z Wang, MA Henderson, GA Kimmel, and I Lyubinetsky. 2012. “Hydrogen Reactivity on Highly-Hydroxylated TiO_2(110) Surfaces Prepared via Carboxylic Acid Adsorption and Photolysis.” *Physical Chemistry Chemical Physics* 14(9):3066-3074. DOI:10.1039/c1cp22515d.

Sponsor: Department of Energy Office of Basic Energy Sciences

Nitric Acid Overcomes Its Fear of Water

Whether in a pond or raindrop, when nitric acid encounters water's surface, it typically falls apart, dissociating into two charged particles. But sometimes it holds together noticeably. Knowing why can help scientists understand and ultimately mitigate the effects of this key component of smog. Combining experiment and theory, researchers from PNNL, the University of California at Irvine, and Helmholtz-Zentrum Berlin discovered that nitric acid dissociates less because it gains structure by building more connections at higher concentrations. When enough acid is present, the molecules build hydrogen bonds that reduce dissociation.

T Lewis, B Winter, AC Stern, MD Baer, CJ Mundy, DJ Tobias, and JC Hemminger. 2011. “Does Nitric Acid Dissociate at the Aqueous Solution Surface?” *The Journal of Physical Chemistry C* **115**(43):21183-21190. DOI: 10.1021/jp205842w.

T Lewis, B Winter, AC Stern, MD Baer, CJ Mundy, DJ Tobias, and JC Hemminger. 2011. “Dissociation of Strong Acid Revisited: X-ray Photoelectron Spectroscopy and Molecular Dynamics Simulations of HNO_3 in Water.” *The Journal of Physical Chemistry B* 115(30):9445-9451. DOI: 10.1021/jp205510q.

Sponsor: Department of Energy Office of Basic Energy Sciences, National Science Foundation, Deutsche Forschungsgemeinschaft, PNNL's Linus Pauling Distinguished Postdoctoral Fellowship

Tasting Carbon with WAFT-ed Light

Getting answers from small samples could save significant costs for researchers. When delving into the nuances of carbon, an instrument designed at PNNL “sips” a tiny sample and reveals information about the different molecules' sources. Using lasers and warm air finesse tuning (WAFTing), the capillary absorption spectrometer measures the ratio of different types of carbon isotopes in a sample. This technique is as precise as technologies requiring 10,000 times more sample. It enables scientists to track the source of nutrients extracted from microbial communities to understand how they convert materials, such as cellulose, into energy-dense compounds, such as glucose. Its extreme sensitivity holds the potential of measuring carbon-14, currently only measured by accelerator mass spectrometers costing several million dollars.

JF Kelly, RL Sams, TA Blake, M Newburn, J Moran, ML Alexander, and H Kreuzer. 2012. “A Capillary Absorption Spectrometer for Stable Carbon Isotope Ratio ($^{13}C/^{12}C$) Analysis in Very Small Samples.” *Review of Scientific Instruments* 83(2):023101. DOI: 10.1063/1.3680593.

Sponsor: PNNL Laboratory Directed Research and Development, EMSL Scientific Partner Proposal

CLIMATE & EARTH SYSTEMS SCIENCE

Dawn breaks over the Raman lidar remote-sensing instrument located at the Atmospheric Radiation Measurement (ARM) Climate Research Facility's Southern Great Plains site. The ground-based laser measures vertical profiles of several cloud and atmospheric properties.

At PNNL, scientists are working to better understand how the planet's human and natural systems interact in the context of climate, as well as other global and regional environmental changes. This research involves working across disciplines and different spatial and temporal scales to integrate theory, measurements, and modeling. Our Climate & Earth Systems Science research tackles key questions and delivers decision-relevant results related to atmospheric aerosols, clouds, and precipitation; human systems, such as agriculture and energy; the cycling of water, carbon, and other important constituents; and the impacts of, and potential responses to, climate change.

Pollution + Storm Clouds = Warmer Atmosphere

Understanding the interactions between clouds and atmospheric particles is important for improving projections of future climate change. Researchers showed for the first time that pollution increases atmospheric warming by invigorating thunderstorm clouds. They conducted a computational study at resolutions high enough to see the clouds develop. In warm summer thunderstorms, pollution particles lead to stronger storms with larger, longer-lasting, anvil-shaped clouds. Compared to cloud anvils that developed in clean air, these larger anvils both warmed and cooled more, though on average, the warming effect dominated. The large amount of heat trapped by pollution-enhanced clouds could potentially impact regional circulation and modify weather systems.

J Fan, D Rosenfeld, Y Ding, LR Leung, and Z Li. 2012. "Potential Aerosol Indirect Effects on Atmospheric Circulation and Radiative Forcing through Deep Convection." *Geophysical Research Letters* 39:L09806. DOI: 10.1029/2012GL051851.

Sponsor: Department of Energy Office of Biological and Environmental Research, the China Ministry of Sciences and Technology

"The large amount of heat trapped by pollution-enhanced clouds could potentially impact regional circulation and modify weather systems."

– Dr. Jiwen Fan, PNNL

Cutting Air Pollution Boosted by Weather

Rain and wind during the 2008 Summer Olympic Games in Beijing were at least as important as emission controls in reducing pollution particles, according to scientists from PNNL and the Chinese Academy of Sciences. They used a coupled meteorological-chemistry model combined with observations to analyze reductions in air pollution before and during the Games. They found that while traffic management and other emission control policies were important, weather conditions also played a key role. The study highlights the importance of accounting for regional-scale interactions when formulating air quality policies.

Y Gao, X Liu, C Zhao, and M Zhang. 2011. "Emission Controls Versus Meteorological Conditions in Determining Aerosol Concentrations in Beijing during the 2008 Olympic Games." *Atmospheric Chemistry and Physics* 11:12437-12451. DOI: 0.5194/acp-11-12437-2011.

Sponsors: Department of Energy Office of Science Scientific Discovery through Advanced Computing, the National Natural Science Foundation of China, the Ministry of Environmental Protection of China

Ice Heating Up Cold Clouds

Competition within clouds in the Arctic is hot. Scientists from PNNL and Environment Canada found that the small amount of heat released when water vapor condenses on ice crystals in Arctic clouds containing both water and ice determines the cloud's survival. The team used data from the 2008 Indirect and Semi-Direct Aerosol (ISDAC) Atmospheric Radiation Measurement (ARM) field campaign. In sophisticated numerical models, they examined the cloud microphysical processes important for cloud maintenance. In mixed-phase clouds, water droplets, ice crystals, and water vapor vie for dominance and co-exist only when the cloud air is constantly moving. When water droplets competing for water vapor lose to ice crystals, an ensuing chain of events drives the cloud toward collapse. In this unstable system, growing ice crystals precipitate out of the cloud, warming, drying, and ultimately destroying it. Better knowledge of the complex interactions in mixed-phase clouds will ultimately help increase accuracy of climate change projections, particularly in the Arctic, which is warming faster than any other region of the world.

M Ovchinnikov, A Korolev, and J Fan. 2011. "Effects of Ice Number Concentration on Dynamics of a Shallow Mixed-Phase Stratiform Cloud." *Journal of Geophysical Research* 116:D00T06. DOI: 10.1029/2011JD015888.

Sponsor: Department of Energy Office of Biological and Environmental Research

The Future of Clean Air

Affluent regions of the world typically regulate air pollution to reduce the risk to human health and ecosystems caused by ozone and particulates. After comparing historical data on regional air pollution and community affluence levels, scientists at PNNL's Joint Global Change Research Institute and the University of North Carolina constructed a reference scenario for future pollutant concentrations that tracks projected regional income trends over the 21st century. With historical analyses guiding scientists' assumptions, they adjusted for data inconsistencies caused by weather, population, geographic location, or growth. The resulting scenarios had greater consistency between income assumptions and simulated pollutant levels than previous approaches.

SJ Smith, JJ West, and P Kyle. 2011. "Economically Consistent Long-Term Scenarios for Air Pollutant Emissions." *Climatic Change* 108:619-627. DOI: 10.1007/s10584-011-0219-1.

Sponsor: Department of Energy Office of Biological and Environmental Research, the Environmental Protection Agency

"This work was a foundational reference case for a scenario that will be used by modeling groups around the globe to make realistic projections of future climate change."

— Dr. Steven J. Smith, PNNL

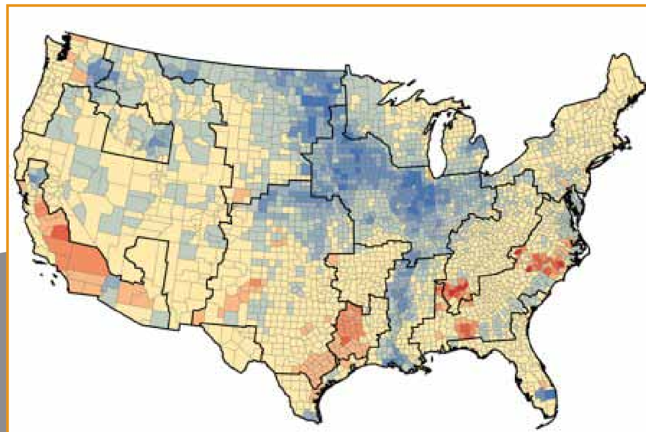
Gauging Water's Future

Population growth, industrialization, and expanding urban areas put pressure on resource managers to meet the increasing demand for water. To provide better information for managing sustainable water supplies, scientists at PNNL, the Chinese Academy of Sciences, and Oak Ridge National Laboratory improved estimates of water runoff in the Community Land Model (CLM). They compared CLM simulations of runoff and land-atmosphere energy exchanges at various locations with data from U.S. Geological Survey stream flow gages and various flux towers across North America.

