2013 Key Scientific ACCOMPLISHMENTS

Pacific Northwest
NATIONAL LABORATORY

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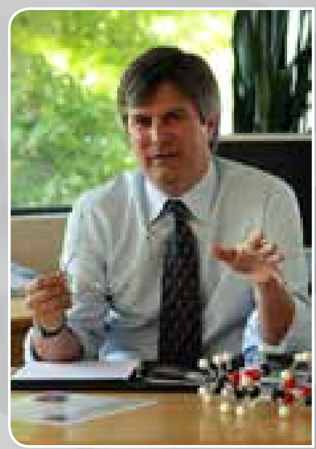
DISCOVE

Cover image: Research within Pacific Northwest National Laboratory's Chemical Imaging Initiative is characterizing chemical and physical interactions of biofilms produced by microbes. This information is used to provide insight on how the tiny microorganisms influence much larger reactions and processes, such as the migration of chemicals and radionuclides underground or precipitation reactions that influence the sequestration of carbon. To study biofilms, researchers must first obtain detailed microscopic images and chemical information. This image, obtained using scanning electron microscopy at EMSL, the Environmental Molecular Sciences Laboratory, shows a biofilm grown on a flat plastic substrate in a constant depth biofilm fermenter.

RY

in Action



In these pages you will find some of the most noteworthy achievements made by Pacific Northwest National Laboratory (PNNL) scientists in 2013. We're proud of our accomplishments' impacts on science and on some of the most important global challenges in energy, security, and environmental sustainability.

In 2013, some of our most exciting research addressed important and challenging questions in microbiology, such as understanding inter- and intracellular metabolic flux distributions in photosynthetic microorganisms for metabolic engineering, and understanding the ecological forces that structure microbial communities. We are also developing new insights into the dynamics of microbial communities with a new high-resolution imaging technique that non-invasively chemically profiles microbial communities with high spatial and temporal resolution. These and other advances portend the predictive manipulation of microbial communities to synthesize valuable products or catalyze important environmental processes.

We also continued to contribute to the global S&T community through our leadership of EMSL, the Environmental Molecular Sciences Laboratory. In these pages, you'll read about the past year's scientific achievements that occurred in EMSL between its researchers and more than 700 users from organizations around the country. Exciting changes are on the horizon as EMSL refines its emphasis to make advances in biosystems design, terrestrial and subsurface ecosystems, energy materials and processes, and atmospheric aerosol research.

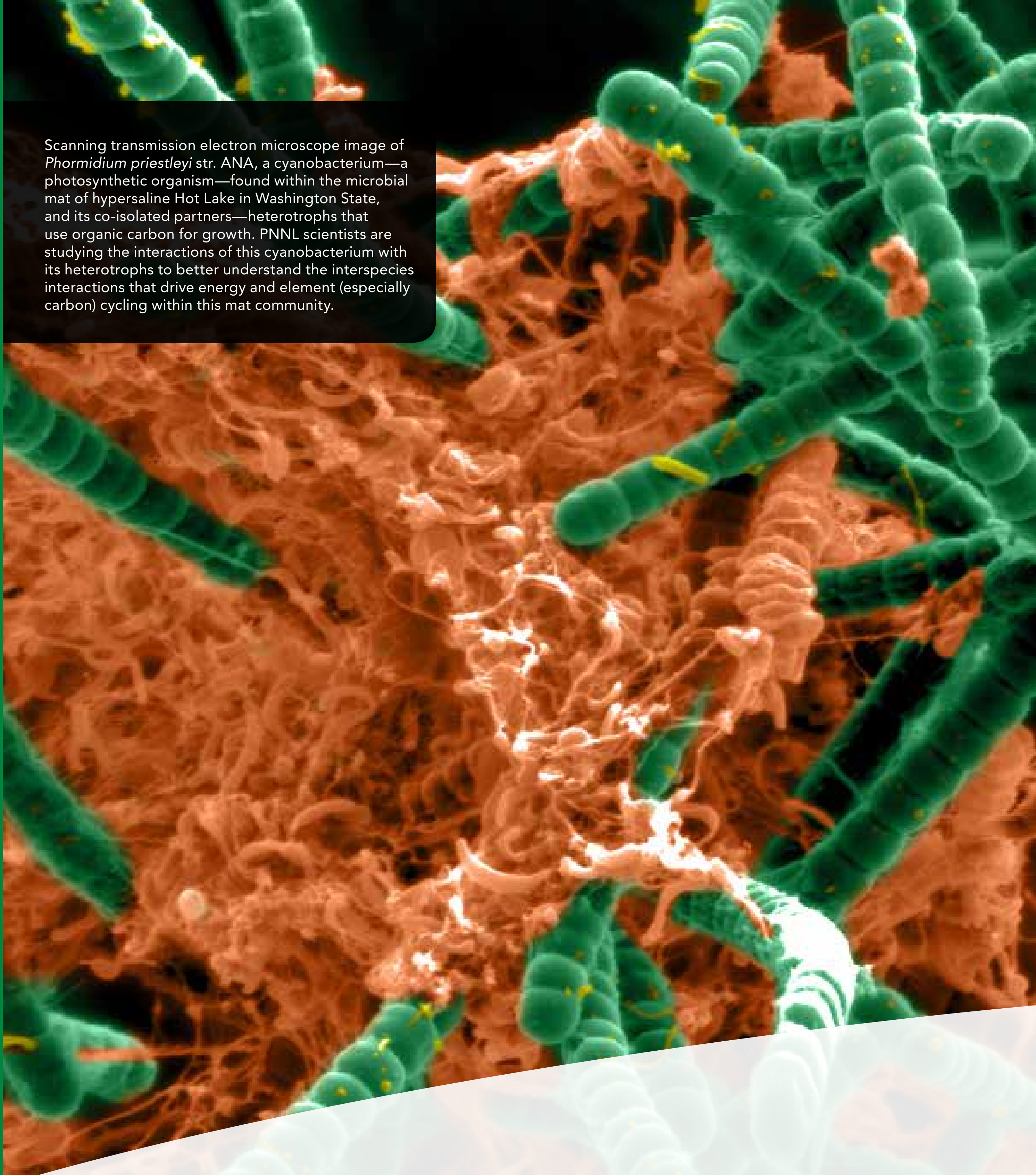
Our technical leadership of another DOE scientific user facility, the Atmospheric Radiation Measurement (ARM) Climate Research Facility, is also leading to key advances in understanding and modeling the atmospheric dynamics driving Earth's climate system. In the coming year, ARM is expanding its horizons for the global research community, adding long-term measurements at the Arctic coast and the Azores to its comprehensive data collection from sites around the world.

We invite you to explore this brochure to learn more about these and other important scientific contributions PNNL staff have made this past year in the fields of biological systems science, climate and earth systems science, chemical imaging, chemistry and geochemistry, materials science, advanced computing, and nuclear and particle physics. If you are interested in collaborating with us or desire additional information, please don't hesitate to contact one of the individuals listed on the back of this booklet.

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

Allison A. Campbell, Ph.D.
Associate Laboratory Director
Environmental Molecular Sciences Laboratory

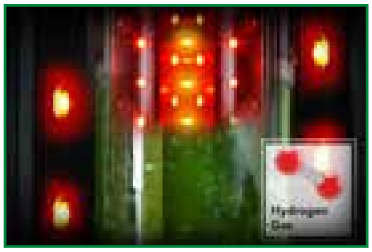
BIOLOGICAL SYSTEMS SCIENCE



Scanning transmission electron microscope image of *Phormidium priestleyi* str. ANA, a cyanobacterium—a photosynthetic organism—found within the microbial mat of hypersaline Hot Lake in Washington State, and its co-isolated partners—heterotrophs that use organic carbon for growth. PNNL scientists are studying the interactions of this cyanobacterium with its heterotrophs to better understand the interspecies interactions that drive energy and element (especially carbon) cycling within this mat community.

Biological systems science encompasses the ability to measure, predict, design, and ultimately control multicellular biological systems and bio-inspired 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 genomics and systems biology approaches. PNNL is recognized internationally for our biological systems science capabilities and leadership in environmental microbiology, systems toxicology, bioenergy, and proteomics and other 'omic technologies. Our expertise also includes cell biology and biochemistry, radiation biology, computational biology, and informatics. PNNL's biological systems science research contributes to advances in bioenergy, biogeochemistry of inorganic contaminants and carbon, human health, and national security.

Cyanobacteria Produces H_2 in O_2's Presence



A photobioreactor designed and developed at PNNL is being used to identify growth limitations of cyanobacteria—important components of major ecosystems and potential catalysts for sustainable biofuel and chemical production.

Hydrogen is appealing as a renewable energy source because it's carbon-neutral, portable, clean, and simple. But it's expensive to produce in sufficient quantities without using fossil fuels. Scientists at PNNL made a significant step toward changing that paradigm. They achieved uninterrupted, sustained hydrogen production from a photosynthetic microbe for more than 100 hours in the presence of oxygen gas, disproving a long-held belief that sustained hydrogen production during photosynthesis was impossible. The team grew cultures of *Cyanothece* sp. ATCC 51142 in a novel photobioreactor designed at PNNL in which the light environment and composition of dissolved nutrients and gas phase could be rigorously controlled and monitored. This gave the microbes the conditions needed to produce hydrogen continuously without significant photodamage or decay in required enzyme activities.

Melnicki MR, GE Pinchuk, EA Hill, LA Kucek, JK Fredrickson, AE Konopka, and AS Beliaev. 2012. "Sustained H_2 Production Driven by Photosynthetic Water Splitting in a Unicellular Cyanobacterium." *mBio* 3(4):e00197-e00212. DOI: 10.1128/mBio.00197-12.

Sponsor: DOE Office of Biological and Environmental Research

"The sustainability of our process is a solid foundation for developing an effective, renewable, and economically efficient bio-hydrogen production process."
–Dr. Alex Beliaev, PNNL

Probing Soil Microbial Communities at the Aggregate Scale

"We want to see the world a microbe sees at the scale at which it operates, because analysis at the right scale enables us to discover fundamental realities of how soil works in nature."
–Dr. Vanessa Bailey, PNNL

In the first efforts to link 1) soil physical structure with microbial community composition in single aggregates, and then 2) composition directly with bioactivity, scientists at PNNL and Argonne National Laboratory studied soil macroaggregates—clumps <1 mm in diameter. At a scale near that of a microbial habitat, they measured physical and bacterial community structure and enzyme function to determine whether the physical structure of soil aggregates constrained composition and function of the microbial community in natural soil. They found that while bacterial communities in single aggregates are significantly less diverse than in whole soil, no apparent link yet exists between the community structure and soil physical structure. These studies demonstrate that analytic measurements at this scale are now feasible and that microbial community composition can be examined jointly with aggregate physical structure or enzymatic activity. This understanding informs land management decisions related to carbon cycling and soil health.

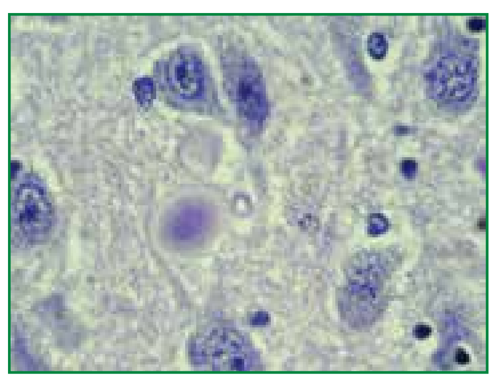
Bailey VL, LA McCue, SJ Fansler, MI Boyanov, F DeCarlo, KM Kemner, and A Konopka. 2013. "Micrometer-Scale Physical Structure and Microbial Composition of Soil Macroaggregates." *Soil Biology and Biochemistry* 65:60-68. DOI: 10.1016/j.soilbio.2013.02.005.

Bailey VL, SJ Fansler, JC Stegen, and LA McCue. 2012. "Linking Microbial Community Structure to β-Glucosidic Function in Soil Aggregates." *ISME Journal* advance online publication. DOI: 10.1038/ismej.2013.87.

Sponsors: PNNL and ANL Laboratory Directed Research and Development Programs

Unlocking the Parkinson's Puzzle

Parkinson's disease is a movement disorder that affects about 1 million people in the U.S. Scientists from PNNL, University of Miami, Baylor College of Medicine, and Rush University have teamed to search for changes that can help predict, diagnose, or monitor the disease. They want to identify components of Lewy bodies—abnormal proteins that form in the nerve cells of Parkinson's patients—and use ultra-sensitive methods to see if any of these proteins have leaked into cerebrospinal fluid or blood. Currently, Lewy bodies' presence can only be determined after death. The team is developing an assay based on biofluid protein measurements using proteomics data obtained from brain tissue samples from 500 cadavers. Proteins expressed exclusively in the tissue will be tested in easily obtained biofluids. Detecting Lewy bodies in living humans could allow direct, accurate diagnosis of Parkinson's onset and progression and help determine drug efficacy during clinical trials.



Micrograph of brain cells containing a Lewy body, the light purple sphere near the center of the image, in a Parkinson's disease patient. A research team led by PNNL is developing a proteomics-based assay for these abnormal proteins.

Sponsor: NIH National Institute of Neurological Disorders and Stroke

A Statistical Approach to Understanding Microbial Community Ecology

To enhance understanding of microbial communities under the Hanford Site, PNNL scientists developed a novel analytical framework that advances ecological understanding. First, it estimates influences of major ecosystem processes, such as ecological selection, microbe dispersal through the environment, or chance events. It then uses ecological patterns to characterize environmental variables that select for particular microbial taxa or constrain microbe movement through the subsurface. The study ultimately synthesizes inferences into a conceptual model of microbial ecology within and between geologic formations beneath the site. The framework showed that spatial turnover in biological community composition is governed simultaneously by multiple ecological processes, and that the relative balance among processes varies across geologic formations and scales. The approach also provides far more ecological knowledge than other approaches. The framework can be used to make direct comparisons across spatial scales, in different ecosystems, and with other taxonomic groupings, resulting in more robust multi-scale predictions.

Stegen JC, X Lin, JK Fredrickson, X Chen, DW Kennedy, CJ Murray, ML Rockhold, and A Konopka. 2013. “Quantifying Community Assembly Processes and Identifying Features That Impose Them.” *The ISME Journal* advance online publication, 6 June 2013. DOI: 10.1038/ismej.2013.93.

