Pacific Northwest
NATIONAL LABORATORY

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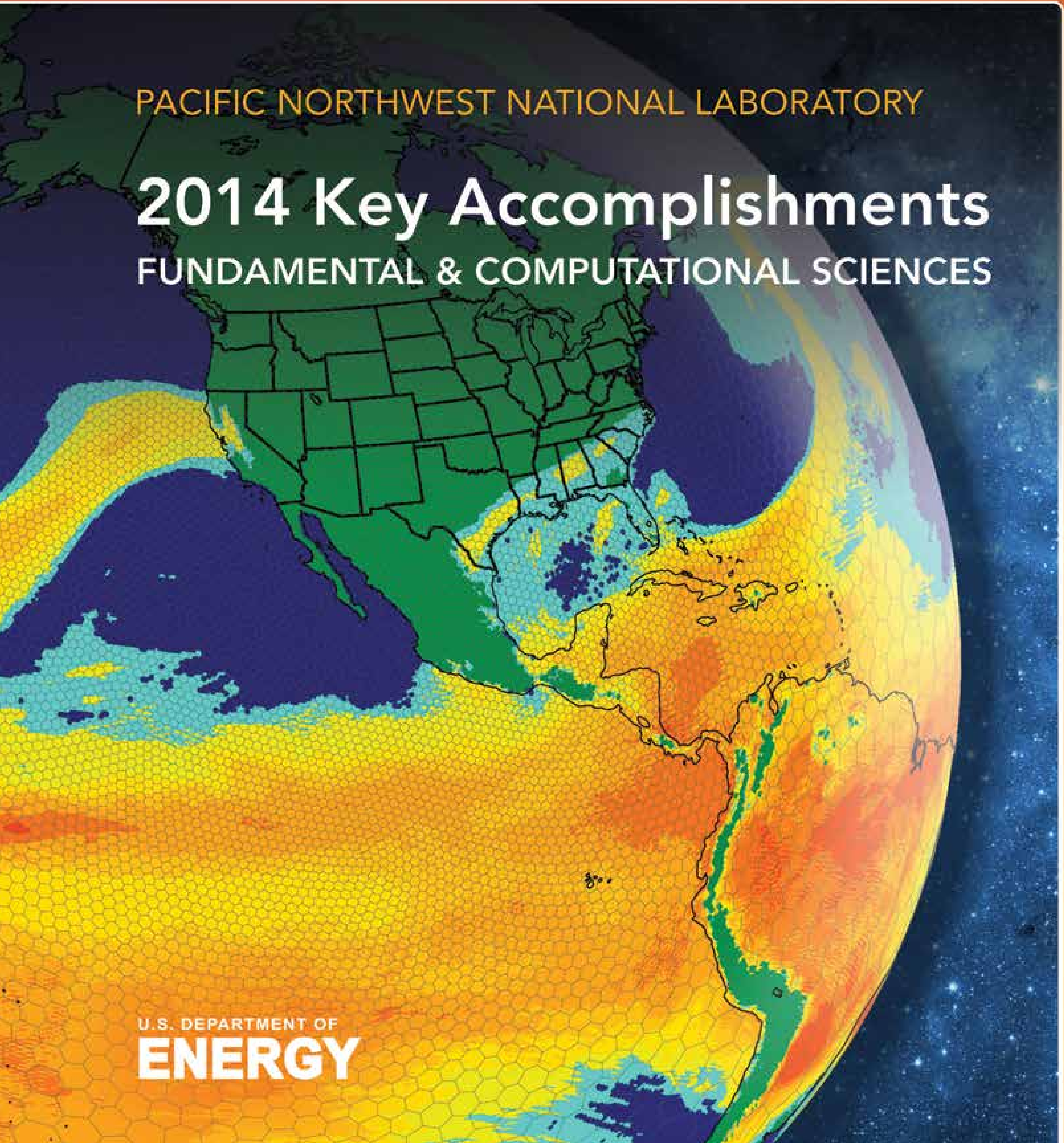
PACIFIC NORTHWEST NATIONAL LABORATORY