Their research demonstrates how soil hydrology affects surface energy and highlights the need for better runoff estimations in land models.

H Li, M Huang, MS Wigmosta, Y Ke, AM Coleman, LR Leung, A Wang, and DM Ricciuto. 2011. "Evaluating Runoff Simulations from the Community Land Model 4.0 Using Observations from Flux Towers and a Mountainous Watershed." *Journal of Geophysical Research - Atmospheres* 116:D24120. DOI: 10.1029/2011JD016276.

Sponsor: Department of Energy Office of Biological and Environmental Sciences



Based on U.S. crop production, scientists determined what regions take in more carbon than they release (blue), and what regions release more carbon than they take in (red).

From Earth to Table to Air

A potato grown in Idaho uses carbon to bulk up, but after being consumed at a Los Angeles bistro, its carbon is released back into the air. Scientists at PNNL, Oak Ridge National Laboratory, and Colorado State University have provided a detailed account of agricultural carbon's journey. Their accounting considers the mobile nature of today's agriculture, where food is often shipped long distances before it is consumed. Understanding how and where agricultural CO_2 is taken up and released can help shape climate change policy. The researchers examined U.S. crop production, the crops' carbon content, and food intake data. Agricultural regions take in large amounts of carbon as crops grow, becoming carbon sinks. Regions with large populations consume those crops and release the carbon, becoming carbon sources. These differences are important for policies aimed at managing CO_2 emissions.

TO West, V Bandaru, CC Brandt, AE Schuh, and SM Ogle. 2011. "Regional Uptake and Release of Crop Carbon in the United States." *Biogeosciences* 8:2037-2046, DOI: 10.5194/bg-8-2037-2011.

Sponsor: National Aeronautics and Space Administration

Researchers found two dominant factors that steer an energy technology transformation.

Driving Change in Technology

Societies will need to make tough decisions to reduce greenhouse gases and limit climate change. To find the most effective ways to encourage those choices, scientists from PNNL and the University of Maryland, working at the Joint Global Change Research Institute, looked at the past 50 years in technology revolutions in biomass and nuclear energy systems in three countries: Brazil, Sweden, and the United States. They found that domestic policy decisions and characteristics of the technology itself are the dominant factors in large-scale energy transitions. Their results show that policies and regulations are powerful motivators to accelerate development and adoption of new technologies.

NE Hultman, EL Malone, P Runci, G Carlock, and K Anderson. 2012. "Factors in Low-carbon Energy Transformations: Comparing Nuclear and Bioenergy in Brazil, Sweden, and the U.S." *Energy Policy* 40:131-146. DOI: 10.1016/j.enpol.2011.08.064.

Sponsor: National Science Foundation

"If we're going to get serious about solving climate change, we'll need a technology revolution. This study breaks new ground in understanding the forces that are most important to make the large-scale move to renewable energy technologies."

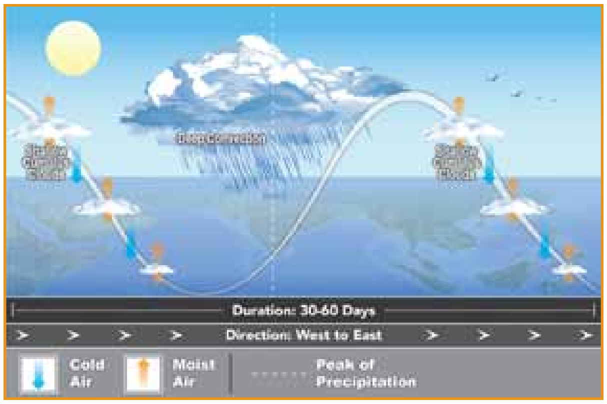
– Dr. Elizabeth Malone, PNNL

Mastering the Mysteries of the MJO

From monsoons in Mumbai to floods and windstorms battering Seattle, the Madden-Julian Oscillation, or MJO, leaves its mark on the world. Climate scientists can now better model this cyclic 30- to 60-day tropical atmospheric wave pattern, thanks to researchers at PNNL and the National Center for Atmospheric Research. Their study shows where the MJO gets energy and how its access to moisture affects the wave's regularity and recurrence. Researchers compared observational data to MJO model simulations with and without restrictions on cloud moistening to capture an accurate depiction of the MJO. They performed a complete thermodynamic budget analysis on the moisture-constrained simulation of the wave that allowed identification of limitations in the current model parameters. Their analyses showed that moisture and temperature are strongly linked in the MJO. Instabilities are created by co-variation of moisture condensation with fluctuations in temperature.

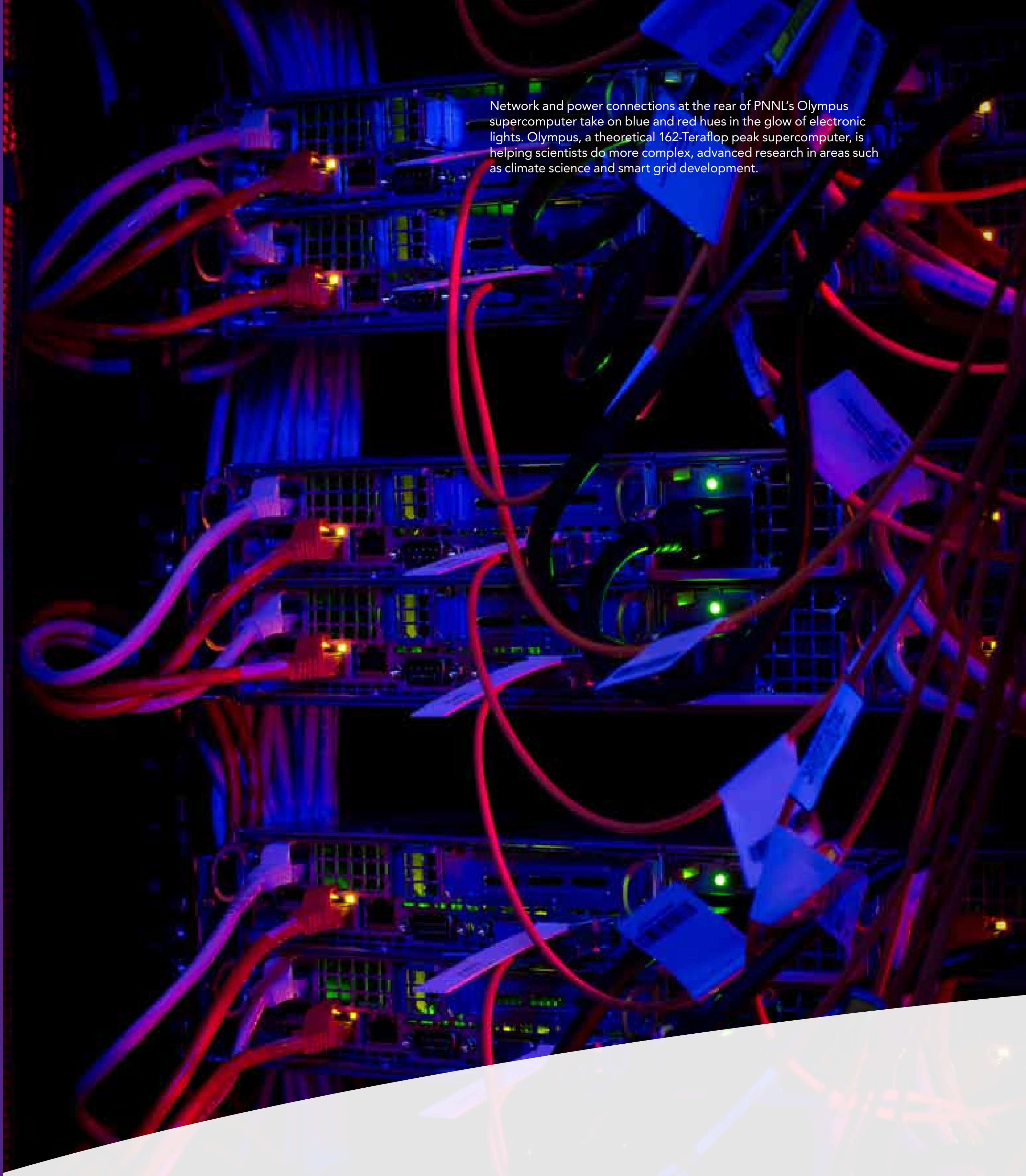
S Hagos, LR Leung, and J Dudhia. 2011. "Thermodynamics of Madden-Julian Oscillation in a Regional Model with Constrained Moisture." *Journal of Atmospheric Sciences* 68(9):1974-1989. DOI: 10.1175/2011JAS3592.1.