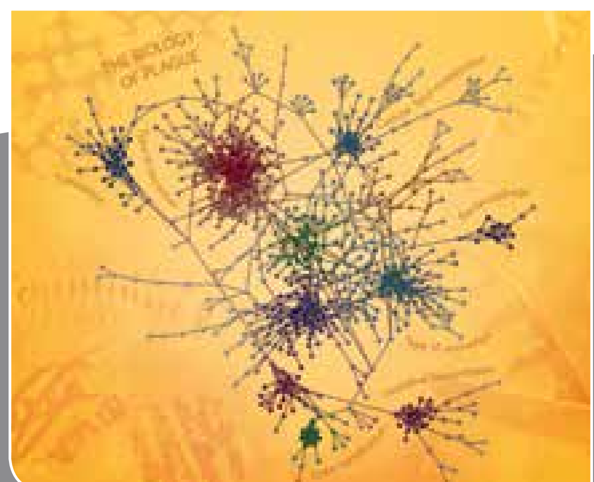
Sponsors: DOE Office of Biological and Environmental Research, PNNL Linus Pauling Distinguished Postdoctoral Fellowship

Understanding Radiation Effects on Skin

Scientists at PNNL developed a mathematical model for inferring radiation-induced changes in cell behavior from tissue-level measurements. They used this model to understand the effect of heavy ion exposures—such as those occuring during space flight and radiotherapy—on tissue and validated key model predictions. They exposed engineered human skin tissues to neon ion irradiation and measured several properties. The complex tissue system makes it hard to determine radiation-induced changes in cells from microscope measurements, so the team developed the model to overcome that challenge. They found that neon ion exposures induce rapid, but transient, changes in cell division, differentiation, and proliferation. Linking radiation-induced cellular and molecular responses to macroscopic processes at the tissue level would improve the ability to understand and predict cancer risk in response to linear energy transfer radiation. This integrated approach can be used to understand multicellular system responses, and can be adapted to other tissues and radiation-exposure scenarios.

von Neubeck C, H Shankaran, MJ Geniza, PM Kauer, RJ Robinson, WB Chrisler, and MB Sowa. 2013. “Integrated Experimental and Computational Approach to Understand the Effects of Heavy Ion Radiation on Skin Homeostasis.” *Integrative Biology* (Accepted). First published online 24 Jul 2013. DOI: 10.1039/C3IB40071A.

Sponsors: DOE Office of Biological and Environmental Research, National Aeronautics and Space Administration



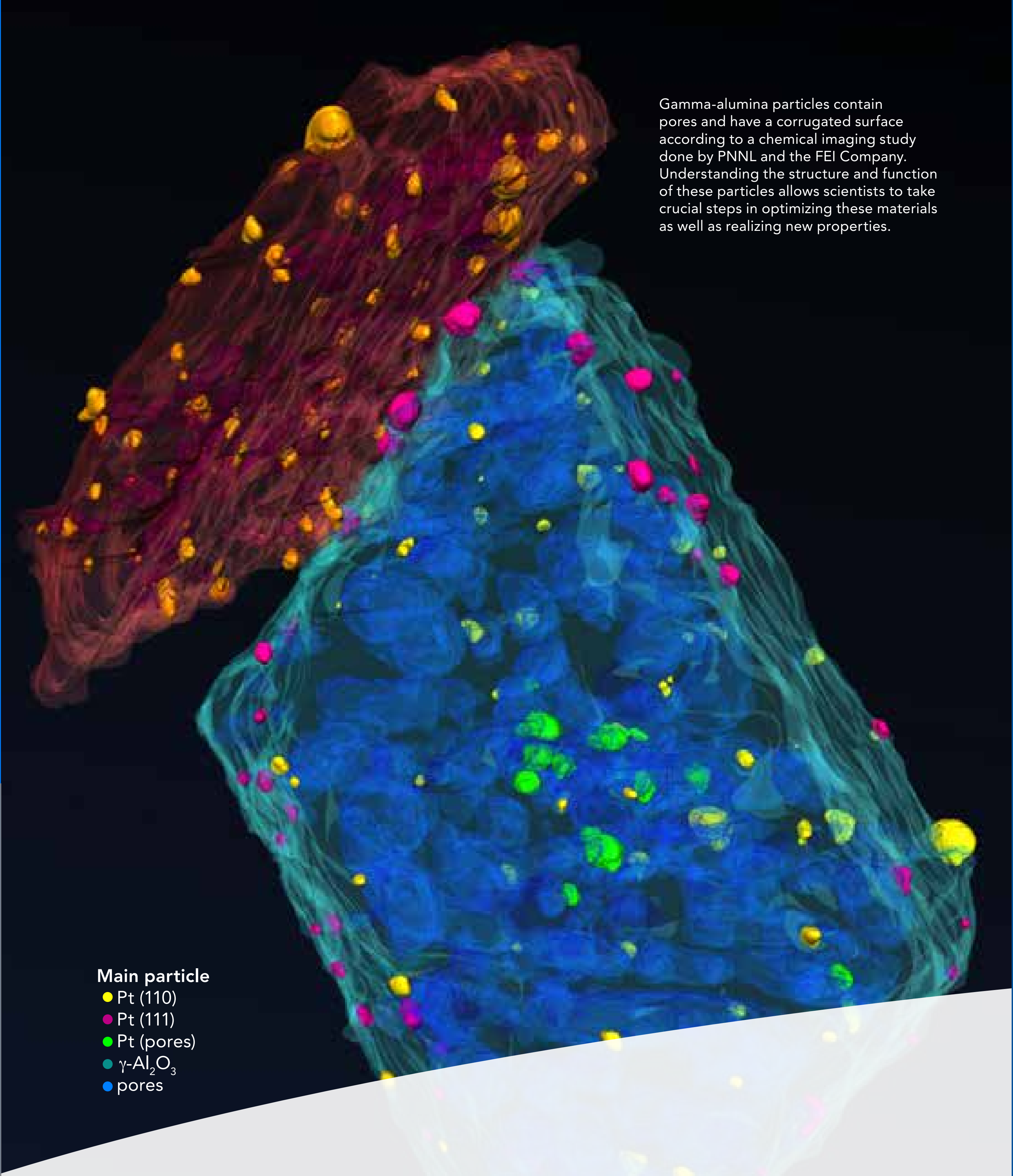
Association network inferred from integrated proteomic and transcriptomic data from three different *Yersinia* strains with varying levels of virulence.

The Biology of Plague

In two strains of the bacteria genus *Yersinia* —a lethal pathogen and its less-virulent form—scientists from PNNL, the J. Craig Venter Institute, and the University of Texas Medical Branch performed multi-omic analyses to determine their differences. They found that how the genes in both are expressed contribute to the striking difference in the diseases they cause. The work, featured on the cover of *Molecular BioSystems*, is the next step in ongoing research on *Yersinia pestis* (YP), which causes high-mortality-rate plague, and *Yersinia pseudotuberculosis* (YPT), an intestinal pathogen with a modest mortality rate. Gene and protein expression levels of shared virulence-related proteins were higher in YP than in YPT, suggesting that adaptation in YP’s regulatory architecture and its unique genetic material may contribute to its pathogenicity. This work provides important information to aid understanding of the different pathogenicities of YP and YPT and ultimately help develop therapeutic targets for this increasingly drug-resistant strain.

Ansong C, AC Rutledge, HD Mitchell, S Chauhan, MB Jones, YM Kim, K McAteer, BL Deatherage, JL DuBois, HM Brewer, BC Frank, JE McDermott, TO Metz, SN Peterson, RD Smith, VL Motin, and JN Adkins. 2012. “A Multi-omic Systems Approach to Elucidating *Yersinia* Virulence Mechanisms.” *Molecular BioSystems* 9:44-54. DOI: 10.1039/C2MB25287B.

Sponsors: NIH National Institutes of Allergy and Infectious Diseases and General Medical Sciences, DOE Office of Biological and Environmental Research

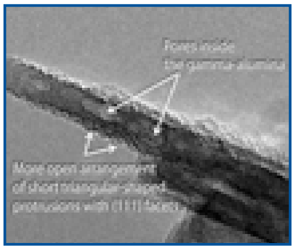


Gamma-alumina particles contain pores and have a corrugated surface according to a chemical imaging study done by PNNL and the FEI Company. Understanding the structure and function of these particles allows scientists to take crucial steps in optimizing these materials as well as realizing new properties.

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 many of today’s tools cannot reach the needed level of clarity. Scientists at PNNL are inventing the tools and techniques to generate in situ, or in-place, images and movies at the nanometer and near-nanometer scales. They are also building the computational tools to analyze the massive data quantities generated.

Seeing a Common Catalyst with New Eyes

Gamma-alumina has been studied extensively for its potential as a durable support material for efficient catalysts, but its atomic arrangement has not been established because of the challenge of getting a detailed view of this complex material. Accurately describing the atomic structure is crucial for understanding and taking advantage of the material's best properties. Scientists at PNNL studded the particles' surfaces with nano-sized catalytic platinum particles and, using a transmission electron microscope at EMSL, obtained ultrahigh-resolution images and chemical data about the particle's surface. They found that the particles were covered with ridges made from a more open, yet symmetrical, arrangement of atoms that covers 70% of the nanoparticle. By understanding the particles' structure and function, scientists can manipulate the properties of these materials. If scientists can characterize the surfaces, they can tailor them for more efficient catalytic applications.



The surface of the plate-like gamma-alumina particles is far from smooth, according to a new transmission electron microscopy study conducted by PNNL and the FEI Company.

Kovarik L, A Genc, C Wang, A Qiu, CHF Peden, J Szanyi, and JH Kwak. 2013. "Tomography and High-Resolution Electron Microscopy Study of Surfaces and Porosity in a Plate-like γ-Al_2O_3." *The Journal of Physical Chemistry C* 117(1):179-186. DOI: 10.1021/jp306800h.

Sponsors: PNNL Laboratory Directed Research and Development, DOE Office of Basic Energy Sciences

"Catalytic research demands this type of state-of-the-art chemical imaging research. Dr. Kovarik's outstanding new images from this powerhouse microscope have yielded unprecedented new information about a catalyst material of enormous practical utility."
–Dr. Charles Peden, PNNL

Motivating Carbon Dioxide

When mixing sunlight and carbon dioxide (CO_2) to link together carbon atoms and create fuels, the CO_2 gets "stuck" on the catalyst's surface and fails to react. PNNL scientists wanted to know what it takes to get the CO_2 to overcome its kinetic energy barrier and fall into catalyst's reactive spot—the oxygen vacancy. They found when warmed to 100 to 160 K, the CO_2 overcomes the kinetic energy barrier and slides into an oxygen vacancy. To make this discovery, the team modified a standard scanning tunneling microscope tip by attaching a single CO_2 molecule at the end. This allowed them to change the contrast of oxygen atoms on the surface and see the CO_2 huddle on the surface or move. Determining the barriers to getting CO_2 into the oxygen vacancies is a fundamental step in creating the needed materials for solar fuels.

Lin X, ZT Wang, I Lyubinetsky, BD Kay, and Z Dohnalek. 2013. "Interaction of CO_2 with Oxygen Adatoms on Rutile TiO_2(110)." *Physical Chemistry Chemical Physics* 15:6190-6195. DOI: 10.1039/c3cp44040k.

Sponsors: PNNL Laboratory Directed Research and Development, DOE Office of Basic Energy Sciences

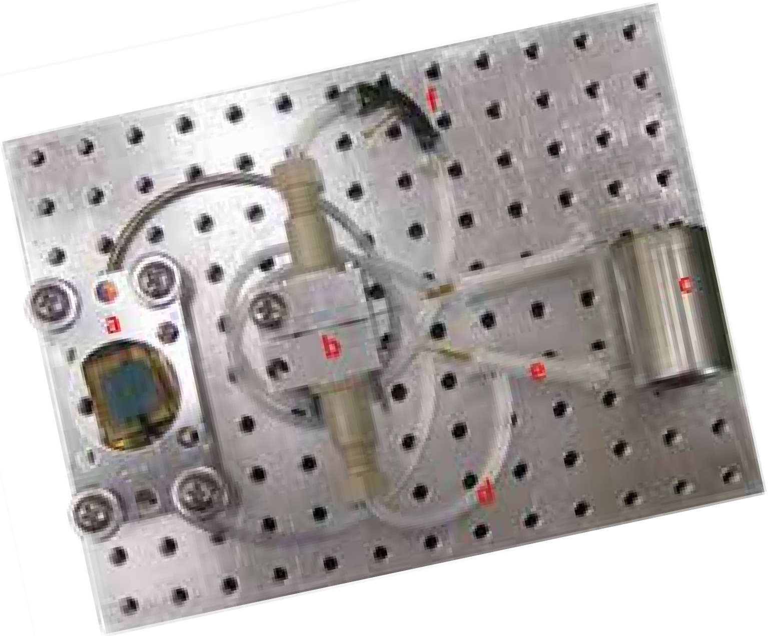
Seeing the Messages Microbes Send

With Nanospray Desorption Ionization Electrospray Mass Spectrometry, or nano-DESI, scientists at PNNL noninvasively profiled the chemicals that a cyanobacterium makes available to others. Over 4 days, *Synechococcus* sp. PCC 7002 steadily secretes sucrose and glucosylglycerol, which could feed nearby bacteria. Using nano-DESI, they chemically profiled the microbial communities in space and time. Built by a team at PNNL, in EMSL, nano-DESI uses two thin glass capillaries to place a small drop of liquid on the microbial colony and then draw some of the now sample-laden liquid off and analyze it in a mass spectrometer for analysis. Understanding microbial behavior could provide basic understanding needed for creating sugars, that is, fuels, from carbon dioxide and sunlight.

Scientists used the nano-DESI to show how bacteria support other colonies to further understanding needed to advance sustainable energy.

Lanekoff I, O Geydebrekht, GE Pinchuk, AE Konopka, and J Laskin. 2013. "Spatially Resolved Analysis of Glycolipids and Metabolites in Living *Synechococcus* Sp. PCC 7002 Using Nanospray Desorption Electrospray Ionization." *Analyst* 138:1971-1978. DOI: 10.1039/C3AN36716A.

Sponsor: PNNL Laboratory Directed Research and Development, EMSL Operating Funds



New Imaging Tool Directly Measures Liquid Surfaces

Designed and fabricated at PNNL, a one-of-a-kind liquid probe continuously pumps liquid samples through a gold-coated microfluidic chamber, presenting these volatile liquids to scientific instruments for thorough analysis. The device's extremely narrow channel provides high linear velocity at the detection window and helps overcome the liquids' tendency to vaporize. Instruments access the liquid via an open viewing port. Tests with electron microscopes and time-of-flight secondary ion mass spectrometers at EMSL prove the device can continuously present complex liquids for up to 8 hours.