2014 Key Accomplishments

FUNDAMENTAL & COMPUTATIONAL SCIENCES



U.S. DEPARTMENT OF
ENERGY

DISCOVE

Cover image: Atmospheric rivers are long and concentrated bands of water vapor originating from the tropics that often result in precipitation extremes and flooding when they hit land. Pictured is a model representation of vertically integrated water vapor at a resolution of 30 kilometers simulated by the Community Atmosphere Model with capability for quasi-uniform and variable resolution modeling. It clearly shows an atmospheric river heading for the U.S. West Coast, transporting abundant moisture from the tropics. In a typical winter, a few atmospheric rivers account for 30–50% of the annual precipitation in California. With accurate modeling of atmospheric rivers, scientists can improve understanding and predictions of climate changes that affect specific regions of the globe.

RY *in Action*

In these pages you will find a selection of the most noteworthy scientific achievements by Pacific Northwest National Laboratory scientists in 2014. We're proud of their impact on science and on some of the most important challenges in energy, security, health and environmental sustainability.

Some of our most important research this past year used unique modeling and simulation approaches to understand and predict the behavior of complex systems, such as the performance of next-generation exascale computing systems, the impact of increased natural gas use on global carbon emissions and the microscopic principles of materials synthesis in solution. We also made notable progress toward a mechanistic understanding of microbial ecology and a multi-scale understanding of how the respiratory system interacts with exogenous chemicals, and the impacts of disease on those interactions—in part via development and use of new computational and imaging approaches.

Molecular-level discoveries were the focus at EMSL, the Environmental Molecular Sciences Laboratory, and the nearly 800 scientists with whom it collaborates each year. In the past year, EMSL strengthened its alignment with the mission of the Department of Energy's (DOE's) Office of Biological and Environmental Research with renewed focus on atmospheric aerosol systems, biosystem dynamics and design, energy materials and processes, and terrestrial and subsurface ecosystems. We continued to advance the power of genomics and molecular characterization with a second collaborative science call for proposals with the DOE Joint Genome Institute. In FY15, we'll launch the 12 resulting projects with collaborators around the nation.

Our technical leadership of another DOE scientific user facility, the Atmospheric Radiation Measurement Climate Research Facility, is advancing knowledge of the atmospheric dynamics driving Earth's climate system. In the last year, ARM enabled PNNL scientists to understand how pollution affects storm clouds, to predict the amount of Earth warming in the coming decades, and to understand the complex factors that impact precipitation and mountain snowpack. In 2014, ARM also began a major shift in operations by closing tropical sites to redistribute instrumentation among the Great Plains and Arctic sites to create data sets to support large eddy simulation modeling.

Please take a few minutes to explore this brochure in more detail to learn about the scientific impact PNNL scientists have made in 2014 in the fields of advanced computing, biological systems science, chemical imaging, chemistry and geochemistry, climate and earth systems science, materials science, 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 brochure.