Sponsor: Department of Energy Office of Biological and Environmental Research



The MJO is a large complex of clouds and rain initiated over the Indian Ocean that slowly progresses around the world along the equator. The MJO has a large effect on tropical monsoons and cyclones, as well as other weather systems outside the tropics.

COMPUTATIONAL SCIENCES & MATHEMATICS



Network and power connections at the rear of PNNL's Olympus supercomputer take on blue and red hues in the glow of electronic lights. Olympus, a theoretical 162-Teraflop peak supercomputer, is helping scientists do more complex, advanced research in areas such as climate science and smart grid development.

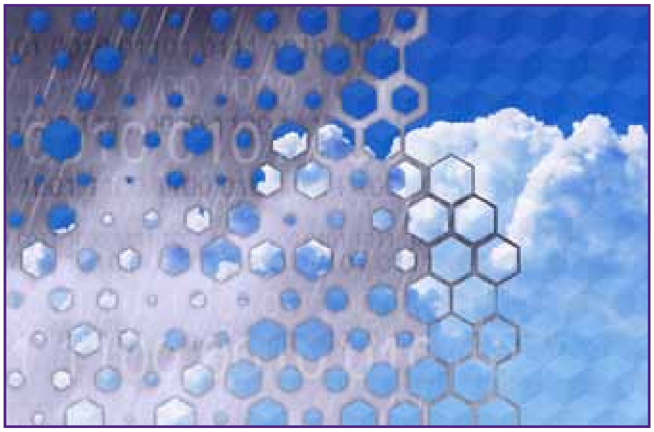
The Computational Sciences & Mathematics Division focuses on creating new computational capabilities to solve problems using extreme-scale simulation and peta-scale data analytics. Our strengths include capabilities in advanced scientific computing, information visualization, and data management. PNNL uses its domain expertise in computing, mathematics, and statistics to develop scalable analysis algorithms, high-performance computing tools and architectures, data intensive information systems, and secure computing infrastructures for scientific discovery, predictive modeling, situational awareness, and decision support.

Taming Uncertainty in Climate Prediction

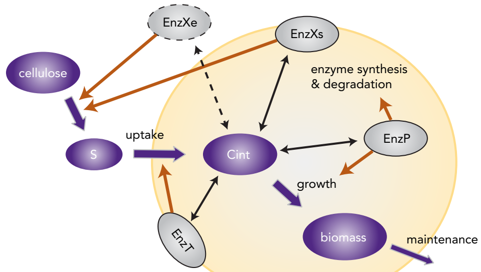
Uncertainty just became more certain. Atmospheric and computational researchers at Pacific Northwest National Laboratory used a scientific approach called "uncertainty quantification," or UQ, that allowed them to better simulate precipitation. Their study is the first to apply a stochastic sampling method to select model inputs for precipitation representations and improve atmospheric simulations within a regional weather research and forecasting model. The approach marks a significant advancement in representing precipitation, one of the most difficult climate components to simulate. Effectively and efficiently representing current weather and climate systems in a computer model paves the way for scientists to apply those same techniques to predict future climate changes.

Yang B, Qian Y, Lin G, Leung R, and Zhang Y. 2012. "Some Issues in Uncertainty Quantification and Parameter Tuning: A Case Study of Convective Parameterization Scheme in the WRF Regional Climate Model." *Atmospheric Chemistry and Physics* 12(5):2409-2427. DOI: 10.5194/acp-12-2409-2012.

Sponsor: Department of Energy Office of Advanced Scientific Computing Research



Results of the uncertainty quantification process show an improved predictive model, making it more reliable in projecting future climate change.



Metabolic network model, its carbon flow paths, and regulatory relationships. Pointed arrows show biochemical reactions, while diamond-head arrows indicate regulatory relationships.

Modeling Microbes to Manage Carbon Dioxide

Scientists are realizing that communities of microbes process energy and materials, which affects their environments. To understand how these communities function in a natural ecosystem, a PNNL research team developed a novel kinetic model that represents microbial community dynamics in soil pores. The model will enable scientists to evaluate consequences of different strategies microbes might use to degrade organic matter, such as cellulose in soil, and analyze how 3D pore structure impacts biological activity. Microbial breakdown of cellulose and related byproducts is a key process in the global carbon cycle. Annually, more than 100 billion tons of cellulose are synthesized by plants and subsequently degraded by microorganisms that, in turn, produce carbon dioxide via respiration.

H Resat, V Bailey, LA McCue, and A Konopka. "Modeling Microbial Dynamics in Heterogeneous Environments: Growth on Soil Carbon Sources." *Microbial Ecology* 63(4):883-897. DOI: 10.1007/s00248-011-9965-x.

Sponsor: PNNL Laboratory Directed Research and Development

Scaling Codes to Enable Faster Data Analysis

The ever-increasing volumes of data generated in scientific research, such as in the areas of bioinformatics and computational biology, results in large repositories of data that current systems are not equipped to analyze quickly. Researchers at PNNL have developed a scalable framework for automatically distributing tasks among processors instead of requiring programmers to handle all the details. The algorithms developed were shown to scale to more than 100,000 cores on the three largest Department of Energy computational platforms: ALCF Intrepid, OLCF Titan, and NERSC Hopper. The framework was used to perform large-scale sequence analysis of datasets on massively parallel supercomputing platforms. The work has been demonstrated on protein data for sequence homology detection and helped scale the analysis from 8,000 cores to 130,000 cores in just 6 weeks.

J Lifflander, S Krishnamoorthy, and L Kale. 2012. "Work Stealing and Persistence-based Load Balancers for Iterative Overdecomposed Applications." In: ACM Symposium on High-Performance Parallel and Distributed Computing.

Sponsors: Department of Energy Office of Advanced Scientific Computing Research, PNNL Laboratory Directed Research and Development

Designing the Next Generation of High-Performance Computing Systems

Standard high-performance computing systems are typically designed and built to solve problems quickly and linearly—taking instructions from a single "thread" in the processor. But many scientific fields have a growing need for irregular data applications to analyze large unstructured datasets and identify connections among seemingly unrelated information. Conventional computing architecture is not set up to accommodate this need. And while multithreaded architectures allow processors to take instruction from more than one thread in a cycle, existing systems were not built to address the volume or new types of data being generated. PNNL researchers developed a process for designing the next generation of these massively multithreaded architectures for irregular applications. New simulation software predicts how a machine will perform before it is built by incorporating design elements, such as necessary hardware, desired outputs, and performance, and identifying design challenges and solutions before building a new system.

A Tumeo, S Secchi, and O Villa. 2012. "Designing Next-Generation Massively Multithreaded Architectures for Irregular Applications." *Computer* 45(8):53-61. DOI: 10.1109/MC.2012.193.

Sponsor: PNNL's Center for Adaptive Supercomputing Software

Enabling Fast, Flexible Development of Complex Modeling and Simulation Environments

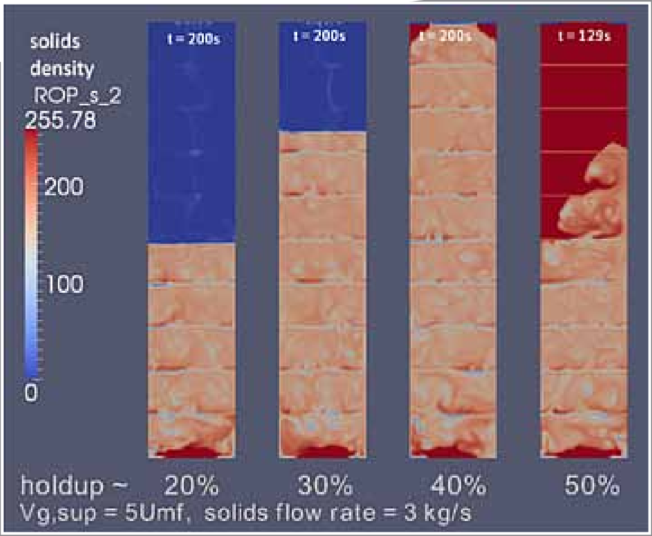
Modeling and simulation are standard elements of virtually all scientific research, but as the scale of computational models and simulations grows to address more complex challenges, it is more difficult to identify the correct inputs and manage and analyze results. Some disciplines have invested significantly in developing comprehensive data management and analysis systems, but they are often limited to a specific domain. A new platform designed by PNNL has demonstrated a design approach that tears down stovepipes across science domains. Velo is a knowledge-management framework that rapidly incorporates domain-specific tools, data, and metadata—offering immediate, high-value capabilities to scientific collaborations. Velo has been deployed to support carbon sequestration, climate modeling, and environmental management and has the flexibility to be adapted for other areas.

I Gorton, C Sivaramakrishnan, GD Black, SK White, S Purohit, CS Lansing, MC Madison, KL Schuchardt, and Y Liu. 2012. "Velo: A Knowledge Management Framework for Modeling and Simulation." *Computing in Science & Engineering* 14(2):12-23. DOI: 10.1109/MCSE.2011.116.