This new tool allows scientists to obtain precise data on interfacial reactions. These interactions are vital for quick, affordable methods of storing electricity from wind turbines and effectively trapping and removing industrial solvents from soil.

Yang L, Z Zhu, XY Yu, E Rodek, L Saraf, T Thevuthasan, and JP Cowin. 2013. "In Situ SEM and ToF-SIMS Analysis of IgG Conjugated Gold Nanoparticles at Aqueous Surfaces." *Surface and Interface Analysis*. DOI: 10.1002/sia.5252.

Yang L, Z Zhu, XY Yu, S Thevuthasan, and JP Cowin. 2013. "Performance of a Microfluidic Flow Cell for In Situ ToF-SIMS Analysis of Selected Organic Molecules at Aqueous Surfaces." *Analytical Methods* 5, 2515-2522. DOI: 10.1039/C3AY26513G.

Yu X-Y, J Cowin, M Iedema, and Z Zhu. August 2013. US Patent 13/047,025 "Studying liquid surfaces under vacuum using ToF-SIMS and SEM via a microfluidic interface."

Sponsors: DOE Office of Basic Energy Research, Office of Biological and Environmental Research, Use at Facility Funds at PNNL, PNNL Laboratory Directed Research and Development

"The discoveries needed to solve today's complex scientific problems aren't something that you're going to get by eyeballing a sample and analyzing a spreadsheet. You need new approaches and new ideas."
–Dr. Louis Terminello, PNNL

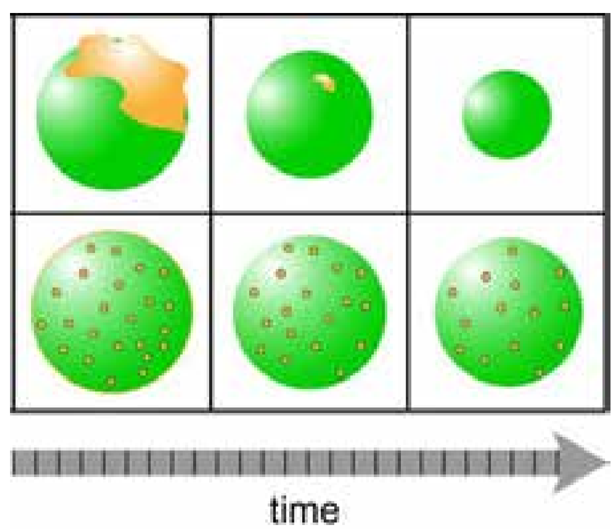
Pollution Hitches Ride to Arctic

Polycyclic aromatic hydrocarbons, or PAHs, produced by fossil fuel and biomass burning reach all the way to the Arctic, even though they should decay long before they travel that far, according to a chemical imaging study by scientists at PNNL, Imre Consulting, and the University of Washington. The team found that atmospherically abundant, carbon-based secondary organic aerosols, or SOAs, allow toxic pollution to tuck inside, providing a vehicle for the pollution's journey. In a one-two punch, the research shows that the PAHs and the SOAs last longer when the pollutants hitch a ride.

For decades, scientists have been trying to explain how atmospheric particles manage to carry harmful pollutants to pristine environments thousands of miles away from their starting point. The results of this study will help scientists understand how pollution is transported over long distances and will help improve air-quality and particle transport models.

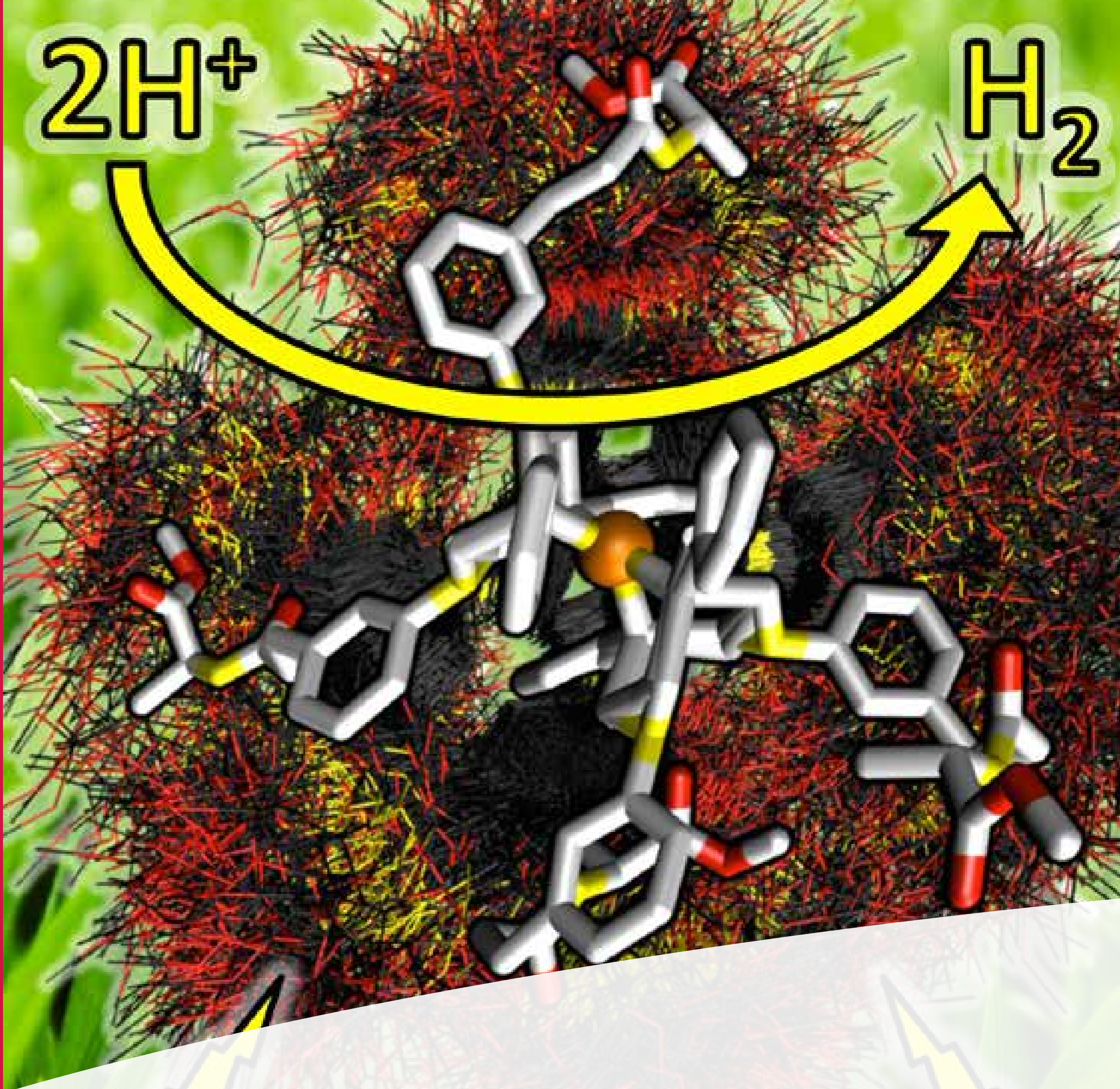
Zelenyuk A, D Imre, J Beránek, E Abramson, J Wilson, and M Shrivastava. 2012. "Synergy Between Secondary Organic Aerosols and Long-Range Transport of Polycyclic Aromatic Hydrocarbons." *Environmental Science & Technology* 46(22):12459-12466. DOI:10.1021/es302743z.

Sponsors: DOE Office of Basic Energy Research, Office of Biological and Environmental Research, Use at Facility Funds at PNNL, PNNL Laboratory Directed Research and Development



When airborne particles (green) form before pollutants known as PAHs (yellow) glob on, the pollutants dissipate quickly, as shown in the top row. But when the particles form in the presence of pollutants, which is what likely happens in nature, the long-lasting particles can take the pollutants for a long-distance ride (bottom).

Scientists at PNNL showed that adding amino acids on a catalyst's outer edge can cause the catalyst to work 5 times faster. This addition to the nickel-based catalyst's outer coordination sphere was inspired by similar features found in natural catalysts.



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 and security issues. At PNNL, scientists conduct research in catalysis, computational chemistry, condensed phase and interfacial chemical physics, geochemistry, separations, and detection. They acquire or 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.

Reactions of Rosettes and Rods

New knowledge about the chemical reactions between stored carbon dioxide and the mineral forsterite is helping determine how much confidence can be placed in using igneous rocks with magnesium-rich olivines for long-term carbon sequestration. Scientists at PNNL determined that the carbon dioxide and forsterite react to form hydrated dypingite, which precipitates from solution. The precipitates grow by different mechanisms and with a different morphology based on whether the starting phase is synthetic or natural forsterite. In synthetic forsterite, magnesium solutions seeped into pores where evaporation left rosettes of dypingite behind. On natural forsterite, dypingite precipitates formed only on the surface and in rod-like structures. This finding, made possible by multimodal high-resolution imaging and spectroscopic analysis, gives new insight into the geochemistry of supercritical carbon dioxide storage.

Arey BW, L Kovarik, O Qafoku, Z Wang, NJ Hess, and AR Felmy. 2013. "Investigation of Mineral Transformations in Wet Supercritical CO_2 by Electron Microscopy." *Microscopy and Microanalysis* 19(2):268-275. DOI: 10.1017/S1431927612014171.

Sponsor: DOE Office of Basic Energy Sciences

New Protein Discovered Gives Insights to Iron's Fate Underground

A protein that steals electrons from iron in one microbe looks a lot like one that adds electrons in another microbe, according to scientists at PNNL and University of East Anglia. Their survey of the genes of common groundwater bacterium *Sideroxydans lithotrophicus* ES-1, which removes electrons from iron, revealed that it contained genes in common with *Shewanella oneidensis* MR-1, which adds electrons to iron. Their results contribute to understanding of the molecular mechanisms by which subsurface microorganisms change the electron configuration of iron and, thus, change its mobility.

Liu J, 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: DOE Office of Biological and Environmental Research

Smashing Glass at the Molecular Level

Whether gas trapped under a layer of amorphous solid water, often called a "frozen" liquid, flows through cracks or bursts out depends on the layer's depth and temperature, according to scientists at PNNL. They proved that in some cases, gases trapped under the water films are released via fissures that form during crystallization. For thicker trapped gas layers, the gas can escape abruptly before crystallization.

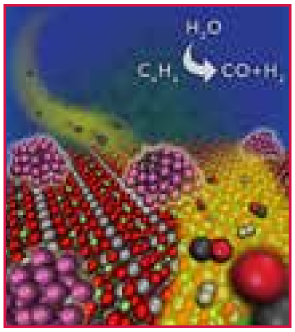
While amorphous solid water does not exist naturally on Earth because of the low temperatures necessary to create and maintain it, understanding the basic principles behind how amorphous solid water releases gases, or doesn't, could answer questions about how astrophysical ices and water on planets form. Here on Earth, this understanding can be used as a model to study the properties and stability of other relevant glasses, which are important in disciplines ranging from materials science and nuclear waste storage to drug delivery and pharmaceuticals.

May RA, RS Smith, and BD Kay. 2013. "The Release of Trapped Gases from Amorphous Solid Water Films. I. 'Top-down' Crystallization-Induced Crack Propagation Probed Using the Molecular Volcano." *The Journal of Chemical Physics* 138:104501. DOI: 10.1063/1.4793311.

May RA, RS Smith, and BD Kay. 2013. "The Release of Trapped Gases from Amorphous Solid Water Films. II. 'Bottom-up' Induced Desorption Pathways." *The Journal of Chemical Physics* 138:104502. DOI: 10.1063/1.4793312.

Sponsor: DOE Office of Basic Energy Sciences

Hydrogen Release Depends on Benzene Bond Scission, Not Absorption

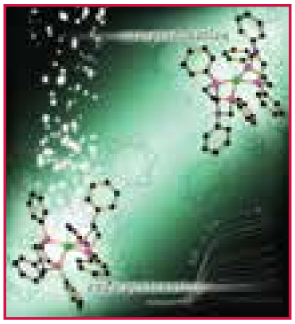


In adding steam to benzene to generate hydrogen, the step that determines the reaction's speed is not the benzene's absorption onto the catalyst, but rather the first benzene bond that breaks, according to scientists at PNNL. The team also found that the speed of hydrogen production could be increased by using small rhodium catalysts on a magnesium aluminum spinel support. This research is helping drive the shift from petroleum to bio-based fuels by building the scientific and engineering foundations.

Mei D, VM Lebarbier, R Rousseau, VA Glezakou, KO Albrecht, L Kovarik, M Flake and RA Dagle. 2013. "Comparative Investigation of Benzene Steam Reforming over Spinel Supported Rh and Ir Catalysts." *ACS Catalysis* 3: 1133-1143.

Sponsor: DOE Office of Biomass Programs

Controlling Proton Source Speeds Catalyst



A new nickel-based catalyst is faster when it and its surrounding acid have the same pKa or proton-donating ability, according to scientists at the Center for Molecular Electrocatalysis, an Energy Frontier Research Center, at PNNL. The catalyst drives turning electrons and protons into a bond between two hydrogen atoms, storing the energy. Making the catalyst faster is vital to designing technologies that can store electrons created by wind turbines. The team's experimental and computational studies focused on the acid that supplies the reaction's protons. When the acid and the catalyst had the same pKa, the speed jumped from 2,400 and 27,000 hydrogen molecules a second to 4,100 to 96,000. This study adds a new level of understanding about how these catalysts interact with their surroundings.

Stewart MP, MH Ho, S Wiese, ML Lindstrom, CE Thogerson, S Raugei, RM Bullock, and ML Helm. 2013. "High Catalytic Rates for Hydrogen Production Using Nickel Electrocatalysts with Seven-Membered Cyclic Diphosphine Ligands Containing One Pendant Amine." *Journal of the American Chemical Society* 135(16):6033-6046. DOI: 10.1021/ja400181a.