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

Allison A. Campbell, Ph.D.
Associate Laboratory Director
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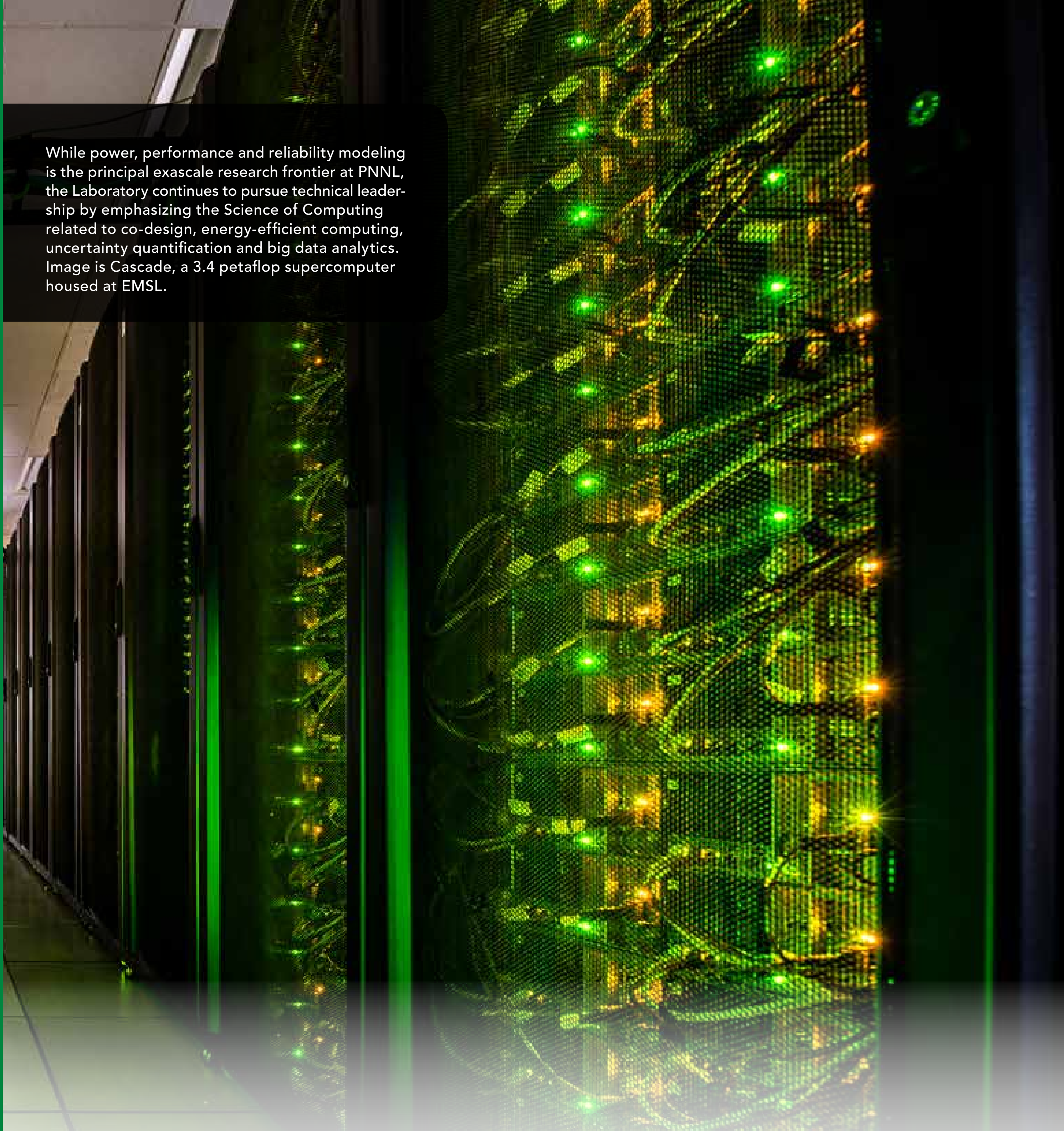


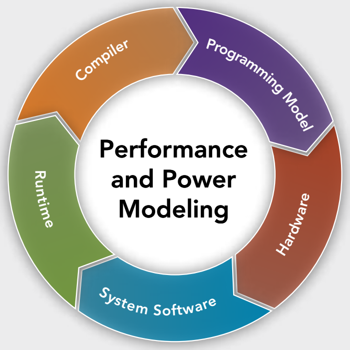
While power, performance and reliability modeling is the principal exascale research frontier at PNNL, the Laboratory continues to pursue technical leadership by emphasizing the Science of Computing related to co-design, energy-efficient computing, uncertainty quantification and big data analytics. Image is Cascade, a 3.4 petaflop supercomputer housed at EMSL.

PNNL's advanced computing research focuses on expanding the national laboratory's computational capabilities and establishing the Laboratory as a national-level computing powerhouse. While this means continuing to provide multifaceted solutions that address significant problems of national interest, it also includes demonstrating a long-term commitment to enhancing the Science of Computing by tackling key strategic computational problems and significantly increasing our computing capabilities. Science of Computing is a leadership direction that will make major contributions toward a foremost grand-challenge scientific goal: achieving high-performance, power-efficient and reliable computing at extreme scales for a spectrum of scientific endeavors.