Sponsor: Department of Energy Office of Environmental Management, PNNL Laboratory Directed Research and Development

Quantifying Carbon Capture Performance

As part of the national Carbon Capture Simulation Initiative sponsored by the Department of Energy, PNNL is leading efforts to develop a multiphase flow simulator to quantify the performance of carbon capture devices. Researchers have applied the techniques using computational tools at a scale never before reached. The work provides a better understanding of how carbon capture devices will work in the real world, increasing confidence in how they will perform amid future carbon capture activities.

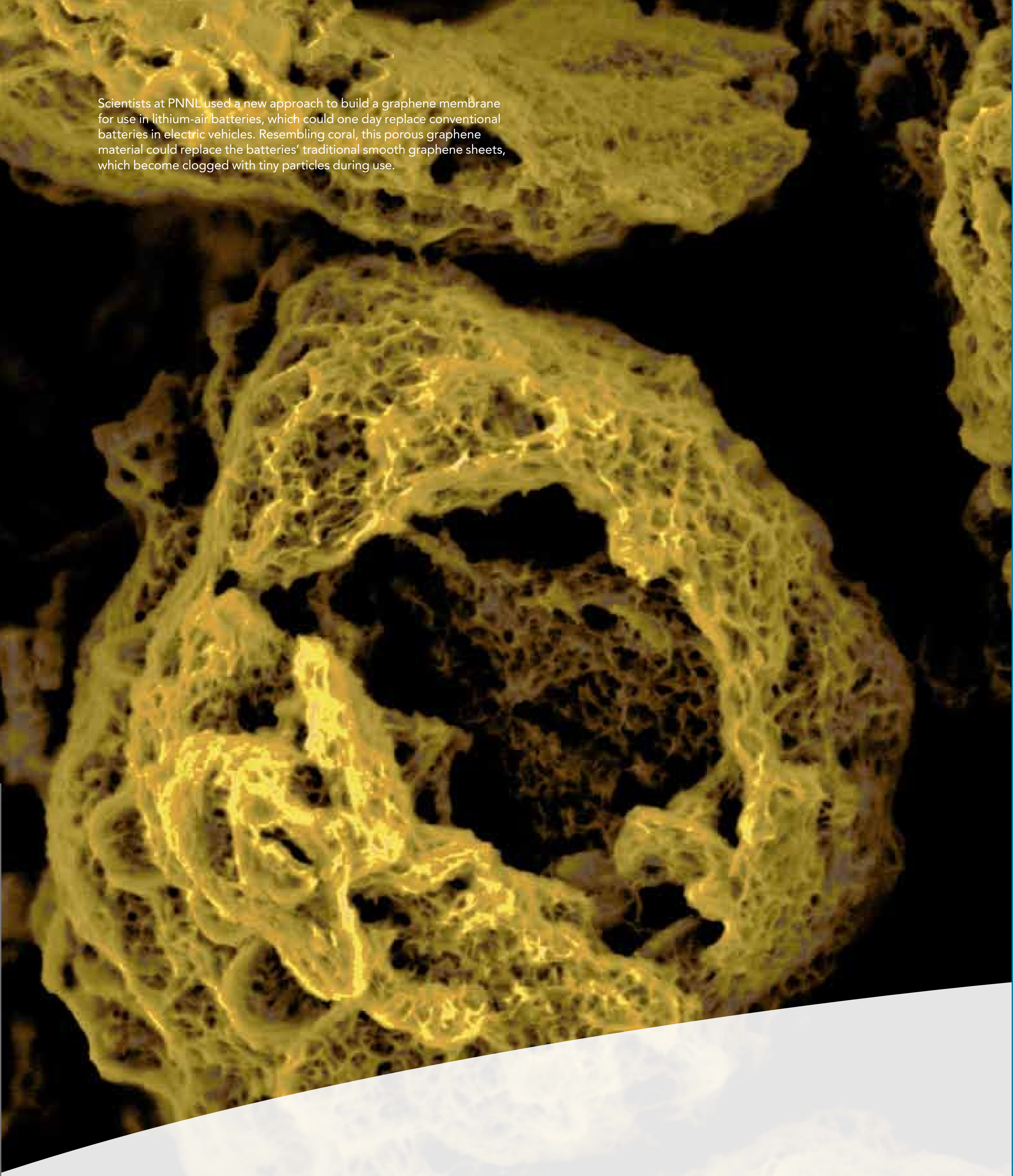


This image depicts columns in a regenerator, a carbon-capture device, and shows the distribution of sorbent particles. Red regions denote a packed bed of particles and blue indicates no particles. PNNL computational scientists are leading development of a carbon-capture device simulator to measure and ultimately optimize device performance.

Z Xu, X Sun, and MA Khaleel. 2012. "A Generalized Kinetic Model for Heterogeneous Gas-Solid Reactions." *Journal of Chemical Physics* 137(7):074702. DOI: 10.1063/1.4740242.

Sponsor: Department of Energy Carbon Capture Simulation Initiative

MATERIAL SCIENCES



Scientists at PNNL used a new approach to build a graphene membrane for use in lithium-air batteries, which could one day replace conventional batteries in electric vehicles. Resembling coral, this porous graphene material could replace the batteries' traditional smooth graphene sheets, which become clogged with tiny particles during use.

Revolutionary materials are needed to produce, use, and store domestically produced energy. These materials are unlikely to be discovered via trial and error, as such an approach is too slow and costly. At PNNL, our research focuses on understanding materials at the molecular and atomic level and then scaling that knowledge to tailor materials to specific situations. Understanding materials often involves understanding how defects and interfaces form and affect the material's behavior. Our defect studies also focus on materials in extreme environments, such as those found in nuclear reactors and orbiting satellites.

Bubbles Help Break Energy Storage Record for Lithium-Air Batteries

Resembling broken eggshells, graphene structures built around bubbles produce a lithium-air battery with the highest energy capacity to date, according to scientists at PNNL and Princeton University. The team created this black, porous material by mixing a binding agent with graphene and water. The solution hardened around the bubbles, which left behind hollow spheres of graphene 10 times smaller than a human hair. The new material could replace traditional smooth graphene sheets in lithium-air batteries, which become clogged with tiny particles during use. As a bonus, the material does not rely on platinum or other precious metals, reducing its potential cost. This hierarchical structure of self-assembled graphene sheets is an ideal design not only for lithium-air batteries but also for many other potential energy applications.

J Xiao, D Mei, X Li, W Xu, D Wang, GL Graff, WD Bennett, Z Nie, LV Sara, IA Aksay, J Liu, and JG Zhang. 2011. "Hierarchically Porous Graphene as a Lithium-Air Battery Electrode." *Nano Letters* 11(11):5071-5078. DOI: 10.1021/nl203332e.

Sponsor: Department of Energy Office of Basic Energy Sciences, PNNL Laboratory Directed Research and Development

"In our process we chose not to use precious metal. This will greatly reduce production costs and increase the adoptability."

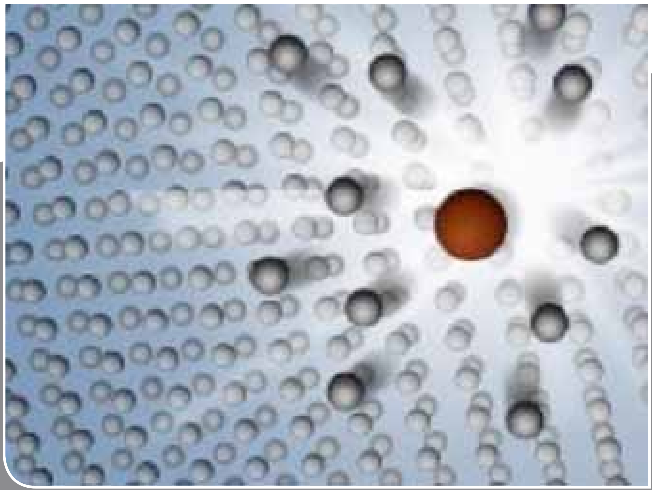
– Dr. Ji-Guang Zhang, PNNL

New Metal Alloy Electrode Designed for Plus-Sized Ions

Storing wind-farm energy and releasing it on demand requires high-capacity, low-cost batteries. Sodium-ion batteries could be part of the answer now, thanks to fundamental insights obtained by scientists at PNNL. Instead of force-fitting larger sodium ions into battery electrodes built for smaller lithium ions, the research team designed an electrode based on the ion's character, not its circumference. The new electrode or anode is built from a tin and antimony alloy with specially designed carbon support. This durable new material can store nearly twice as much energy as a carbon electrode in the popular lithium-ion battery and is much cheaper, and it has more capacity and is sturdier than sodium-ion batteries. The new alloy could be vital to creating a durable, high-capacity anode while keeping battery costs down—factors vital to implementing large-scale energy storage systems.

L Xiao, Y Cao, J Xiao, W Wang, L Kovarik, Z Nie, and J Liu. 2012. "High Capacity, Reversible Alloying Reactions in SnSb/C Nanocomposites for Na-Ion Battery Applications." *Chemical Communications* 48:3321-3323. DOI: 10.1039/C2CC17129E.

Sponsor: Department of Energy Office of Basic Energy Sciences



Researchers at PNNL developed nuclear-reaction analytical methods used to study oxygen behavior in solid samples. The methods can be used to investigate ceramic oxide materials with potential in future nuclear energy systems, security devices, and space vehicles.