Sponsors: DOE Office of Basic Energy Sciences, Energy Frontier Research Center, DOE Faculty and Student Team program

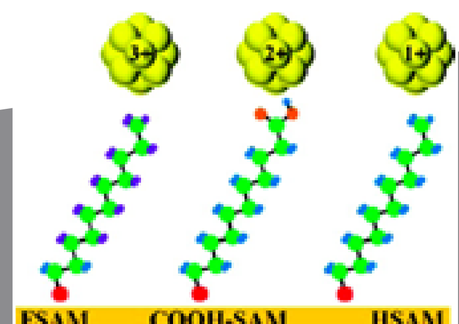
Synthetic Molecule First Electricity-Making Catalyst to Use Iron to Split Hydrogen Gas

A fast and efficient iron-based catalyst that splits hydrogen gas to make electricity—necessary to make fuel cells more economical—was reported by researchers at the Center for Molecular Electrocatalysis, based at PNNL. The catalyst's speed peaked at about two molecules per second, thousands of times faster than the closest, non-electricity-making iron-based competitor. In addition, they determined its overpotential, a measure of how efficient the catalyst is. Coming in at 160 to 220 millivolts, the catalyst revealed itself to be similar in efficiency to most commercially available catalysts. The result moves chemists and engineers a step closer to widely affordable fuel cells. Fuel cells generate electricity out of a chemical fuel, usually hydrogen. The bond within a hydrogen molecule stores electricity, where two electrons connect two hydrogen atoms like a barbell.

Liu T, DL DuBois, and RM Bullock. 2013. "An Iron Complex with Pendent Amines as a Molecular Electrocatalyst for Oxidation of Hydrogen." *Nature Chemistry* 5:228-233. DOI: 10.1038/nchem.1571.

Sponsor: DOE Office of Basic Energy Sciences

Electrons have a much easier time getting to the positively charged gold clusters on the slightly polar HSAM surface than they do on the highly polar fluorine-based FSAM surface, according to scientists at Pacific Northwest National Laboratory.



Soft Landing and Particle Coverage Key to Keeping or Losing Charge on Surfaces

Reliable, renewable energy sources demand catalysts with specific physical and chemical properties that are controlled by the size and electrical charge of the catalyst's metal nanoparticles. Scientists at PNNL have discovered how to precisely control both the size and charge of the gold particles. To effectively distribute metal clusters across a catalytic support, a layer of tethering molecules may be used. The team found that the polarity of the tethering molecules determines the propensity of electron tunneling through the layer, which has a strong effect on the charge of the metal clusters.

The team also found that covering the surface in a denser layer of multiply charged gold clusters changed the clusters' charges. The greater number of multiply charged clusters deposited on the surface built up a sufficient potential to allow the electrons from the surface to tunnel to the gold clusters, reducing their charge state. Understanding how these barriers break down gives scientists the knowledge they need to control material's charges.

Johnson GE, T Priest, and J Laskin. 2012. "Charge Retention by Gold Clusters on Surfaces Prepared Using Soft Landing of Mass Selected Ions." *ACS Nano* 6(1):573-582. DOI: 10.1021/nn2039565.

Johnson GE, T Priest, and J Laskin. 2012. "Coverage Dependent Charge Reduction of Cationic Gold Clusters on Surfaces Prepared Using Soft Landing of Mass-Selected Ions." *The Journal of Physical Chemistry C* 116(47):24977-24986. DOI:10.1021/jp308795r.

Sponsors: PNNL Laboratory Directed Research and Development, DOE Office of Basic Energy Sciences, DOE's Science Undergraduate Laboratory Internship at PNNL

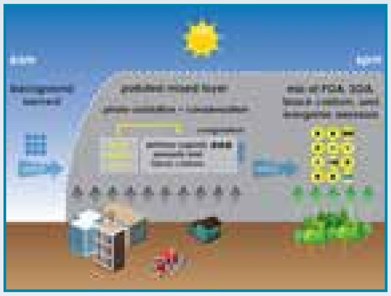
CLIMATE & EARTH SYSTEMS SCIENCE

Fair-weather cumulus clouds appear innocuous. But they play an important role in regulating Earth's temperature, and pollution particles are changing their properties over many areas of the globe. Understanding and accurately modeling changes in clouds are among the most important challenges for climate prediction. Photo over the ARM Climate Research Facility Southern Great Plains site in Oklahoma, a DOE scientific user facility.

How do human activities and natural systems interact to affect the Earth's climate? Ultimately, that is the question challenging scientists at Pacific Northwest National Laboratory. We are expanding knowledge of fundamental atmospheric processes, developing and applying state-of-the-art modeling capabilities, and improving understanding of how climate, energy, water, and land systems interact. This requires working across disciplines and integrating theory, measurements, and modeling at scales ranging from molecular to global.

Research from the Carbonaceous Aerosols and Radiative Effects Study (CARES)

In the 2010 CARES field campaign, funded by DOE's Atmospheric Radiation Measurement (ARM) Climate Research Facility, scientists led by PNNL amassed a rich dataset that will shed light on how carbonaceous aerosols (carbon-based particles) form, travel, interact, undergo chemical transformations, and ultimately affect the Earth's climate. Laying the groundwork for future analyses, the scientists identified three observation periods when the aerosols in the sampling area could be attributed primarily to natural sources, primarily by emissions related to human activities, and when both types of emissions mixed together. This research provides a roadmap for future data analyses and modeling studies of the complex interactions between the urban and natural carbonaceous aerosols.



Black carbon and other carbon-containing (organic) aerosol particles are emitted directly into the atmosphere through human activities. Secondary organic aerosols (SOAs) are formed through complex physical and chemical interactions between pre-existing aerosols in the atmosphere and trace organic gases emitted from both human-caused and natural sources.

Zaveri RA, et al. 2012. "Overview of the 2010 Carbonaceous Aerosols and Radiative Effects Study (CARES)." *Atmospheric Chemistry and Physics* 12(16):7647-7687. DOI:10.5194/acp-12-7647-2012.

Sponsor: DOE Office of Biological and Environmental Research

The New Frontier in SOA Modeling

Fortified with new evidence of particles' true properties, scientists developed a multi-dimensional modeling framework that predicts their formation and evolution in the atmosphere. Instead of treating secondary organic aerosols (SOAs), created by a mix of natural and human-caused emissions, as liquid-like volatile solutions as has traditionally been done, they modeled them as non-volatile semi-solids. The team applied state-of-the-art instrumentation and approaches to characterize properties of SOA particles in both laboratory and field settings to show that the particles are not at equilibrium as assumed by traditional models. Instead, researchers found the particles to be nearly non-volatile and highly viscous. For the first time, the team expanded their model to include a multi-dimensional framework to represent the multi-generational aging of gas-phase SOA precursors.

"This work opens new frontiers in the field of SOAs. We have taken the first step to improve the model's representation of SOAs based on our new experimental findings of low volatility and high viscosity of secondary organic aerosols."
– Dr. Manish Shrivastava, PNNL

Shrivastava M, A Zelenyuk, D Imre, R Easter, J Beránek, RA Zaveri, and J Fast. 2013. "Implications of Low Volatility SOA and Gas-phase Fragmentation Reactions on SOA Loadings and their Spatial and Temporal Evolution in the Atmosphere." *Journal of Geophysical Research-Atmospheres* 118(8):3328-3342. DOI: 10.1002/jgrd.50160.

Sponsors: DOE Office of Biological and Environmental Research, Office of Basic Energy Sciences

When Pollution Gets a Whiff of Trees

Scientists are working to describe the natural and human-caused sources of atmospheric carbon, which is 30 to 90 percent of the total particle mass in the atmosphere. To understand how these sources mix and react with the other and affect the climate, PNNL led a multi-institutional field study called CARES. Using CARES data, researchers found that polluted city emissions travel miles away, eventually mixing with forest emissions producing levels of new carbon-containing particles called secondary organic aerosols in amounts greater than previously expected. These added atmospheric particles can have a large impact air quality, visibility, human health, and, ultimately, the climate. Accurately predicting how these particles form will help scientists and policy makers understand and predict future global climate change.

"This process is a result of human activities and is not yet well understood. The level of organic aerosol produced from mixes of city and tree emissions is greater than we expected, which may impact the way we look at future climate change."
– Dr. John Shilling, PNNL

Shilling JE, RA Zaveri, JD Fast, L Kleinman, ML Alexander, MR Canagaratna, E Fortner, JM Hubbe, JT Jayne, A Sedlacek, A Setyan, S Springston, DR Worsnop, and Q Zhang. 2013. "Enhanced SOA Formation from Mixed Anthropogenic and Biogenic Emissions During the CARES Campaign." *Atmospheric Chemistry and Physics* 13(4):2091-2113. DOI:10.5194/acp-13-2091-2013.

Sponsor: DOE Office of Biological and Environmental Research

Fresh Water Feeds Hurricanes' Fury

When hurricanes blow over ocean regions swamped with fresh water, the storm can unexpectedly intensify. PNNL-led research brought new insight to the conditions that make these storms, which affect millions of lives around the world, more intense and destructive. The researchers found that layers of fresh water between the warm ocean surface and the colder ocean below prevent mixing and cooling of the surface layer by strong winds, a process that normally limits hurricane intensification. The team supported their analysis with a computer model, comparing tropical cyclones over regions with and without these freshwater "barrier" layers.

Hurricane Omar wreaked destruction over the Carribean islands in 2008. A large influx of fresh water sets up conditions in the ocean that form a layer between the surface and the colder ocean below—a barrier layer that prevents ocean layer mixing. Omar's most intense activity occurred when it traveled over this layer. *Satellite image courtesy of NASA Earth Observatory.*

Balaguru K, P Chang, R Saravanan, LR Leung, Z Xu, M Li and JS Hsieh. 2012. "Ocean Barrier Layers' Effect on Tropical Cyclone Intensification." *Proceedings of the National Academy of Sciences of the United States of America* 109(36):14343-14347. DOI: 10.1073/pnas.1201364109.

Sponsor: DOE Office of Biological and Environmental Research

"Sixty percent of the world's population lives in areas affected by tropical cyclones. Though we can predict the paths cyclones take, we need to predict their intensity better to protect people susceptible to their destructive power."
– Dr. Karthik Balaguru, PNNL

New River-Routing Model Improves Simulations of Water Movement

A new river-routing model improves computer simulations of the magnitude and timing of water flow through the landscape and into the ocean, thanks to research led by PNNL. The MOdel for Scale Adaptive River Transport (MOSART) is a new, physically based tool for simulating streamflow and river dynamics. When coupled with established land and Earth system models, MOSART outperforms other river routing models and provides the basis for a better understanding of water-land interactions. It also serves as a cornerstone for integrating and understanding impacts of human activities, such as irrigation and reservoir operation, on the water cycle at different spatial scales.

Li H, MS Wigmosta, H Wu, M Huang, Y Ke, AM Coleman, and LR Leung. 2013. "A Physically Based Runoff Routing Model for Land Surface and Earth System Models." *Journal of Hydrometeorology* 14(3):808-828. DOI: 10.1175/JHM-D-12-015.1.

Sponsors: DOE Office of Biological and Environmental Research, PNNL Laboratory Directed Research and Development

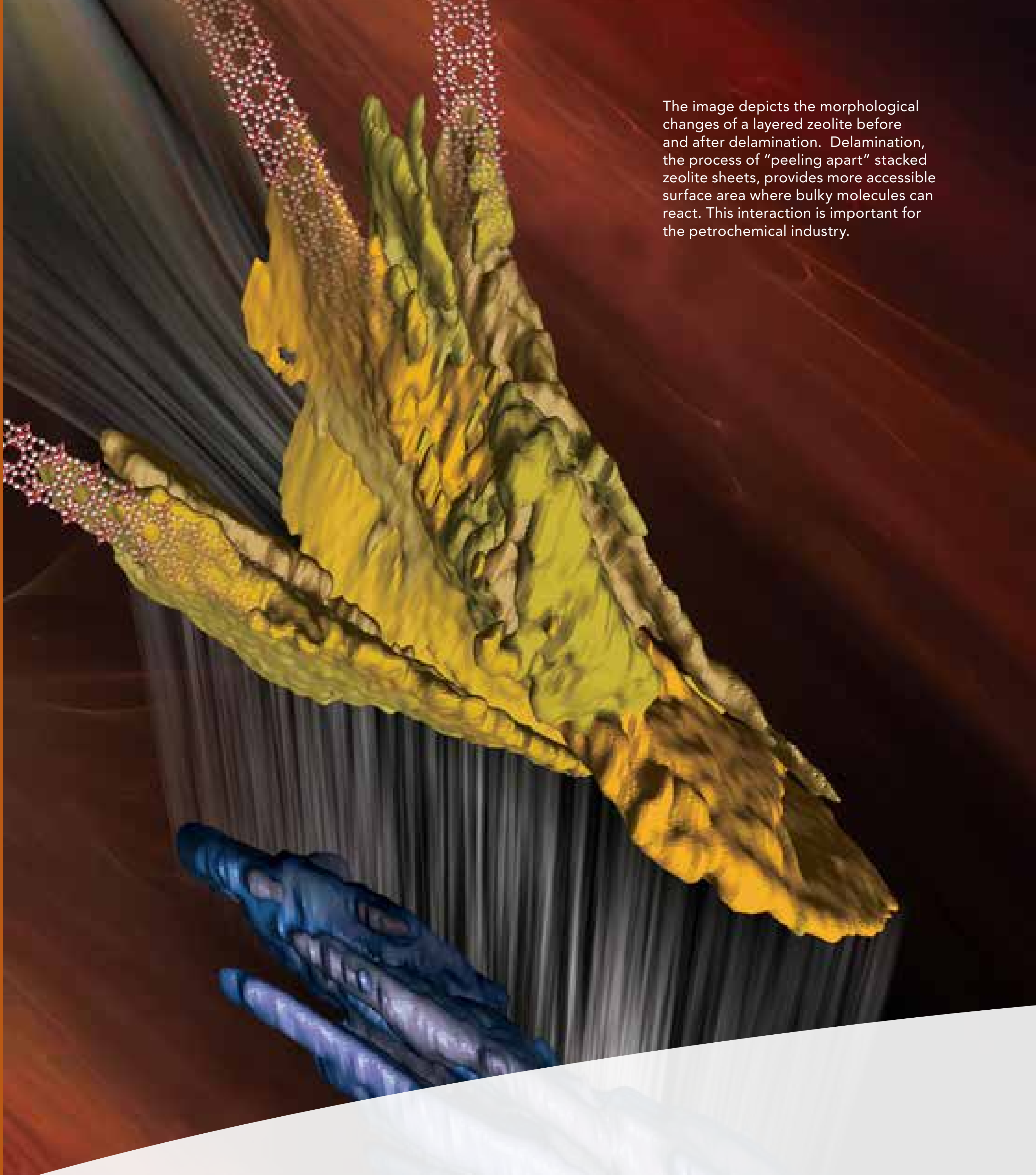
Water for Power

Today, electrical power plant cooling uses about 15 percent of the world's water. Generating electricity using new low-emissions technologies is not likely to increase water demand through the end of the century, according to PNNL and collaborators at the University of Alberta. To find how the choice of technologies to generate electrical power may impact the global and regional economy, water use and emissions, researchers turned to the Global Change Assessment Model (GCAM)—a partial equilibrium integrated assessment model developed at PNNL—to understand future costs and decisions. Even with the higher costs associated with cooling methods other than water, they found that low-emission technologies can be a viable choice for power generation. The research team developed a technology-level database of water demands per power generation technology in each of 14 global macro-regions, consistent with available water demand estimates in various countries.