Advanced computing is multidisciplinary and capability-based, built on technical pillars of high-performance computing, data science and computational mathematics. This approach encompasses broad applications of expertise in computing toward scientific breakthroughs affecting all of PNNL's core pursuits—energy, the environment, national security and fundamental science.

Powering Performance at the Exascale

The Performance and Architecture Laboratory, or PAL, at PNNL takes on power and energy problems affecting high-performance computing. These issues may impact achieving practical performance at the extreme scale of computing. For researchers, it is critical to understand the power consumption by a system at any given time. Thus, building self-aware, self-adaptive computing software that manages changing power characteristics is essential. PAL scientists have developed power-aware algorithms that use an accurate per-core proxy power sensor model to estimate the active power of each processing core. The new methods have afforded the first workload-specific quantitative power modeling capability that accurately captures workload phases, their impact on power consumption and the effects of system architecture and processor clock speeds. These methods assure next-generation supercomputers will have the power and energy efficiencies required to deliver practical and sustainable exaflop performance.



PNNL's Performance and Architecture Laboratory develops an integrated approach to co-design of the hardware-software stack through integrated performance and power modeling.

Hoisie A, K Barker, R Gioiosa, DJ Kerbyson, G Kestor, J Manzano, A Marquez, S Song, N Tallent, A Tumeo and A Vishnu. 2013. "Tackling the Power and Energy Wall for Future HPC Systems, Performance and Architecture Lab (PAL) at PNNL: A Perspective from the Pacific Northwest National Laboratory." *HPCwire* December 17, 2013.

Sponsors: DOE Office of Science, Office of Advanced Scientific Computing Research, Defense Advanced Research Projects Agency, PNNL Laboratory Directed Research and Development

Palm: Making Application Modeling Easier

Application performance modeling is an important methodology for diagnosing performance-limiting resources, optimizing application and system performance and designing large-scale machines. However, because creating analytical models can be difficult and time-consuming, application developers often forgo the insight that these models can provide. To simplify things, computer scientists at PNNL developed the Performance and Architecture Lab Modeling tool, or Palm. Palm constructs a model by automating common modeling tasks and providing a mechanism for modelers to incorporate human insight. With Palm, reproducing a model is straightforward. Given the same input, Palm generates the same model. Meanwhile, the modeling language divides the modeling task into sub problems and formally links an application's source code with its model. This link makes defining rules for generating models according to source code organization possible. Palm represents a first step toward enabling the open distribution and cross-team validation of models.

Tallent NR and A Hoisie. 2014. "Palm: Easing the Burden of Analytical Performance." In *ICS'14 Proceedings of the 28th ACM International Conference on Supercomputing*, pp. 221-230. Association for Computing Machinery, New York, N.Y. DOI: 10.1145/2597652.2597683.

Sponsor: DOE Office of Science, Office of Advanced Scientific Computing Research

Simplifying Exascale Application Development

Hiding the complexities that underpin exascale system operations from application developers is a critical challenge facing teams designing next-generation supercomputers. One way that computer scientists at PNNL are attacking the problem is by developing formal design processes based on Concurrent Collections (CnC), a programming model that combines task and data parallelism. Using these processes, scientists have transformed the Livermore Unstructured Lagrangian Explicit Shock Hydrodynamics (LULESH) proxy application code that models the motion of materials relative to each other when subjected to forces into a complete CnC specification. Systems that capture data and control dependencies, as well as separate computations from implementation issues, can hide the complexities of exascale systems. These processes will dramatically decrease development costs and increase opportunities for automatic performance optimizations.

"The formalization of scientific applications as graphs is extremely important and enlightening. In addition to providing a natural and obvious pathway for application development, we identified communications and optimization issues that could be addressed with added clarity before the computation steps were even implemented."