When Atoms Collide

A novel technique for materials research is contributing unexpectedly to nuclear safety. Scientists at PNNL developed the method for measuring the concentration of oxygen atoms at different depths in solid samples. Because this method can be used to validate theoretical models describing nuclear reactions, the International Atomic Energy Agency included data from it in an extensive, publicly available database used by the research community. These data also have relevance to the structural materials used to build nuclear reactors, security devices, and space vehicles.

W Jiang, V Shutthanandan, S Thevuthasan, DE McCready, and WJ Weber. 2003. "Oxygen Analysis Using Energetic Ion Beams." *Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms* 207(4):453-461. DOI: 10.1016/S0168-583X(03)01123-6.

Sponsor: Department of Energy Office of Basic Energy Sciences

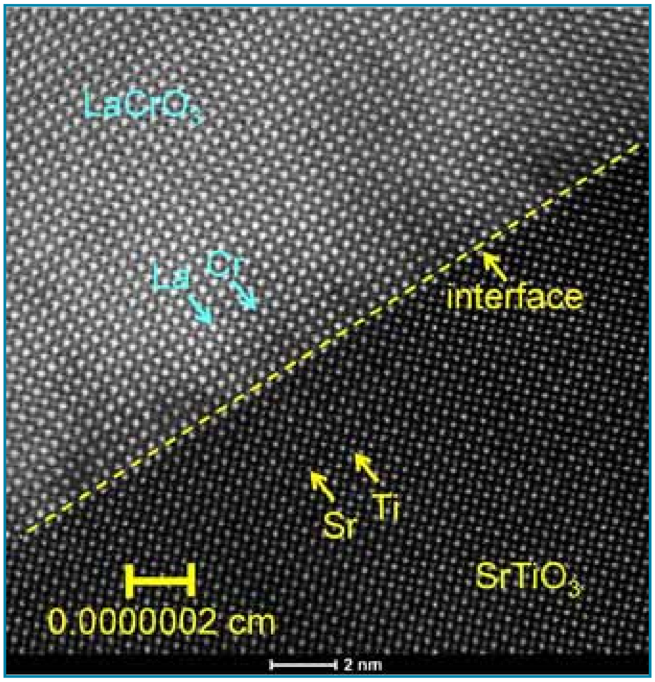
An About-Face on Electrical Conductivity at the Interface

To improve the electronic devices that keep our hyper-connected world organized, scientists are investigating an unusual form of electrical conductivity that takes place at the junction of two oxides, materials made of oxygen and metal. When an oxide made up of alternating positively and negatively charged layers—called polar—is placed in contact with a nonpolar oxide, the interface between the two can conduct electricity in a way that could make some novel electronic devices possible.

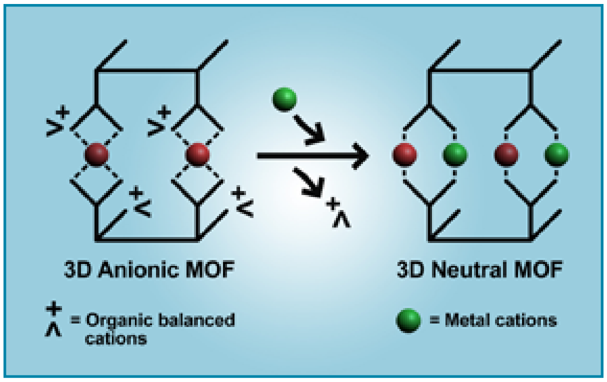
But scientists from PNNL and University College London found the interface of two particular complex oxides did not conduct electricity, contradicting the current model, which assumes precise, clear-cut regions exist for each oxide material. These results suggest that the popular model is too simplistic to be as universal as it is claimed to be.

SA Chambers, L Qiao, TC Droubay, TC Kaspar, BW Arey, and PV Sushko. 2011. "Band Alignment, Built-In Potential, and the Absence of Conductivity at the $LaCrO_3/SrTiO_3$ (001) Heterojunction." *Physical Review Letters* 107(20):206802. DOI: 10.1103/PhysRevLett.107.206802.

Sponsors: Department of Energy Office of Basic Energy Sciences, the Royal Society



A cross-sectional scanning transmission electron micrograph of the interface between the polar lanthanum chromium oxide ($LaCrO_3$) and the nonpolar strontium titanium oxide ($SrTiO_3$). Although the interface appears to be atomically abrupt, detailed spectroscopic measurements show that cation mixing occurs in the interfacial region.



Researchers at PNNL studied a metal organic framework with a negative charge (anionic MOF) and a flexible structure. The framework captured positively charged metal ions, and, in the process lost its charge, becoming a neutral framework.

Flexible Molecular Cages Expand to Pack in Multiple Metals

By expanding and rearranging certain connections, a rare molecule packs in two different metals, not just one, according to scientists at PNNL. They created a metal organic framework, or MOF, that expands by 33 percent when it takes in metals. Unlike most MOFs, the molecule forms and breaks bonds with the charged metals it carries. It is also highly selective, taking in only metals that are missing two electrons. As a bonus, this unusual MOF works as a solid. Manipulating the MOF's carrying capacity could benefit work in batteries, sensors, nuclear fuel, and electroplating.

J Tian, LV Saraf, B Schwenzer, SM Taylor, EK Brchin, J Liu, SJ Dalgarno, and PK Thallapally. 2012. "Selective Metal Cation Capture by Soft Anionic Metal-Organic Frameworks via Drastic Single-Crystal-Single-Crystal Transformations." *Journal of the American Chemical Society* 134(23):9581-9584. DOI: 10.1021/ja303092m.

Sponsors: Engineering and Physical Sciences Research Council, Department of Energy Office of Basic Energy Sciences

"To the best of our knowledge, this is the first documented report of capturing metal ions with soft anionic metal organic frameworks in the solid state."

– Dr. Praveen Thallapally, PNNL

SUBSURFACE SCIENCE

Capturing and storing carbon dioxide (CO_2) and other greenhouse gases deep underground is one of the most promising options for fighting climate change. Scientists at PNNL are using electron microscopes to understand the reaction of CO_2 and minerals found underground. This picture shows the aftermath of fayalite reacting with the CO_2 to form siderite, thereby capturing gaseous CO_2 in a solid, stable form.

PNNL is an international leader in subsurface science, which involves developing and applying basic understanding of biogeochemical reactions, energy, and mass transfer to predict, assess, mitigate, design, and operate environmental processes. Our expertise includes molecular-to-field-scale biogeochemistry and reactive and multiphase transport modeling; laboratory-to-field-scale geohydrology, hydrology, and multiphase flow modeling; ecological assessment, management, and monitoring; human health and environmental risk assessment; and environmental systems technology development and deployment. We apply this expertise toward protecting water sources and aquatic ecosystems and understanding the terrestrial carbon cycle. We are national leaders in mitigating greenhouse gases through geologic sequestration science.

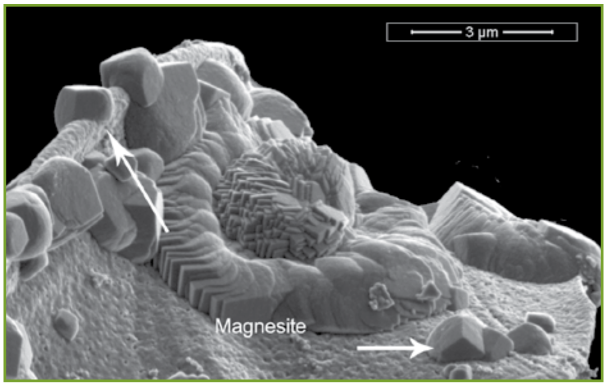
The Preferences of Uranium

Uranium prefers petite particles, according to scientists at PNNL. The radionuclide attaches quickly and abundantly to smaller subsurface grains, while gravel and other large bits adsorb less uranium(IV) than smaller grains and also adsorb it more slowly. From these findings, the team wrote a series of mathematical formulas to predict uranium adsorption and desorption affinity and kinetics in sediments containing different grain sizes. They tested their predictions on sediment from the Hanford Site in southeastern Washington State, where uranium from weapons production is spreading out and migrating toward the Columbia River. To keep the uranium from the river, scientists need to know how uranium moves through the complex subsurface. This study shows a way to get such information for wide areas. With these and other results, PNNL scientists are shaping how uranium's behavior is considered by scientists, cleanup experts, and regulators.

J Shang, C Liu, Z Wang, and JM Zachara. 2011. "Effect of Grain Size on Uranium(VI) Surface Complexation Kinetics and Adsorption Additivity." *Environmental Science & Technology* 45(14):6025-6031. DOI: 10.1021/es200920k.

Sponsor: Department of Energy Office of Biological and Environmental Research

More than 200,000 kg of uranium have been released to the vadose zone at the Hanford Site near the Columbia River. Plumes of uranium exist in the groundwater and vadose zone.



High-resolution scanning electron microscopic images of the reacted forsterite indicating the formation of magnesite (cubes).