Kyle P, EGR Davies, JJ Dooley, SJ Smith, LE Clarke, JA Edmonds, and M Hejazi. 2013. "Influence of Climate Change Mitigation Technology for Global Demands of Water for Electricity Generation." *International Journal of Greenhouse Gas Control* 13:112-123. DOI:10.1016/j.ijggc.2012.12.006.

Sponsor: DOE Office of Biological and Environmental Research

MATERIALS SCIENCES



The image depicts the morphological changes of a layered zeolite before and after delamination. Delamination, the process of "peeling apart" stacked zeolite sheets, provides more accessible surface area where bulky molecules can react. This interaction is important for the petrochemical industry.

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.

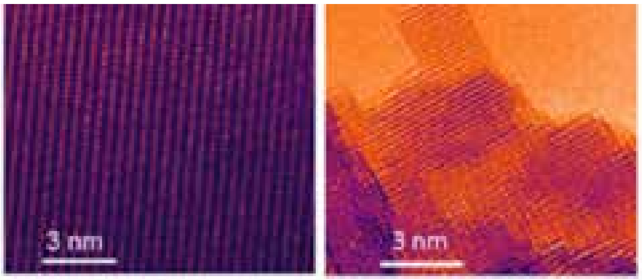
Batteries Lose in Game of Thorns

Starting as a few atoms long, thorns forming on the electrode surface in a layered lithium battery cause the battery to gradually fade, according to scientists at PNNL and Argonne National Laboratory. Using powerful imaging technologies at ANL and EMSL, they determined that a crystallographic spinel structure grows out of the electrode material and eventually completely converts the whole electrode material into the spinel structure. Further, this growth liberates lithium oxide molecules, causing cracking and pitting. The damaged electrode thereby fades, releasing less energy with each charge/discharge cycle.

Increasing independence from fossil fuels for the nation's transportation fleet requires innovation in energy storage. A lithium-rich layered composite could increase batteries' energy density by more than 50 percent. However, the voltage and amount of energy that can be stored and released gradually declines with use. By analyzing atomic-resolution images of the battery's electrode before and after use, the team determined how and where the transformations or phase transitions occur in the composite.

Gu M, I Belharouak, J Zheng, H Wu, J Xiao, A Genc, K Amine, S Thevuthasan, DR Baer, JG Zhang, ND Browning, J Liu, and C Wang. 2013. "Formation of the Spinel Phase in the Layered Composite Cathode Used in Li-Ion Batteries." *ACS Nano* 7(1):760-767. DOI: 10.1021/nn305065u.

Sponsors: PNNL Laboratory Directed Research and Development, DOE Assistant Secretary for Energy Efficiency and Renewable Energy, DOE Office of Vehicle Technologies, DOE Office of Basic Energy Sciences, DOE Freedom CAR and Vehicle Technologies Office

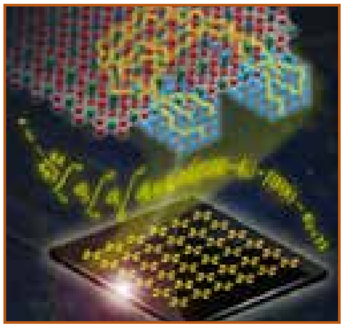


High-angle annular dark-field scanning transmission electron microscopy images showing the structural transformation from layered (left) to spinel (right) during the cyclic charge/discharge process.

"Atomic-level imaging provides the opportunity to get a fundamental picture of how does this type of subtle change evolves."
– Dr. Chongmin Wang, PNNL

How to Overcome the Oxide Barrier

Scientists at PNNL have discovered an ultra-low resistance electrical contact for strontium titanate, an important prototypical oxide semiconductor, and elucidated the atomistic reasons for its favorable properties. Oxide semiconductors are likely to be critical to creating next-generation electronic devices; however, they develop a large energy barrier at the contact point with most metals. This study showed that chromium doesn't generate any barrier to electron entry or exit into strontium titanate.



Atomistic diagram for crystalline chromium metal (light blue) on strontium titanate (top), an equation that describes the transport process (middle), and an array of metal contacts on a strontium titanate wafer (bottom).

The equivalent of 1 or 2 atomic layers of chromium diffuse into the strontium titanate and occupy interstitial sites. These chromium atoms transfer electrons to titanium atoms in the top few atomic planes, removing the energy barrier. Unlike other metal/oxide interfaces with low resistance, this junction is structurally and compositionally well defined and spatially confined. The insights gained in this work are transferable to finding low-resistance metals for other oxide semiconductors.

Chambers SA, ND Browning, M Gu, C Wang, H Yang, and PV Sushko. 2013. "Ultra-low Contact Resistance at an Epitaxial Metal/Oxide Heterojunction through Interstitial Site Doping." *Advanced Materials* 25(29):4001-4005. DOI: 10.1002/adma201301030.

Sponsor: DOE Office of Basic Energy Sciences

Modeling Materials at the Mesoscale

PNNL's Applied Computational Mathematics and Engineering (ACME) group stands apart with its signature capabilities in integrated computational materials engineering (ICME) and is taking aim at the mesoscale. With microstructure-based predictive modeling tools designed to understand the influences of mesoscale defects and heterogeneities—and their evolution kinetics on the overall mechanical properties of engineering materials—PNNL is bridging lower-length-scale material science and discovery to the larger-length-scale materials engineering and application. ACME currently is developing ICME-based predictive capabilities in lightweight metallic materials, including nuclear fuel and structural materials; multiphase advanced high-strength steels; magnesium castings; aluminum sheets; and amorphous glass systems for transparent armor applications.

Askari H, HM Zbib, and X Sun. 2012. "Multiscale Modeling of Inclusions and Precipitation Hardening in Metal Matrix Composites: Application to Advanced High Strength Steels." *Journal of Nanomechanics and Micromechanics* 3(2):24-33. DOI: 10.1061/(ASCE)NM.2153-5477.0000052.

Sun X, KS Choi, and DS Li. 2013. "Predicting the Influence of Pore Characteristics on Ductility of Thin-Walled High Pressure Die Casting Magnesium." *Materials Science and Engineering A* 572(10 June 2013):45-55. DOI: 10.1016/j.msea.2013.02.026.

Sponsors: DOE Offices of Energy Efficiency and Renewable Energy, Fossil Energy, and Nuclear Energy; U.S. Army

Team Led by Argonne National Lab Selected as DOE's Batteries and Energy Storage Hub

PNNL contributes expertise to 5-year $120 million Joint Center for Energy Storage Research

JCESR will combine the R&D firepower of five DOE national laboratories, five universities, and four private firms in an effort aimed at achieving revolutionary advances in battery performance. Advancing next-generation battery and energy storage technologies for electric and hybrid cars and the electrical grid are critical to help reduce America's reliance on foreign oil and lower energy costs for U.S. consumers.

PNNL will tap into its extensive experience in fundamental and applied sciences, including advanced materials synthesis, characterization, and modeling, as well as electrical grid infrastructure, grid storage, and management, to help improve the performance, reliability and life-span of batteries. PNNL will also play an important role in developing new technologies for stationary storage to enable widespread use of renewable energy.

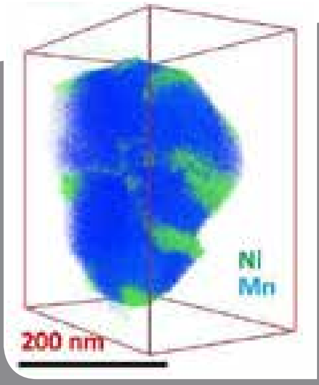
Unique research tools and imaging expertise from researchers in EMSL, DOE's Environmental Molecular Sciences Laboratory at PNNL, will help the team understand complex electrochemical reactions as they occur within working batteries, as well as determine why batteries ultimately fail.

PNNL's expertise in materials synthesis and processing will also contribute to the development of low-cost, high-capacity electrode materials for advanced batteries with unprecedented energy density and power.

JCESR will be centered at Argonne, outside of Chicago. The State of Illinois will provide $35 million to construct a 45,000-square-foot home for JCESR.

JCESR will bring together some of the most advanced energy storage research programs in the U.S. today. JCESR partners include:

- **DOE research centers**–Argonne National Laboratory, Lawrence Berkeley National Laboratory, Pacific Northwest National Laboratory, Sandia National Laboratories, and the Stanford Linear Accelerator Collider.
- **Research universities**–Northwestern University; University of Chicago; University of Illinois, Chicago; University of Illinois, Urbana-Champaign; and the University of Michigan.
- **Industry**–Applied Materials, Clean Energy Trust, Dow, and Johnson Controls.



While manganese (blue) fills out this battery nanoparticle evenly, nickel (green) clumps in certain regions, interfering with the material's smooth operation.

Nickelblock: An Element's Love-Hate Relationship with Battery Electrodes

Anyone who owns an electronic device knows that lithium-ion batteries could work better and last longer. Now, scientists examining battery materials on the nano-scale reveal how nickel forms a physical barrier that impedes the shuttling of lithium ions in the electrode, reducing how fast the materials charge and discharge. The researchers created high-resolution three-dimensional images of electrode materials made from lithium-nickel-manganese oxide layered nanoparticles, mapping the individual elements. These maps showed that nickel formed clumps at certain spots in the nanoparticles. A higher magnification view showed the nickel blocking the channels through which lithium ions normally travel when batteries are charged and discharged.

Many ideas to reduce the nation's oil addiction require an effective battery. For example, hybrid or all-electric vehicles need batteries that can perform for a long time between recharging. Lithium-ion batteries are a popular option, because pound for pound, they are some of the most energetic rechargeable batteries available. One of the greatest challenges facing lithium-ion battery development is the gradual capacity fading that accompanies each charge and discharge.

Gu M, I Belharouak, A Genc, Z Wang, D Wang, K Amine, F Gao, G Zhou, S Thevuthasan, DR Baer, JG Zhang, ND Browning, J Liu, and C Wang. 2012. "Conflicting Roles of Ni in Controlling Cathode Performance in Li-ion Batteries." *NanoLetters* 12(10):5186-5191. DOI:10.1021/nl302249v.

NUCLEAR & PARTICLE PHYSICS

The Belle Detector at KEK Laboratory, Tsukuba, Japan

Nuclear and particle physics is the study of the fundamental constituents of matter and the forces of nature. The frontiers of nuclear and particle physics are advanced through cathedral-sized detector systems, novel materials, and high-performance computer systems. The nuclear and particle physics program at PNNL is built upon capabilities in low background materials; precision assays; ultra-low background high-purity germanium detectors; ultra-high-rate high-purity germanium detectors; detector design and engineering; remote handling; irradiation testing; microwave detection; and data-intensive computing. PNNL management, scientists, and engineers are eager to apply this experience and technology to address the key scientific questions in nuclear and particle physics today.

COUPP60 Bubble Chamber–now taking data at SNOLAB

The Frontiers of Nuclear and Particle Physics Research

For more than 30 years PNNL has developed cutting-edge radiation detectors for environmental monitoring, national security, and fundamental physics research. Applications 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 standoff radiation detection and radiological threat characterization.

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.

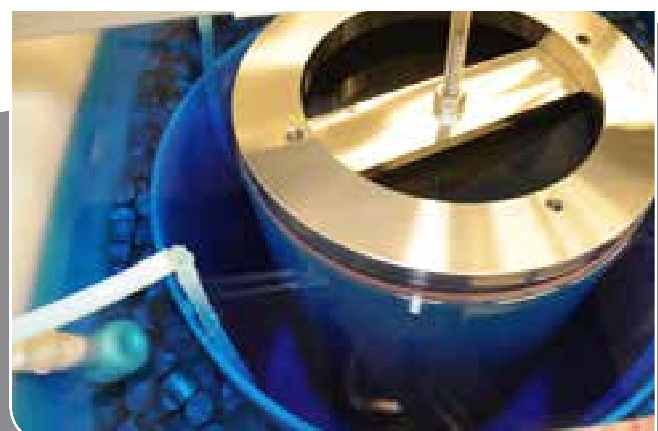
Dark Matter: At the Cosmic Frontier of Particle Physics

Despite being invisible to our telescopes, dark matter is known by its gravitational effects throughout the universe. PNNL is involved in the search for signals from dark matter particle interactions in the CoGeNT, PICO[1], SuperCDMS, and MAJORANA experiments. These experiments involve extremely low-background radiation detectors in deep underground laboratories.

CoGeNT and SuperCDMS use unique germanium detectors to search for dark matter interactions. CoGeNT employs state-of-the-art energy resolution to resolve backgrounds, while SuperCDMS uses cryogenic (~50 mK) bolometry to discriminate signal from background events. PICO is based on continuously sensitive bubble chambers—sensitive only to nuclear interactions and not to most radiometric backgrounds.

PNNL's expertise in ultra-low-background materials helps reduce the natural and cosmically induced background that could overwhelm the extremely rare dark matter events—the common challenge for all these experiments. PNNL's expertise in copper electroforming, ultra-sensitive assay, especially for uranium and thorium, and detector assembly are helping these experiments make order-of-magnitude improvements in sensitivity.

[1]In 2013, the COUPP and PICASSO collaborations merged, adopting the name PICO.