Turning Down the Heat for Carbon

One option to reduce the impact of carbon dioxide (CO_2) from coal-fired power plants and other sources is to pump the CO_2 into underground reservoirs and have it become part of the mineral formations. Trapping the CO_2 through transformation into minerals takes place more readily at high temperatures. But scientists at PNNL discovered a reaction that breaks the rules. At relatively low temperatures and while recycling the water it needs, this reaction transforms CO_2 into the mineral magnesite. By understanding such fundamental sequestration reactions, scientists can inform policymakers and others about mitigation options. Industries that form minerals could also benefit from the team's discovery, as it offers a pathway to make valuable products with lower energy costs.

AR Felmy, O Qafoku, BW Arey, JZ Hu, MY Hu, HT Schaef, ES Ilton, NJ Hess, CI Pearce, J Feng, and KM Rosso. 2012. "Reaction of Water-Saturated Supercritical CO_2 with Forsterite: Evidence for Magnesite Formation at Low Temperatures." *Geochimica et Cosmochimica Acta* 91(15):271-282. DOI: 10-1016/j.gea.2012.05.016.

Sponsor: Department of Energy Office of Basic Energy Sciences

Protein Gives Insights to Iron's Fate Underground

It's almost an evil twin story: a protein that steals electrons from iron in one microbe looks like one that adds electrons in another, according to scientists at PNNL and the University of East Anglia. Their survey of the genes of groundwater bacterium *Sideroxydans lithotrophicus* ES-1, which removes electrons from iron, showed it contained genes in common with *Shewanella oneidensis* MR-1, an electron adder.

These results contribute to understanding the molecular mechanisms by which microorganisms change the electron configuration of iron and, thus, its mobility. The protein, MtoA, is the first member of its specific family to be purified and characterized from an Fe(II)-oxidizing bacterium.

J Liu, Z Wang, SM Belchik, MJ Edwards, C Liu, DW Kennedy, ED Merkley, MS Lipton, JN Butt, DJ Richardson, JM Zachara, JK Fredrickson, KM Rosso, and L Shi. 2012. "Identification and Characterization of MtoA: a Decaheme c-type Cytochrome of the Neutrophilic Fe(II)-Oxidizing Bacterium *Sideroxydans lithotrophicus* ES-1." *Frontiers in Microbiological Chemistry* 3:37. DOI: 10.3389/fmicb.2012.00037.

Sponsor: Department of Energy Office of Biological and Environmental Research

Same Samples, Different Analyses, Complementary Inferences

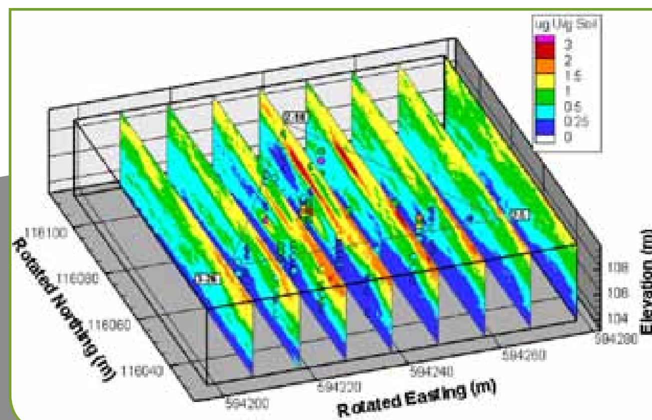
Results of two separate but complementary analyses on 400 samples of Hanford Site groundwater provide insights that, when combined, offer a better understanding of environmental effects on microbial community composition and the communities' influence on the biogeochemistry of subsurface sediments. Scientists at PNNL analyzed ~200,000 gene sequences from the groundwater's bacteria and archaea. The first study analyzed the rate at which community composition changed over time and space. It showed that river water intrusion more than 200 meters inshore from the Columbia River impacted the composition. Moreover, the effects were greatest near the top of the water table during the river's seasonal rise.

In the second study, scientists combined plant ecology tools with a randomization model to predict microbial community behavior when all organisms are ecologically similar, resulting in the random assembly of ecological communities. They discovered that river intrusion can indeed impact microbial communities, but only when combined with specific geologic features. When those conditions are not met, microbial community composition changed stochastically through time. Community studies like these can help scientists predict changes in microbial community dynamics caused by climate change or pollution.

X Lin, JP McKinley, CT Resch, RM Kaluzny, C Lauber, JK Fredrickson, RC Knight, and A Konopka. 2012. "Spatial and Temporal Dynamics of the Microbial Community in the Hanford Unconfined Aquifer." *The ISME Journal,* 6(9):1665-1676. DOI: 10.1038/ismej.2012.26.

Stegen JC, X Lin, A Konopka, and JK Fredrickson. 2012. "Stochastic and Deterministic Assembly Processes in Subsurface Microbial Communities." *The ISME Journal,* 6(9):1653-1664. DOI: 10.1038/ismej.2012.22.

Sponsor: Department of Energy Office of Biological and Environmental Research, PNNL's Linus Pauling Distinguished Postdoctoral Fellowship



3D model of uranium in sediment samples from a plume on the Hanford Site. Areas of higher concentration are spatially variable in the upper portion of grid (lower vadose zone)

Modeling the Underground Landscape

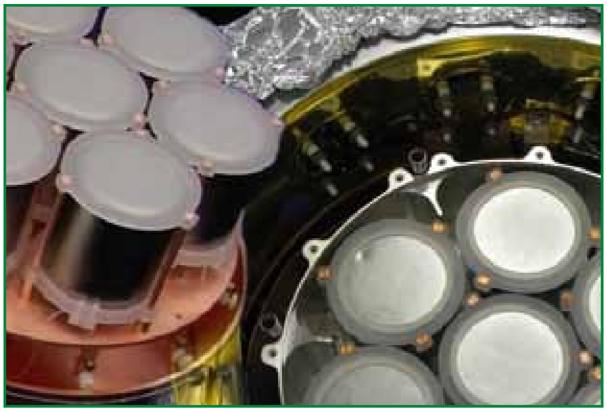
Scientists have built a computer model of the concentration and spatial distribution of mobile uranium attached to sediments within a plume that may date back to World War II. The model draws on soil samples taken from within the plume, located on the Hanford Site adjacent to the Columbia River in Washington State. With it, scientists can estimate the mobile uranium mass across a larger, varied site and the uncertainty associated with their predictions. The plume has lasted far longer than predicted, and this study provides information that can help determine why. Understanding and halting uranium is of interest to the Department of Energy, state governments, and others who want to effectively and economically protect the river.

CJ Murray, JM Zachara, JP McKinley, A Ward, YJ Bott, K Draper, and D Moore. 2012. "Establishing a Geochemical Heterogeneity Model for a Contaminated Vadose Zone – Aquifer System." *Journal of Contaminant Hydrology*, DOI: 10.1016/j.jconhyd.2012.02.003.

Sponsor: Department of Energy Office of Biological and Environmental Research

WEAK INTERACTION PHYSICS

Physics has two working models of reality: Einstein's general relativity theory dealing with space, time, and gravity, and the Standard Model, which incorporates three fundamental interactions between the particles making up all matter, electromagnetism and the strong and weak nuclear forces. Researchers are exploring the "strong" and "weak" forces to get a well-rounded understanding of the universe. Guided by the Standard Model, weak interaction physics at PNNL focuses on experimental measurements of lepton number violation, neutrino mass, dark matter, heavy quark physics, and astrophysics. We focus on breakthroughs in the field by merging our interdisciplinary team with technical expertise uniquely suited for experimental studies of rare processes.



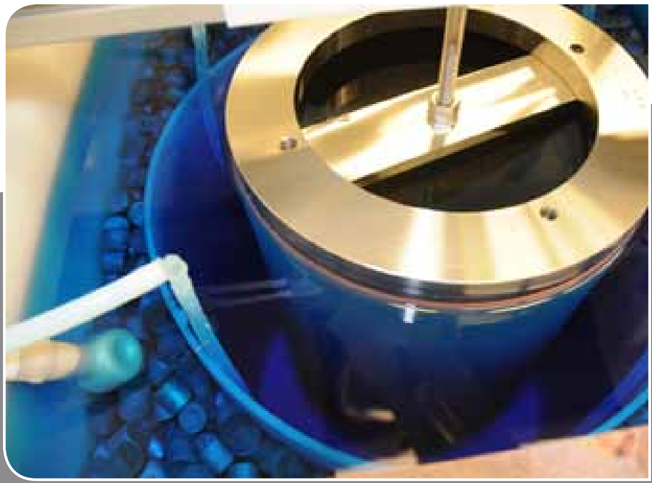
Germanium detector array.

The Frontiers of Nuclear & Particle Physics Research

For more than 30 years, PNNL has developed cutting-edge germanium (Ge) detectors for environmental monitoring, national security, and fundamental physics research. Applications of this technology have ranged from ultra-low-background detectors for measuring trace environmental radionuclides to high rate detectors for evaluating Hanford waste tank composition to large arrays for stand-off radiation detection and characterization of radiological threats. Throughout this history, there has been a synergistic relationship between applied research developments for environmental monitoring and national security and fundamental physics searches for neutrinoless double-beta decay, axions, and dark matter.

A CoGeNT Look at Dark Matter

Dark matter is well known by its gravitational effects observed throughout the universe, despite being invisible to our telescopes. The CoGeNT Dark Matter Experiment is the direct search for signals from dark matter particle interactions. It is being conducted in Soudan Underground Laboratory (Soudan, MN). PNNL's expertise in ultra-low-background materials has been applied to reduce the natural and cosmically induced background that could overwhelm the extremely rare events. To reduce the detector threshold to unprecedented levels and access more of the signal region, which rises exponentially at low energy, PNNL is developing the ultra-low-background cryostat for the next evolution of CoGeNT, C4, which will increase the sensitivity tenfold. CoGeNT data show possible indications of dark matter. The C4 experiment is poised to make a conclusive scientific discovery, whether the observed excess of events in the CoGeNT data are dark matter or come from some other phenomenon.

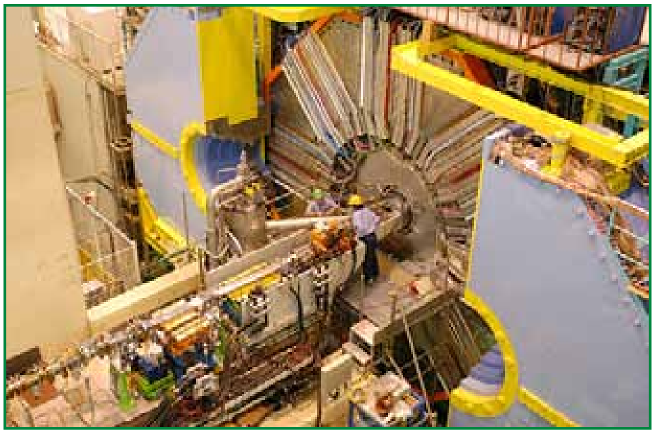


Electroforming copper.

MAJORANA: In Search of Rare Radioactive Decay

PNNL is bringing its signature capability in ultra-low-level counting to help search for a rare form of radioactive decay, called "neutrinoless double-beta decay." This effort is part of the MAJORANA DEMONSTRATOR project, which could help determine the mass and understand the properties of neutrinos, one of nature's fundamental subatomic particles.

The project will be conducted in the Sanford Underground Laboratory at the 4850-foot level of the Homestake Mine in South Dakota. The deep underground location shields against cosmic radiation on the Earth's surface. The project requires the lowest possible radioactive background environment, so copper used to shield the experiment is being manufactured underground using a PNNL-developed technology to protect against any naturally occurring radioactive impurities. This copper will be the highest purity copper in the world.



Belle detector.

Belle and Belle II

The Belle particle physics experiment, conducted by the Belle Collaboration, is an international effort investigating matter-antimatter interaction asymmetries at the High Energy Accelerator Research Organization (KEK) in Tsukuba, Japan. The Belle detector is a multilayer particle detector that recorded electron-positron interactions near 10 GeV center-of-mass energy from 1999-2010. It is used in research, including rare decay studies; exotic particles searches; and precision measurements of B mesons, D mesons, and tau particles, and has resulted in more than 300 publications in physics journals.

Recently, physicists observed two long-sought quantum states in the bottomonium family of subatomic particles in data from the KEK particle accelerator, the analysis of which was led by PNNL scientists. The results will help them better understand one of the four fundamental forces of the universe—the strong force—that helps govern matter interactions.

PNNL provides high-performance computational capabilities to support Belle scientists in data analysis, handling, and transfer and server infrastructure. Since July 2011, a high-performance computing capability for Belle has been available at PNNL, with 95 international user accounts as of July 2012.

Alongside high-energy physicists from 17 countries, PNNL is DOE's lead laboratory for the Belle II project, an upgrade to the detector system to view collisions from the upgraded KEK-B accelerator that will lead to a 50-fold increase in data available for precision studies and discovery science.

Sponsors: PNNL Laboratory Directed Research and Development, Department of Energy Office of High Energy Physics, Office of Nuclear Physics

Project X—Nuclear Energy Station

Project X is a high-intensity continuous wave proton beam accelerator being built at Fermilab (Batavia, IL) in the next decade. PNNL is an official collaborating institution on Project X with a specific focus on a Nuclear Energy Experimental Station that includes research topics, experimental approach, design, and engagement with the nuclear energy community. PNNL produced a report on how the Nuclear Energy Station could enable research and testing of materials for fission and fusion reactors, isotope production, and fundamental research in nuclear physics. PNNL will lead a workshop in November 2012, bringing together the scientific and applied research programs to develop the research agenda and the conceptual nuclear energy experimental station design.

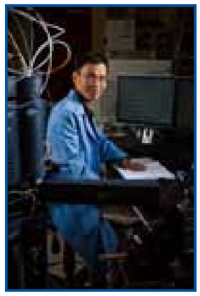
Answering Questions About the Universe

Unique capabilities in ultra-low-background radiation detection, signature science, and high-performance computing contribute to PNNL's growing expertise in high-energy physics that seeks to answer the most fundamental questions about the universe. In addition to the projects summarized already, PNNL is engaged in these longer-term programs:

- The Mu2e experiment at Fermilab will be one of the most sensitive rare decay searches ever conducted. It will use PNNL's expertise in HPGe detectors developed for national security.
- PNNL provides expertise in radio frequency and microwave engineering to Project 8, which is developing a method for measuring neutrino mass based on detection of cyclotron radiation emitted by magnetically trapped electrons.
- The proposed International Linear Collider particle accelerator has a planned collision energy of 500 GeV, with a possible upgrade to 1000 GeV (1 TeV). PNNL's computing and physics capabilities are contributing to the development of the science case for this facility.
- PNNL's involvement in detector development for future high energy and nuclear physics experiments keeps us at the forefront of the field and offers opportunities for adapting cutting-edge technologies to other missions in national security and environmental science. This is a principal aim of investments being made through the Laboratory's Ultra-Sensitive Nuclear Measurements Initiative, which began in Fiscal Year 2012.

WEI-JUN QIAN

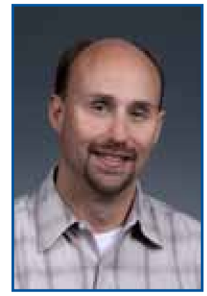
Wins Government's Highest Science and Engineering Award



Bioanalytical chemist Wei-Jun Qian was named winner of a Presidential Early Career Award for Scientists and Engineers (PECASE) for his work in proteomics. The PECASE is the highest honor given by the U.S. government to scientists and engineers who are at the start of their careers. Qian and his fellow PECASE winners were honored at a White House ceremony on Oct. 14, 2011.

JOSHUA ADKINS

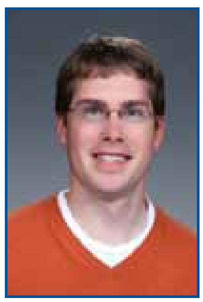
Keck Futures Initiative Conference



Josh Adkins was invited to participate in the ninth annual National Academies Keck Futures Initiative Conference, Nov. 10-13, 2011 in Irvine, California. The conference brings together the country's leading researchers to jointly tackle a complex, pressing problem via multidisciplinary approach. Adkins leads the National Institutes of Health Center for Systems Biology of EnteroPathogens at PNNL.

SAM PAYNE

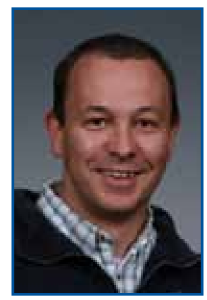
DOE Early Career Research Award



Bioinformaticist Sam Payne received an Early Career Research Award from the Department of Energy to advance his research identifying proteins that could be used in biofuel production. His grant will total $2.5 million over 5 years.

BORA AKYOL

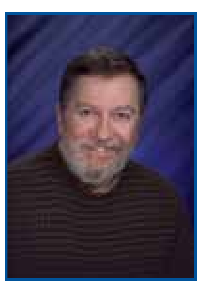
National Board of Information Security Examiners



Computational research scientist Bora Akyol was selected as a Fellow on the National Board of Information Security Examiners. As a member of the NBISE Smart Grid Security Panel, he will work with a distinguished group of cyber security experts to create a certification for smart grid cyber security professionals. Akyol also serves as a focus area lead for PNNL's Future Power Grid Initiative.

CHARLES TIMCHALK, TORKA POET

Best Biological Modeling Paper



Charles Timchalk

Toxicologists Charles Timchalk and Torka Poet co-authored "Development of a Source-to-Outcome Model for Dietary Exposures to Insecticide Residues: An Example Using Chlorpyrifos," selected as the best modeling paper of 2011 by the Society of Toxicology's Biological Modeling Specialty Section. They described a model linking exposure and dose information for the agricultural pesticide chlorpyrifos. They expanded an existing model to describe the impact of chlorpyrifos when ingested as crop residue.

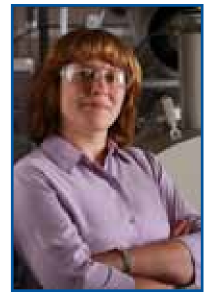
DANIEL CHAVARRIA

Top 40 Under 40

Senior computational research scientist Daniel Chavarria was recognized by *Hispanic Engineer & Information Technology* magazine as one of its "Top 40 Under 40," which features early-career Hispanics excelling in science, technology, engineering, and other science-related fields. Chavarria was recognized for his work in parallel and distributed systems, compilers for high-performance and parallel computing, reconfigurable computing, programming languages, and interactions of architectural features with software systems.