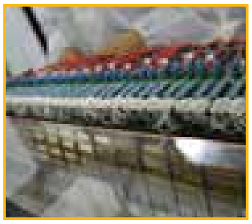


Electroforming copper

MAJORANA: In Search of Rare Radioactive Decay

As one of the founding members of the MAJORANA experiment, involving 20 institutions, PNNL is bringing its signature capability in ultra-low-level detection to help search for a rare form of radioactive decay in germanium (^{76}Ge)—never before detected—called "neutrinoless double beta decay" ($0\nu\beta\beta$). If observed, $0\nu\beta\beta$ would demonstrate neutrinos are Majorana-type particles. This discovery would show neutrinos are unique among fundamental particles, having a property whereby the matter and anti-matter version of this particle are indistinguishable. Scientists from PNNL are developing the necessary equipment to detect and measure the properties of these particles. Ultrapure electroformed copper created in PNNL's Shallow Underground Laboratory and the Sanford Underground Research Facility is key to the success of the detection technology. Measuring the Majorana nature of neutrinos from the previously unobserved $0\nu\beta\beta$ process would give clues about the formation of the universe and why we observe more matter than antimatter in the universe.

Belle and Belle II


Belle II particle identification detector prototype

The international Belle particle physics experiment is investigating matter-antimatter interaction asymmetries at the High Energy Accelerator Research Organization (KEK) in Tsukuba, Japan. The Belle detector is a house-sized collection of precise radiation sensors that recorded electron-positron interactions of near 10 GeV center-of-mass energy from 1999-2010. The data from this experiment continues to be used in rare decay studies, exotic particle searches, and precise measurements of B and D mesons and tau leptons and has resulted in nearly 400 publications in physics journals.

Alongside more than 500 high-energy physicists from 23 countries, PNNL is DOE's lead laboratory for the Belle II Project, an upgrade to the detector system to view collisions from the upgraded SuperKEK-B accelerator that will lead to a 50-fold increase in data available for precision studies and discovery science.

PNNL's Belle II computing center will store and (re)process the raw data samples, generate simulation samples and re-distribute data to European collaborators and U.S. institutions.

In the next decade, Belle II is expected to produce one of the world's largest scientific data samples – total data volume of a few hundred petabytes – driving the transpacific network bandwidth requirements.

Project X – Materials Irradiation Facility

Project X is a high-intensity continuous wave proton beam accelerator proposed to be built at Fermi National Accelerator Laboratory (FNAL) in the next decade. While the primary driver for Project X is particle physics research, the high beam power and intensity offer the potential for a flexible target station to address questions in nuclear energy, fusion energy science, and nuclear physics. PNNL collaborates on Project X focusing on the energy station concept to support high-priority research and development needs for DOE Office of Nuclear Energy, Office of Fusion Energy, and Office of Nuclear Physics as well as the accelerator target issues identified within the Accelerator Community.

PNNL co-organized and led a workshop in January 2013 of 45 accelerator, particle physics, and nuclear energy experts who identified the unique mission priorities that a Project X Target Station could provide, such as fusion and fast-reactor structural materials irradiation, separate-effects phenomena in fuels or materials, and integral effects testing of fast-reactor fuel. PNNL is actively engaged in follow-on activities.

At FNAL's request, PNNL has written technical reports on the broader impacts of the Project X spallation source, presented at international conferences, and facilitated dialogue between the physics and nuclear energy communities.

Answering Questions About the Universe

Unique capabilities in ultra-low-background radiation detection and exploration of dark matter contribute to PNNL's growing expertise in nuclear and particle physics. This research will help answer the most fundamental questions about the universe. In addition to the projects summarized above, PNNL is engaged in these longer term programs:

» The mu2e experiment, one of the most sensitive rare decay searches ever conducted, will benefit from our expertise in HPGe high rate detectors developed for international safeguards.

» We are working with the Darkside dark matter collaboration to purify low-activity argon extracted from underground sources. PNNL uses this unique resource for national security projects and environmental science.

» We provide expertise in radio frequency and microwave engineering to Project 8, which is developing a method to measure neutrino mass based on detecting cyclotron radiation emitted by magnetically trapped electrons.

» Our computing and physics capabilities contributed to the recently published Technical Design Report for the International Linear Collider particle accelerator, which has a planned collision energy of 500 GeV and a possible upgrade to 1,000 GeV (1 TeV).

» Detector development for future nuclear and particle physics experiments keeps us at the forefront of the field and offers opportunities to adapt cutting-edge technologies to national security and environmental science missions through the Laboratory's Ultra-Sensitive Nuclear Measurements Initiative, which began in FY12.

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

ADVANCED COMPUTING

Access to PNNL's 162-Teraflop peak supercomputer, Olympus, is available via the PNNL Institutional Computing, or PIC, program that allows PNNL researchers to apply for allocations of cluster time, data storage, or test beds by submitting a brief proposal at any time.

The Advanced Computing Research Area at PNNL focuses on creating advanced computational capabilities and provides multifaceted solutions to solve significant problems of national interest to the energy, environment, and national security sectors, as well as fundamental science. Our approach to Advanced Computing is multi-disciplinary and covers a large spectrum of expertise. It enables scientific breakthroughs using 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. Our Advanced Computing capabilities also include state-of-the-art computational capabilities to enable computing at extreme-scale.

Managing Uncertainty Clears Up the Rain

Using uncertainty quantification methods, scientists can better simulate precipitation, one of the most difficult climate elements to represent in climate models.

Variable and difficult to predict, precipitation is one of the most challenging climate elements to represent in a computer model. Yet, having computational confidence to predict future climate scenarios based on accurate present-day modeling is crucial. Using a unique uncertainty quantification technique, scientists calibrated the ratio between showery and stormy rain for simulations in the Community Atmospheric Model (CAM5), the popular atmospheric component of the Community Earth System Model. The multi-institutional team employed a simulated stochastic approximation annealing algorithm that capitalizes on two techniques, allowing the algorithm to efficiently arrive at optimal results. For the first time, scientists combined precipitation rates and types from two observation sources to calculate convective precipitation ratios and compared them with simulations in CAM5. They also analyzed the sensitivity of precipitation and circulation to key parameters in the model to assess the impact of these improved simulations on global circulation and climate modeling.

Yang B, Y Qian, G Lin, LR Leung, PJ Rasch, GJ Zhang, SA McFarlane, C Zhao, Y Zhang, H Wang, M Wang, and X Liu. 2013. "Uncertainty Quantification and Parameter Tuning in the CAM5 Zhang-McFarlane Convection Scheme and Impact of Improved Convection on the Global Circulation and Climate." *Journal of Geophysical Research-Atmospheres* 118:395-415. DOI: 10.1029/2012JD018213.

Sponsors: DOE Biological and Environmental Research and Advanced Scientific Computing Research

Better Chemistry Through Computing

While massively parallel computers can intricately simulate complex physical motions of atoms and molecules, currently accessible time scales limit how well structural equations evolve to demonstrate more realistic chemical phenomena. To calculate atomic forces in areas such as aerosol chemistry and human health more efficiently, scientists from EMSL; University of Chicago; and University of California, San Diego developed and assessed parallel in time algorithms, where forward integration of Newton equations is distributed over many processors and applied to atomic-level molecular dynamics (MD) or ab initio molecular dynamics (AIMD) simulations. Similar in size and complexity to actual materials chemistry problems, they tested a 1,000 silicon atom liquid MD and an $HCl+4H_2O$ AIMD simulation. For the parallelized MD simulation, the algorithm achieved a maximum speedup of 3.0, while the AIMD demonstrated speedups up to 14.3. In both cases, the speedups occurred across slow networks, indicating these algorithms can be used for long time dynamics AIMD simulations with machines connected via WiFi or the Internet. Moreover, these timings afford meaningful—and real-world applicable—dynamic simulations at a modest cost.

Bylaska EJ, JQ Weare, and JH Weare. 2013. "Extending Molecular Simulation Time Scales: Parallel in Time Integrations for High-Level Quantum Chemistry and Complex Force Representations." *Journal of Chemical Physics.* Accepted.

Sponsors: DOE Offices of Advanced Scientific Computing Research, Basic Energy Sciences, Biological and Environmental Research

The Most Scalable Work Distribution Strategies

Persistence-based load balancers and work-stealing algorithms quickly balance work distribution among millions of computer processor cores.

Balancing work among the millions of processor cores found in supercomputers is an extremely challenging and time-consuming procedure. However, scientists receive the fastest results when all processors are fully automated and effectively used. Researchers from PNNL and the University of Illinois at Urbana-Champaign found that persistence-based load balancers and work-stealing algorithms improve the efficiency of problem solving by actively finding and redistributing work. Persistence-based load balancers continually check for optimum routes processors can use to complete a given set of tasks, redistributing work based on measured performance profiles from previous iterations. In work stealing, calculations are automatically balanced across processors by having idle processors grab work units from other busy processors. Used in combination or as an alternative to persistence-based load balancing, work stealing is a viable alternative for applications with severe workload imbalances that need correcting or cannot be easily profiled. Using a coupled-cluster quantum chemistry application, scientists demonstrated this approach was effective in achieving reduced time-to-solution on several leadership-class supercomputing systems.

Lifflander J, S Krishnamoorthy, and L Kale. 2012. "Work Stealing and Persistence-Based Load Balancers for Iterative Overdecomposed Applications." In: *Proceedings of the 21st International Symposium on High-Performance Parallel and Distributed Computing (HPDC '12)*, pp. 137-148. ACM, New York. DOI: 10.1145/2287076.2287103.

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

Mesoscale Simulations See into Sickle Cells

Using a systematic, dissipative particle dynamics-based (a stochastic simulation technique for complex fluids) simulation study of individual sickle red blood cells (SS-RBCs) in shear flow, scientists from Princeton and Brown universities and PNNL examined the biophysical characteristics surrounding vasoocclusion crisis, vascular blockage that occurs when sickle-shaped cells obstruct circulation, which primarily affects people with sickle cell anemia. In mesoscopic simulations of postcapillary SS-RBC flow, they identified cell groups and the respective adhesion strengths that led to full or transient occlusion states. In this study, blood occlusion occurred mainly in postcapillaries with diameters smaller than 12–14 μm, which agreed with other experimental results. Under inflammation-stimulated conditions, the scientists documented how adherent white blood cells can trap SS-RBCs and lead to vasoocclusion in venular (small vein) flow, especially in larger vessels. These simulations also revealed and quantified the multi-interactional and multistage nature of vasoocclusion, which can inform processes to generate effective biomarkers and therapeutic treatments for sickle cell anemia. Moreover, the resulting computational framework can be paired with microfluidic experiments for future clinical research.

Lei H and GE Karniadakis. 2013. "Probing Vasoocclusion Phenomena in Sickle Cell Anemia via Mesoscopic Simulations." *Proceedings of the National Academy of Sciences of the United States of America* 110(28):11326-11330. DOI: 10.1073/pnas.1221297110.

Sponsor: National Institutes of Health

Energy-Efficient Computing at the Exascale

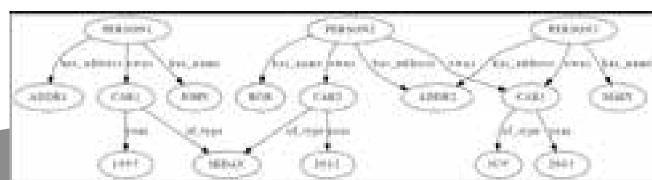
PNNL is at the forefront of energy-efficient computing research, exploring energy and power efficiency aspects affecting next-generation exascale (10^{18} operations/sec) supercomputers. To identify opportunities for power savings under DOE Exascale Co-Design Center workloads, PNNL scientists have developed an accurate sensor model that estimates the active power of each computer core by inspecting its activity. This enables scientists to develop power-aware algorithms and characterize applications to identify power-savings.

Because data movement is a major limitation in achieving power and energy efficiency, they modeled the energy cost of moving data across the memory hierarchy of current systems and for scientific applications. They answered questions, such as the amount of energy spent in data movement with respect to an application's total energy consumption, and identified dominant components of data movement energy for current and future parallel applications.

Kestor G, R Gioiosa, DJ Kerbyson, and A Hoisie. 2013. "Enabling Accurate Power Profiling of HPC Applications on Exascale Systems." In *Proceedings of the 3rd International Workshop on Runtime and Operating Systems for Supercomputers*, pp. 4:1-4:8. Association for Computing Machinery, ACM, New York. DOI: 10.1145/2491661.2481429.

Kestor G, R Gioiosa, DJ Kerbyson, and A Hoisie. 2013. "Quantifying the Energy Cost of Data Movement in Scientific Applications." (Best paper candidate.) In *Proceedings of the IEEE International Symposium on Workload Characterization* (In Press).

Sponsor: DOE Advanced Scientific Computing Research



An example semantic graph structure. These graphs have labels on the edges and nodes and can scale with enormous data sizes.

Discovering Knowledge in Semantic, Web-Scale Datasets

Data collection and analysis of web-scale semantic data is rapidly changing the way scientific, national security, and business communities operate. Using current database systems, based on the relational data model, to discover complex semantic relationships is especially difficult as the systems are not designed to support subgraph isomorphism, typed path traversal, and community detection. In response to these analytic challenges, PNNL researchers developed Semantic Graph Engine Multithreaded, or SGEM. The framework has three components: 1) a SPARQL (query language for databases) front end to transform SPARQL to data parallel C code; 2) a semantic graph engine with scalable multithreaded algorithms for query processing; and 3) a custom multithreaded runtime layer for scalable performance on conventional cluster systems. The platform scales with data sizes and maintains query throughput as system size grows by running on conventional clusters with large memory nodes, maintaining all data in memory, using multithreading to hide memory latencies, and aggressively aggregating memory requests to maximize system bandwidth.

Castellana VG, A Tumeo, O Villa, D Haglin, and J Feo. 2013. "Composing Data Parallel Code for a SPARQL Graph Engine." In: *2013 ASE/IEEE International Conference on Big Data*, September 8-14, 2013, Washington D.C., In press.

Sponsor: PNNL Center for Adaptive Supercomputing Software

Scientists are studying the mineral/biological associations in the rhizosphere to better understand the role of the soil microbes in the soil-mineral weathering process. Pictured here are conidia (spores) of *Penicillium* sp., a ubiquitous soil fungus that lives mainly on organic biodegradable substances. The spores were imaged using instrumentation at EMSL.

EMSL, the Environmental Molecular Sciences Laboratory, is a national scientific user facility sponsored by DOE's Office of Science and located at PNNL. EMSL provides an open, collaborative environment for scientific advances in biosystems design, terrestrial and subsurface ecosystems, energy materials and processes, and atmospheric aerosol research. Integration of theory and experiment requires advancement of new technologies that enable EMSL's user community to discover novel insights and approaches relevant to the missions of the Office of Biological and Environmental Research and DOE.

Getting to the "Root" of Symbiosis

Because of their extensive genomes, it's difficult to use conventional proteomics technologies to get meaningful information from plants. However, the complete genome available for soybean root hairs provides an excellent model for examining single-cell systems biology. Using EMSL's highly sensitive proteomics tools, scientists analyzed the processes involved when soybean root hair systems become infected by rhizobia—symbiotic, nitrogen-fixing soil bacteria. They provide water and nutrient uptake from the soil but are also the dominant rhizobia infection site. The root hairs were monitored for changes over 72 hours. Nine time points were analyzed separately then combined to establish the reference proteome map, cataloging more than 5,700 proteins involved in cell functionality. The scientists also labeled peptides to track how the cell permitted rhizobia infection. The infected area forms a nodule where bacteria fix nitrogen for the host, acting as built-in fertilizer. Comprehensive understanding of symbiosis could help in redesigning plants and improving crop yields, benefitting food and biofuel production.

Brechenmacher L, THN Nguyen, K Hixson, M Libault, JT Aldrich, L Pasa-Tolic, and G Stacey. 2012. "Identification of Soybean Proteins from a Single Cell Type: The Root Hair." *Proteomics* 12(22):3365-3373. DOI: 10.1002/pmic.201200160.

Nguyen THN, L Brechenmacher, J Aldrich, T Clauss, M Gritsenko, K Hixson, M Libault, K Tanaka, F Yang, Q Yao, L Pasa-Tolic, D Xu, HT Nguyen, and G Stacey. 2012. "Quantitative Phosphoproteomic Analysis of Soybean Root Hairs Inoculated with *Bradyrhizobium japonicum." Molecular and Cellular Proteomics* 11(11):1140-1155. DOI: 10.1074/mcp.M112.018028.

Sponsors: United Soybean Board, National Science Foundation, DOE Office of Biological and Environmental Research

Participants: University of Missouri National Center for Soybean Biotechnology, Biochemistry Division, and C.S. Bond Life Sciences Center; EMSL; Vietnam Education Foundation; PNNL; University of Oklahoma Botany and Microbiology Department

Predictive Biogeochemistry Models More Accurate, Scalable

Predictive models of biogeochemical interactions in soils are more accurate and scalable—from the pore scale to the field scale—if they consider the reaction chemistry that occurs in distinct soil pore structures, or domains, according to a team of EMSL scientists and users. The team conducted integrated computational and experimental pore-scale reaction kinetics studies. They built a silicon micromodel with a pore-scale structure mimicking that found in nature and coated it with a thin film of hematite (Fe_2O_3), then injected reduced flavin mononucleotide ($FMNH_2$), a form of vitamin B2 and effective electron transfer agent, and studied Fe_2O_3 dissolution by $FMNH_2$ both in situ and in real time. Hematite reaction kinetics were distinctly different in three domains: an advection domain where fluid flows with relative freedom, a macropore domain where diffusion dominates but that is well connected to the advection domain, and a micropore domain where fluid is stagnant and resides in soil aggregates. Predictive models accounting for these domains will be more effective at predicting the environmental impact of geochemical and microbial activities in soil and can help design improved remediation strategies.

Zhang C, C Liu, and Z Shi. 2013. "Micromodel Investigation of Transport Effect on the Kinetics of Reductive Dissolution of Hematite." *Environmental Science & Technology* 47(9):4131-4139. DOI: 10.1021/es304006w.

Sponsor: DOE Office of Biological and Environmental Research

Participants: EMSL, PNNL

Biofilms move electrons surprisingly long distances across two distinct layers.

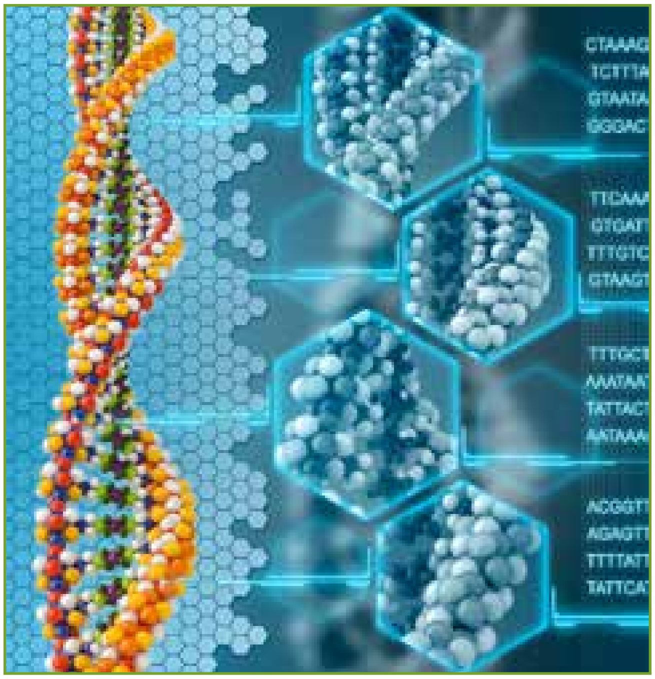
Biofilms Move Electrons Long Distances

Bacteria can move electrons at least half a millimeter across a scaffolding made by themselves, of themselves. This new finding challenges the conventional belief that electrical resistance within biofilms would restrict long-range electron transfer, and offers new insight into bacteria-metal electron exchange. Researchers used *Geobacter sulfurreducens* and a novel electrochemical-nuclear magnetic resonance microimaging system, designed and built by EMSL staff and users, that makes it possible for the first time to conduct simultaneous electrochemical and NMR studies on biofilms. They showed that *Geobacter* biofilms have a top layer of metabolically active bacteria sitting on an inactive layer. The inactive layer provides a bioscaffold on which electrons flow from the biofilm top to the electrode surface on which the biofilm grew. This finding will influence design of bioelectrochemical systems for producing hydrogen or enhancing wastewater treatment methods, while simultaneously generating electricity; improve predictive models of electron transfer, and provide better understanding of biofilm behavior and roles in the environment.

Renslow RS, JT Babauta, A Dohnalkova, MI Boyanov, KM Kemner, PD Majors, JK Fredrickson, and H Beyenal. 2013. "Metabolic Spatial Variability in Electrode-Respiring *Geobacter sulfurreducens* Biofilms." *Energy and Environmental Science* 6(6):1827-1836. DOI: 10.1039/C3EE40203G.

Sponsors: U.S. Office of Naval Research, DOE Office of Biological and Environmental Research

Participants: Washington State University, EMSL, Argonne National Laboratory, PNNL



EMSL contributed to research published in *Science* that expands what is known about bacteria capable of performing bioremediation from handfuls of genes to tens of complete or nearly complete genomes.

New Bacteria, Metabolic Roles at IFRC Site

New bacteria and details about the bacteria's metabolic roles were discovered in microbial communities collected from a subsurface aquifer as part of DOE's Integrated Field Research Challenge (IFRC). Researchers sequenced nearly 150,000 genes from IFRC samples and were able to assign these genes to, or reconstruct the genomes in part or in whole for, 87 different bacterial species, and 49 of the genomes belong to species never before characterized at the genome level. Some of these organisms fell into a new phylogenetic classification named PER, or Peregrine. Proteomics tools at EMSL provided valuable data about the metabolic activity of the bacteria in their native subsurface environment, showing that they may play roles in carbon cycling, sulfur cycling, and hydrogen production. The team's groundbreaking results could lead to improved methods to stimulate bacteria to uptake atmospheric carbon, thus reducing greenhouse gases, and to better apply microbes to remediate toxic metal-contaminated environments.

Wrighton KC, BC Thomas, I Sharon, CS Miller, CJ Castelle, NC VerBerkmoes, MJ Wilkins, RL Hettich, MS Lipton, KH Williams, PE Long, and JF Banfield. 2012. "Fermentation, Hydrogen and Sulfur Metabolism in Multiple Uncultivated Bacterial Phyla." *Science* 337(6102):1661-1665. DOI: 10.1126/science.1224041.

Sponsor: DOE Office of Biological and Environmental Research

Participants: University of California, Berkeley; Lawrence Berkeley National Laboratory; Oak Ridge National Laboratory; PNNL

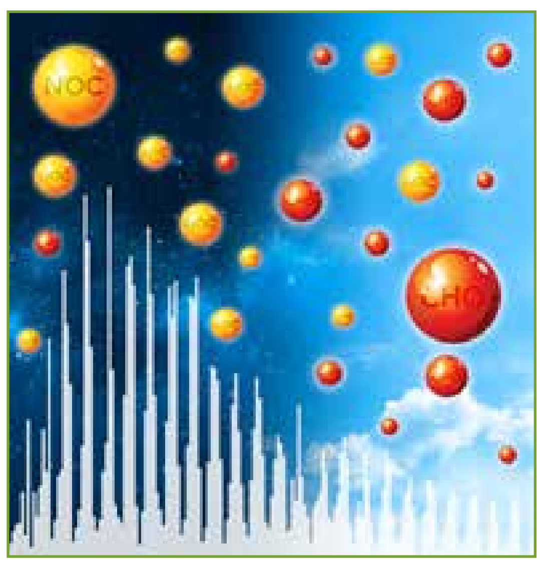
Deciphering Atmospheric Organic Aerosols

Current understanding of molecular composition of atmospheric organic aerosols, or OA, is limited, so their impact on climate change and the environment cannot be accurately predicted and mitigated. To probe the chemical compositional changes that occur in OA during a diurnal cycle and examine the OA species distribution across multiple scales, scientists employed EMSL's nanospray desorption electrospray ionization coupled with high-resolution mass spectrometry capabilities to characterize more than 850 unique molecular species in a Bakersfield, California, study area. The analyses revealed patterns, such as increased nitrogen-containing organic compounds (NOC) in samples taken at night with more OA containing only carbon, hydrogen, and oxygen (CHO) in the afternoon. The NOC showed evidence of being formed by reactions that transform carbonyls (carbon and oxygen compounds) into imines (compounds derived from ammonia). This requires aqueous-phase chemistry of ammonium and organic compounds in liquid-phase particles. The scientists hypothesized ammonium chemistry may be an important pathway for NOC formation in OA. This work provides an alternate technique for investigating OA and offers another step toward clarifying the chemical transformations that determine OA composition.

O'Brien RE, A Laskin, J Laskin, S Liu, R Weber, LM Russell, and AH Goldstein. 2013. "Molecular Characterization of Organic Aerosol Using Nanospray Desorption/Electrospray Ionization Mass Spectrometry: CalNex 2010 field study." *Atmospheric Environment* 68:265-272. DOI: 10.1016/j.atmosenv.2012.11.056.

Sponsors: California Air Resources Board, DOE Office of Biological and Environmental Research, DOE Office of Basic Energy Sciences

Participants: University of California, Berkeley; University of California, San Diego; EMSL; PNNL



Observed nighttime enhancement of NOC showed evidence of being formed by reactions that transform carbonyls into imines, leading scientists to hypothesize that ammonium chemistry may be an important pathway for NOC formation in OA.

SELECTED AWARDS & HONORS

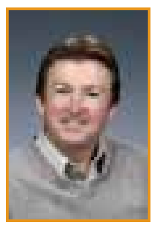
YUEHE LIN

American Institute for Medical and Biological Engineering's College of Fellows

Laboratory Fellow **Yuehe Lin** was named to the American Institute for Medical and Biological Engineering's College of Fellows for his leadership and scientific contributions. Lin's research focuses on developing nanobioelectronic devices and nanomaterials for diagnosis and drug delivery. These technologies could be used for early diagnosis of diseases and for effectively delivering drugs to fight diseases.

NIGEL BROWNING

Microscopy Society of America, AAAS Fellow



Laboratory Fellow **Nigel Browning** was elected as a Fellow of the Microscopy Society of America and the American Association for the Advancement of Science (AAAS) for his advances in scanning transmission electron microscopy, and for developing spatial, temporal and spectroscopic techniques to better understand foundational issues in physical and life sciences. Browning has been pushing the limits of electron microscopy and spectroscopy since the early 1990s, when he applied the new technology to determine the composition of individual planes of atoms.

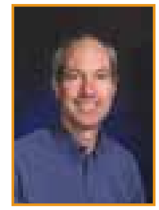
DANIEL CHAVARRÍA

Presenter at 2013 IEEE CCGrid Conference

Computer scientist **Daniel Chavarría**, presented "Scalable PGAS Metadata Management on Extreme Scale Systems" to the 2013 Institute of Electrical and Electronics Engineering (IEEE) and Association for Computing Machinery Cluster, Cloud and Grid Computing Conference. His paper was one of only 57 accepted. Chavarría's presentation described improving computational scalability by reducing metadata space requirements on next-generation trans-petascale systems.

WAYNE HESS, HONGFEI WANG

American Physical Society Fellows



Wayne Hess

Hongfei Wang

Physical chemist **Wayne Hess** and EMSL lead scientist **Hongfei Wang** were named American Physical Society Fellows for outstanding research and seminal contributions in their fields. Hess was recognized for his contributions to understanding the dynamics and reactions of electronically excited crystalline solids and laser desorption of atoms and molecules. Wang was recognized for his exceptional contributions to the physics enterprise, including seminal contributions to the development of surface nonlinear vibrational spectroscopy and to the understanding of molecular interaction and structure at interfaces.

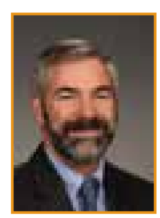
JOHANNES LERCHER

2013 Tanabe Prize for Catalysis

Johannes Lercher, Director of PNNL's Institute for Integrated Catalysis, received the 2013 Tanabe Prize for Acid-Base Catalysis. He was selected for this international award for "his substantial contributions to the field of acid-base catalysis." His research is focused on the fundamentals of catalytic materials and processes and includes research on catalyzed reactions involving fossil fuels and alternative feedstocks such as biomass.

JAMES DE YOREO

Outstanding Materials Science Award



Laboratory Fellow **James De Yoreo** was honored with the 2013 American Association for Crystal Growth Award for his foundational insights into the processes underlying biomineralization and biomolecular assembly. De Yoreo pioneered in situ imaging with atomic force microscopy to understand the growth of crystals, from proteins to bones. His work includes discovering the stereochemical relationship between proteins and crystal structures that allow biological systems to manipulate the energies associated with crystallization and creating a first-of-its-kind model that describes how molecular bonds break when pulled apart, changing the conventional wisdom.

JAMES DOOLEY
Technical Program Committee for GHGT-12

Atmospheric scientist **James Dooley** was invited to serve on the Technical Program Committee for the 12th International Conference on Greenhouse Gas Control Technologies (GHGT-12), the premier international technical conference in the field of carbon dioxide capture and storage. The committee is responsible for organization and programming of all technical sessions for the conference.