JULIA LASKIN

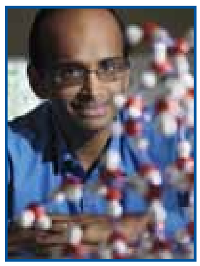
Inaugural American Chemical Society Award



Laboratory Fellow Julia Laskin received the first Rising Star Award from the Women Chemists Committee of the American Chemical Society. The award honors 10 women in the chemical enterprise who have made outstanding contributions in their fields of study. Laskin was selected for her work in gas-phase ion chemistry and mass spectrometry of complex molecules.

RAM DEVANATHAN

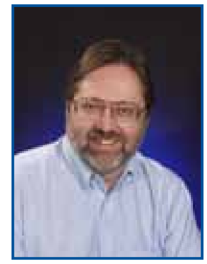
Fulrath Award of the American Ceramic Society



Materials scientist Ram Devanathan received the American Ceramic Society's Richard M. Fulrath Award for his leading-edge research on fuel cells, radiation-resistant semiconductors, nuclear fuels, and nanoscale processes in ceramics. The award promotes technical and personal friendships between Japanese and American ceramic engineers and scientists and encourages a greater understanding among the diverse cultures surrounding the Pacific Rim.

JOEL POUNDS

National Review Panel for Lead Effects



Laboratory Fellow Joel Pounds chaired a panel that reviewed findings in a draft National Toxicology Program report on the health effects of low levels of lead. The nine-member international panel concurred with the report's overall conclusion that there is sufficient evidence for adverse health effects in children and adults at lead levels in the blood below 5 micrograms per deciliter.

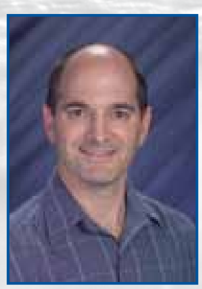
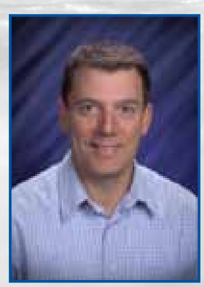
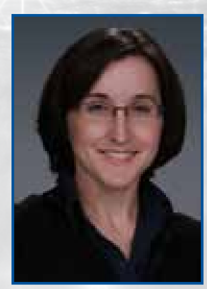
The 4STAR instrument (inset) is installed through the upper hull of the G-1 research aircraft.

BEAT SCHMID, GENE DUKES, CONNOR FLYNN, JOHN HUBBE, and CELINE KLUZEK

NASA Group Achievement Award

Climate and Aircraft Team members Beat Schmid, Gene Dukes, Connor Flynn, John Hubbe, and Celine Kluzek received the prestigious 2011 National Aeronautics and Space Administration Group Achievement Award. As part of the 4STAR Development Team, which included NASA collaborators, this team expanded the scientific, engineering, and aviation capabilities for sun and sky tracking measurements.



From left:
Beat Schmid,
Gene Dukes,
Connor Flynn,
John Hubbe,
Celine Kluzek

GUANG LIN
Early Career Achievement Award

Computational mathematician Guang Lin received the Laboratory Director's 2012 Ronald L. Brodzinski Award for Early Career Exceptional Achievement for his leading-edge research in uncertainty quantification and petascale data analytics applied to climate models. The awards recognize distinguished staff who have made notable contributions to the scientific or engineering communities.

ALESSANDRO MORARI and ROBERTO GIOIOSA
Best Paper at International Conference

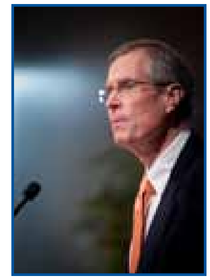
Roberto Gioiosa

Computational research scientists Alessandro Morari and Roberto Gioiosa won the best paper award in the software category at the International Parallel & Distributed Process Symposium (IPDPS) in China for "Evaluating the Impact of TLB Misses on Fugure HPC Systems." IPDPS is a premier international forum for engineers and scientists from around the world to present their latest research findings in all aspects of parallel computation.

KEQI TANG and RYAN KELLY
Technology Transfer Award

Research scientists Keqi Tang and Ryan Kelly received a 2012 Excellence in Technology Transfer Award from the Federal Laboratory Consortium for transferring a method to manufacture emitters for mass spectrometry to Bruker-Michrom of Auburn, California. The consortium is a nationwide network that encourages federal laboratories to transfer lab-developed technologies to commercial markets.

JAE EDMONDS
Highest Battelle Honor

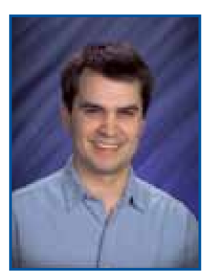


Veteran economist James "Jae" Edmonds was named a Battelle Fellow, the organization's highest recognition for individual achievement in science and technology. The honor, shared by only five other Laboratory staff, recognizes Edmonds for his pioneering work in the field of integrated assessment of energy and environment, including the development of the Global Climate Assessment Model, a foundational model of human and natural Earth systems for the global community. He has a long record of service to national and international climate science communities, including the Intergovernmental Panel on Climate Change assessments since 1990. He conducts his research at the Joint Global Change Research Institute, a collaboration between PNNL and the University of Maryland.

GOURIHAR KULKARNI
Small Business Technology Transfer Grant

Atmospheric scientist Gourihar Kulkarni was awarded Phase II funding in the prestigious Department of Energy Small Business Technology Transfer program. He will work with Droplet Measurement Technologies to develop an ice nucleation chamber. A major challenge in cloud formation research is understanding how ice particles form. Kulkarni's ice nucleation chamber will characterize one of five formation mechanisms. This development will bring the team closer to unlocking additional ice formation mechanisms.

Keqi Tang



Ryan Kelly

Fellows

2012 AAAS Fellows

Two scientists were named American Association for the Advancement of Science Fellows for their exceptional efforts to advance science and apply it to real-world problems. They were honored at the annual meeting in Vancouver, B.C., in February.

KARIN RODLAND

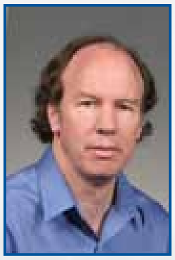
For distinguished contributions in the application of proteomics to cancer biology and for contributions to the development of biomedical research at PNNL. Rodland, a PNNL Laboratory Fellow, has an international reputation for using proteomics to identify biomarkers that can provide early detection of cancer and other diseases.

HUSSEIN ZBIB

For distinguished contributions to the field of mechanics and materials science and engineering, particularly for multi-scale theoretical modeling and predictions of the thermo-mechanical behavior of advanced nanomaterials. Zbib, a PNNL Laboratory Fellow, focuses on establishing models that can predict the mechanical behavior of materials at nano- to micro-scales.

STEVE GHAN

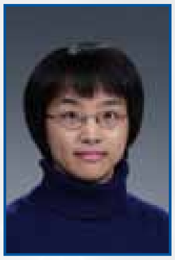
Laboratory Fellow



Climate scientist Steven Ghan was named a Laboratory Fellow, a top honor in science and engineering given at PNNL. He is a world-renowned expert in cloud-aerosol interactions and advancements in worldwide climate modeling research. Ghan's scientific contributions include research to represent sub-grid atmospheric processes, including aerosol-cloud interactions within global climate models. He is highly recognized for his expertise in developing, evaluating, and applying parameterizations for climate models .

HUI WAN

Linus Pauling Distinguished Postdoctoral Fellow

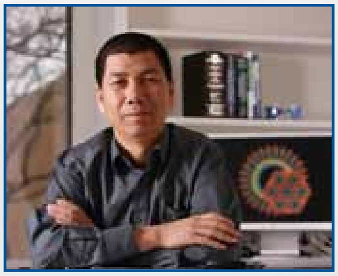


Atmospheric scientist Hui Wan was chosen for one of three 2011 Linus Pauling Distinguished Postdoctoral Fellowships awarded at the Laboratory. The Fellowship supports the next generation of scientists and engineers to lead discoveries pushing the frontiers of foundational science and solving compelling challenges for the nation and world. Wan was formerly at the Max Planck Institute for Meteorology in Hamburg, Germany. Her research targets decreasing the uncertainty in climate predictions by improving the way that model components are coupled in global climate models.

JUN LIU

Materials Research Society Fellow

PNNL Laboratory Fellow Jun Liu was elected a Fellow of the Materials Research Society, an international organization that strives to advance interdisciplinary materials science to solve vital issues and improve the quality of life, for his contributions to materials research and the scientific community. At PNNL, Liu has advanced nanomaterials and catalysis synthesis and characterization for energy and environmental applications. His recent work includes developing graphene and metal oxide nanocomposites for advanced lithium battery applications.



About Pacific Northwest National Laboratory

Pacific Northwest National Laboratory is a Department of Energy Office of Science national laboratory where interdisciplinary teams advance science and technology and deliver solutions to America's most intractable problems in energy, the environment, and national security. PNNL employs 4,700 staff, has an annual budget of nearly $1.1 billion, and has been managed by Ohio-based Battelle since the Laboratory's inception in 1965.

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