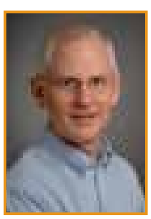
SRIRAM KRISHNAMOORTHY
DOE Early Career Research Award

High-performance computing scientist **Sriram Krishnamoorthy** has been awarded DOE's Early Career Research Program funding. Of 770 applicants, he is one of 61 scientists to receive the award. Krishnamoorthy will pursue "Concrete Ingredients for Flexible Programming Abstractions on Exascale Systems," which will fundamentally transform exascale programming models and runtime systems for scientific applications.

JAE EDMONDS, LIZ MALONE, RICHARD MOSS, RUBY LEUNG
National Leadership in the National Academies

Jae Edmonds

Elizabeth Malone

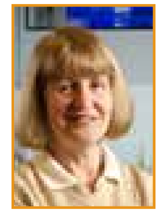


Richard Moss

Ruby Leung

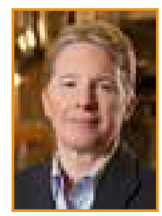
Battelle Fellow **Jae Edmonds**, scientists **Elizabeth Malone** and **Richard Moss**, and Laboratory Fellow **L. Ruby Leung** served on committees for the National Research Council (NRC), contributing national leadership and technical expertise addressing some of the world's most pressing climate change issues. The NRC brings together experts in all areas of science and technology to address critical national issues and inform public and federal government policy. Edmonds and Leung served as members of the study committee that produced the report *A National Strategy for Advancing Climate Modeling*. Malone served on a committee that produced the report *Himalayan Glaciers: Climate Change, Water Resources, and Water Security*. Moss was appointed Chair of the newly established Board on Environmental Change and Society.

KARIN RODLAND
NIH Cancer Biomarkers Study Chair



Karin Rodland, Laboratory Fellow and science lead of National Institutes of Health programs at PNNL was invited to serve as a chairperson of the NIH's Cancer Biomarkers Study Section. Dr. Richard Nakamura, Director of the NIH's Center for Scientific Review, said this of her Rodland's inclusion, "the skill and leadership offered by the chairperson determine to a significant extent the effectiveness and efficiency of the review group. I want to emphasize the importance of Dr. Rodland's participation in assuring the quality of the NIH peer review process."

AAAS FELLOWS
Doug Ray and Allison Campbell



Douglas Ray, Associate Laboratory Director of the Fundamental & Computational Sciences Directorate at PNNL, was inducted as a American Association for the Advancement of Science Fellow for "distinguished contributions to physical chemistry and molecular spectroscopy, and for building a world-class chemistry organization at PNNL." **Allison Campbell**, director of EMSL, a DOE scientific user facility at PNNL, and an Associate Laboratory Director at PNNL, was inducted for her work in the "synthesis of thin films for ceramics and biomaterial development."

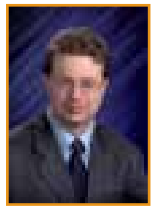
TOXICOLOGISTS
Received Best Paper Award from International Society

A journal article by a team of PNNL toxicologists was selected as the 2012 best paper by the Biological Modeling Specialty Section of the Society of Toxicology from more than 1,000 publications. "Comparative Computational Modeling of Airflows and Vapor Dosimetry in the Respiratory Tracts of Rat, Monkey, and Human" describes development of the first-ever computational fluid dynamic models for upper and lower respiratory airways of a rat, a monkey, and a human. The models will help assess potential risks for exposure to gases and vapors. The authors are **Richard Corley, Dan Einstein, Senthil Kabilan, Andrew Kuprat, James Carson, Kevin Minard, Rick Jacob,** and **Chuck Timchalk**.

ALEX SHVARTSBURG, KEQI TANG

FLC Tech Transfer Award

Scientists **Alex Shvartsburg** and **Keqi Tang** were awarded a 2013 Federal Laboratory Consortium Excellence in Technology Transfer Award for their work on the Next-Generation Microchip Ion Mobility Spectrometer. The dime-sized device accelerates ion mobility spectrometry separations by more than 100 times. The scientists teamed with Owlstone Nanotech to develop these microchips.



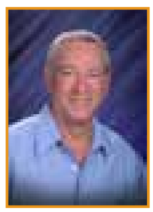
Alex Shvartsburg

Keqi Tang

CHARLES LONG

2012 World Meteorological Organization Väisälä Award

Atmospheric scientist **Charles Long**, together with an international research team, received the 23rd Professor Dr. Vilho Väisälä Award for an Outstanding Research Paper on Instruments and Methods of Observation. "Optimized Fractional Cloudiness Determination from Five Ground-based Remote Sensing Techniques" was published in the *Journal of Geophysical Research*. Long is the only two-time winner of this international award to date.



NOVEL INTEGRATION

of Mass Spectrometry Techniques Wins R&D 100 Award

An instrument that quickly and effectively analyzes complex biological and environmental samples is one of 2012's 100 most significant scientific and technological products or advances. The Combined Orthogonal Mobility & Mass Evaluation Technology (CoMet), developed at PNNL in EMSL, won an R&D 100 Award from *R&D Magazine*. CoMet separates and identifies specific molecules in complex biological and environmental samples, integrating two complementary analysis techniques—multiplexed ion mobility spectrometry and ultrafast quadrupole time-of-flight mass spectrometry—within a single instrument. The PNNL developers are **Dick Smith, Gordon Anderson, Erin Baker, Kevin Crowell, William Danielson III, Yehia Ibrahim, Brian LaMarche, Matthew Monroe, Ronald Moore, Randolph Norheim, Daniel Orton, Alex Shvartsburg, Gordon Slysz,** and **Keqi Tang**.

STEVEN GHAN

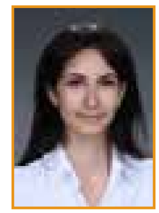
Editor-in-Chief for JGR-Atmospheres

Laboratory Fellow **Steven Ghan** was appointed Editor-in-Chief of the Atmospheres section of the *Journal of Geophysical Research*. He was appointed by the American Geophysical Union's Council to lead the journal's editorial direction for the next 4 years.

MARIA VLACHOPOULOU

IEEE's "New Face of Engineering"

Computer engineer **Maria Vlachopoulou** was named the New Face of Engineering by IEEE, given for contributions of engineers age 30 or younger, for her breakthrough research in computer algorithms and mathematical models supporting the transition of the U.S. power grid to a more secure, efficient, and robust system. She also works with high school and middle school students to generate interest in science, technology, engineering and mathematics careers.



DARREN KERBYSON, SRIRAM KRISHNAMOORTHY

INCITE Award

Computer scientists **Darren Kerbyson** and **Sriram Krishnamoorthy** were awarded time on the leadership-class computing systems of the DOE Office of Science through the Innovative and Novel Computational Impact on Theory and Experiment (INCITE) Awards. The program awards time with this special class of computing systems to execute grand challenge research that could not otherwise be performed. Kerbyson, a coinvestigator on the "Performance Evaluation and Analysis Consortium (PEAC) End Station" was awarded 85 million core hours on three supercomputers to focus on computer science research on performance analysis, optimization, and modeling of extreme-scale systems. Krishnamoorthy is a co-investigator on the "Developing and Testing Future Application and Operating Systems for Exascale" project. He was awarded 50 million core hours on two supercomputers to focus on designing task-based programming models for dynamic load-balancing and fault tolerance.

Darren Kerbyson

Sriram Krishnamoorthy

CHUN ZHAO

Guest Editor of *Aeolian Research*

Atmospheric scientist **Chun Zhao** was guest editor of a special issue of *Aeolian Research* focused on contributions in mineral-dust properties, the dust cycle, and effects of dust on Earth systems. He was chosen for his extensive experience in development and application of regional and global models to investigate challenging issues in modeling aerosols and their effects on the climate.

MORRIS BULLOCK

Royal Society of Chemistry Award

Morris Bullock, Director of the Center for Molecular Electrocatalysis, a DOE Energy Frontier Research Center led by PNNL, received the biannual Royal Society of Chemistry's Homogeneous Catalysis Award. Bullock was recognized for his "seminal work on transition metal hydrides, his pioneering use of inexpensive metals for homogeneous catalysis and the development of a new programme on molecular electrocatalysis."

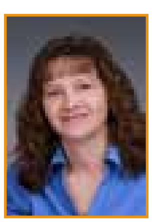
KEQI TANG

Battelle Distinguished Inventor

Scientist **Keqi Tang** has been named a Battelle Distinguished Inventor, an annual award given to Battelle staff who have 14 or more U.S. patents to their credit. Tang has been granted 17 U.S. patents and 4 foreign patents for methods, instruments, and devices in the fields of microfluidics and mass spectrometry. He joins more than 60 inventors from the Battelle-managed labs, 21 of which have been from PNNL, in receiving this honor.

KATRINA WATERS

National EPA Advisory Panel



Katrina Waters, computational biologist and bioinformaticist, was invited to participate in the Environmental Protection Agency Scientific Advisory Panel. The panel, convened under the Safe Drinking Water Act, will discuss and make recommendations on how to prioritize the listing of chemicals that have the highest potential to interact with the human estrogen receptor system.

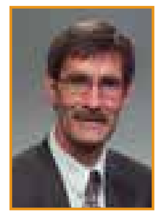
DICK SMITH

Distinguished Contribution in Mass Spectrometry

Director of proteomics **Richard (Dick) D. Smith** received the 2013 Award for a Distinguished Contribution to Mass Spectrometry from the American Society for Mass Spectrometry. He was selected for the development of the electrodynamic ion funnel, designed for ion focusing and manipulation at elevated pressures. Originally created in 1997, the ion funnel has been adapted and modified for a range of applications, including enabling application in ion mobility spectrometry and new mass spectrometer ion sources.

MARK ENGELHARD

American Vacuum Society Fellow



The American Vacuum Society (AVS) Science and Technology Society has named **Mark Engelhard** a Fellow, the society's premier membership recognition, for "sustained creative application and novel adaptation of surface analytical tools to address a wide range of energy and environmental problems and for service to the surface analysis community." Since 1978, Engelhard, an EMSL senior research scientist specializing in interface spectroscopy and diffraction, has used surface-sensitive techniques to study surface and interphase chemistry.

DAVE KOPPENAAL

American Chemical Society Fellow

Dave Koppenaal, chief technology officer for EMSL, has been selected for the rank of Fellow in the American Chemical Society for his "outstanding achievements in and contributions to science and the profession of chemistry." He is responsible for directing the development and scientific application of new, transformational instruments and tools for EMSL. His research has focused on low-level, ultra-trace detection and analysis of metals and radionuclides for environmental or nonproliferation purposes.

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 4,400 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.

For more information, contact:

Douglas Ray, Ph.D.
Associate Laboratory Director
Fundamental & Computational Sciences
Pacific Northwest National Laboratory
P.O. Box 999, MSIN K9-80
Richland, WA 99352
509-375-2500
doug.ray@pnnl.gov

Allison A. Campbell, Ph.D.
Associate Laboratory Director
EMSL
Pacific Northwest National Laboratory
P.O. Box 999, MSIN K8-84
Richland, WA 99352
509-371-6000
allison.campbell@pnnl.gov

Charlette A. Geffen, Ph.D.
Director, Atmospheric Sciences & Global Change Division
Laboratory Research Manager for Climate & Earth Systems Sciences
509-375-3646
ca.geffen@pnnl.gov

Jim K. Fredrickson, Ph.D.
Interim Director, Biological Sciences Division
Laboratory Research Manager for Biological Systems Sciences
509-371-6943
jim.fredrickson@pnnl.gov

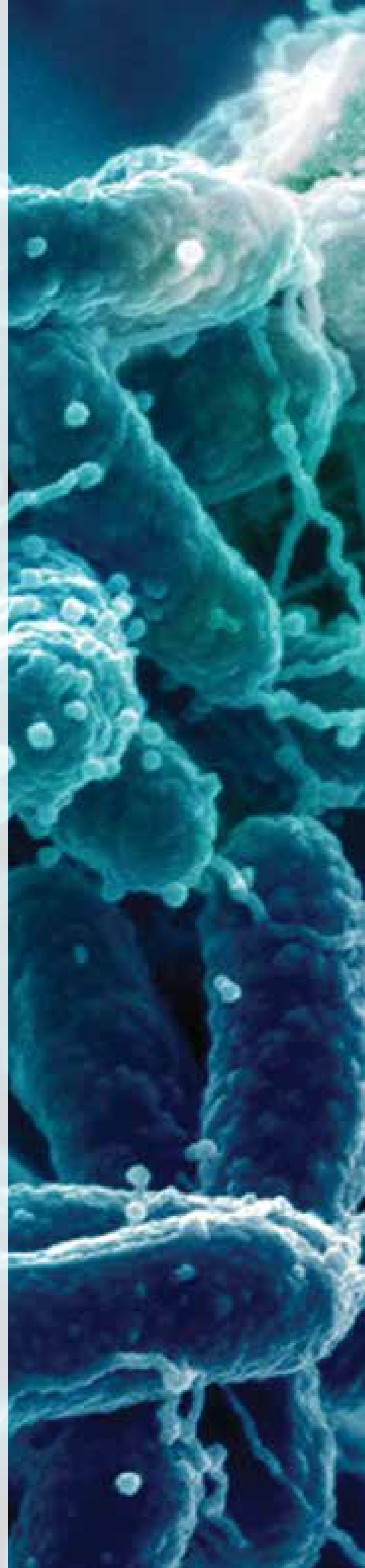
Louis Terminello, Ph.D.
Chief Scientist
Laboratory Research Manager for Chemical Imaging and Materials Sciences
509-371-6790
louis.terminello@pnnl.gov

Bruce C. Garrett, Ph.D.
Director, Physical Sciences Division
Laboratory Research Manager for Chemistry and Geochemistry
509-372-6344
bruce.garrett@pnnl.gov

Adolfy Hoisie, Ph.D.
Laboratory Fellow
Laboratory Research Manager for Advanced Computing
509-372-4957
adolfy.hoisie@pnnl.gov

David M. Asner, Ph.D.
Laboratory Fellow
Laboratory Research Manager for Particle Physics
509-375-1689
david.asner@pnnl.gov

Richard T. Kouzes, Ph.D.
Laboratory Fellow
Laboratory Research Manager for Nuclear Physics
509-372-4858
rkouzes@pnnl.gov



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PNNL-SA-97879 | August 2013