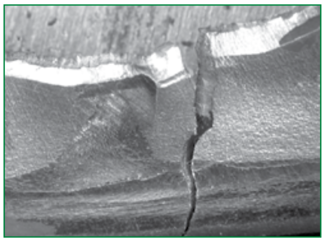
—Dr. John Feo, Director, PNNL Center for Adaptive Supercomputing Software

Sponsors: DOE Office of Science, Office of Advanced Scientific Computing Research, Department of Defense, National Science Foundation

ADVANCED COMPUTING

Automotive Body Building

To achieve higher fuel efficiency standards, car manufacturers consistently seek to use advanced lightweight materials to build their vehicles. As part of ongoing work with Ford Motor Company, PNNL scientists have developed a new integrated manufacturing process simulation framework that offers an enhanced understanding of what occurs as aluminum alloy sheets, a quality material primarily used for automotive paneling, undergo shearing or trimming in preparation for the subsequent forming process. These simulations show how manufacturing processes influence material failures by providing a more complete picture of tensile failure behaviors of previously trimmed edges. Under various trimming conditions, the manufacturing process simulation predicted that tensile stretchability decreased with increased trimming clearances. The ability to predict what aspects of the trimming process contribute to edge fractures in automotive materials could generate lighter, more durable alloy sheets and further improve automobile fabrication. The method also can examine the tensile stretchability of other materials, such as steel sheets.



The ability to predict what aspects of the aluminum alloy sheet trimming process contribute to edge fractures could generate lighter, more durable material and further improve automobile fabrication.

"Our goal with this work is to develop an integrated modeling framework for predicting tensile stretchability by considering multiple factors, most important the manufacturing history the sheet has gone through. We want to be able to identify the key factors that are detrimental to trimmed edge stretchability and provide practical solutions to mitigate edge fracture in production."

—Dr. Xin Sun, PNNL Laboratory Fellow

Hu XH, X Sun and SF Golovashchenko. 2014. "Predicting Tensile Stretchability of Trimmed AA6111-T4 Sheets." *Computational Materials Science* 85:409-419. DOI: 10.1016/j.commatsci.2014.01.015.

Sponsor: DOE Office of Energy Efficiency and Renewable Energy

Inverse Modeling of X-Ray Imaging to Combat Nuclear Materials Trafficking

As an ongoing effort to curtail illicit trafficking of nuclear materials, scientists from PNNL and the University of Texas at Austin studied inverse modeling of spectral X-ray radiography to determine the presence of nuclear materials in small containers. Researchers applied an inversion algorithm to synthetic radiographs of objects composed of layers of plutonium, cotton, steel, lead, aluminum and copper to estimate the quantities of these materials within the layers. Their work showed that coupling the algorithm with current-generation commercial detectors has the potential to distinguish small quantities of nuclear materials, such as nuclear material stowed within airline passenger luggage. Extending existing imaging technology to detect small amounts of plutonium or highly enriched uranium hidden in composite objects could provide a major advance in combating the threat of nuclear materials trafficking.

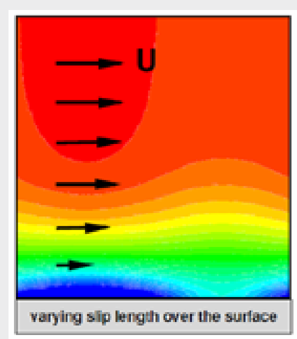
Gilbert AJ, BS McDonald, SM Robinson, KD Jarman, TA White and MR Deinert. 2014. "Non-Invasive Material Discrimination Using Spectral X-Ray Radiography." *Journal of Applied Physics* 115(15):154901. DOI: 10.1063/1.4870043.

Sponsor: National Nuclear Security Administration

Surpassing Boundaries in Fluid Dynamics

To improve the numerical methods and algorithms used to analyze and model physical phenomena associated with fluid flows and the forces that affect them at various scales and boundary conditions, scientists from PNNL and the University of South Florida demonstrated the viability of a new method: smoothed particle hydrodynamics-continuous boundary force (SPH-CBF). Their novel method solves Navier-Stokes equations (used to describe fluid motion) subjected to Robin boundary conditions using an SPH method for solving partial differential equations, providing a significant advancement to existing SPH theory.

The formulation also uses SPH strengths in modeling diverse physics problems, such as those involving atmospheric systems, energy materials and processes, subsurface flow and transport and high-strength materials, which are relevant to important DOE mission objectives.

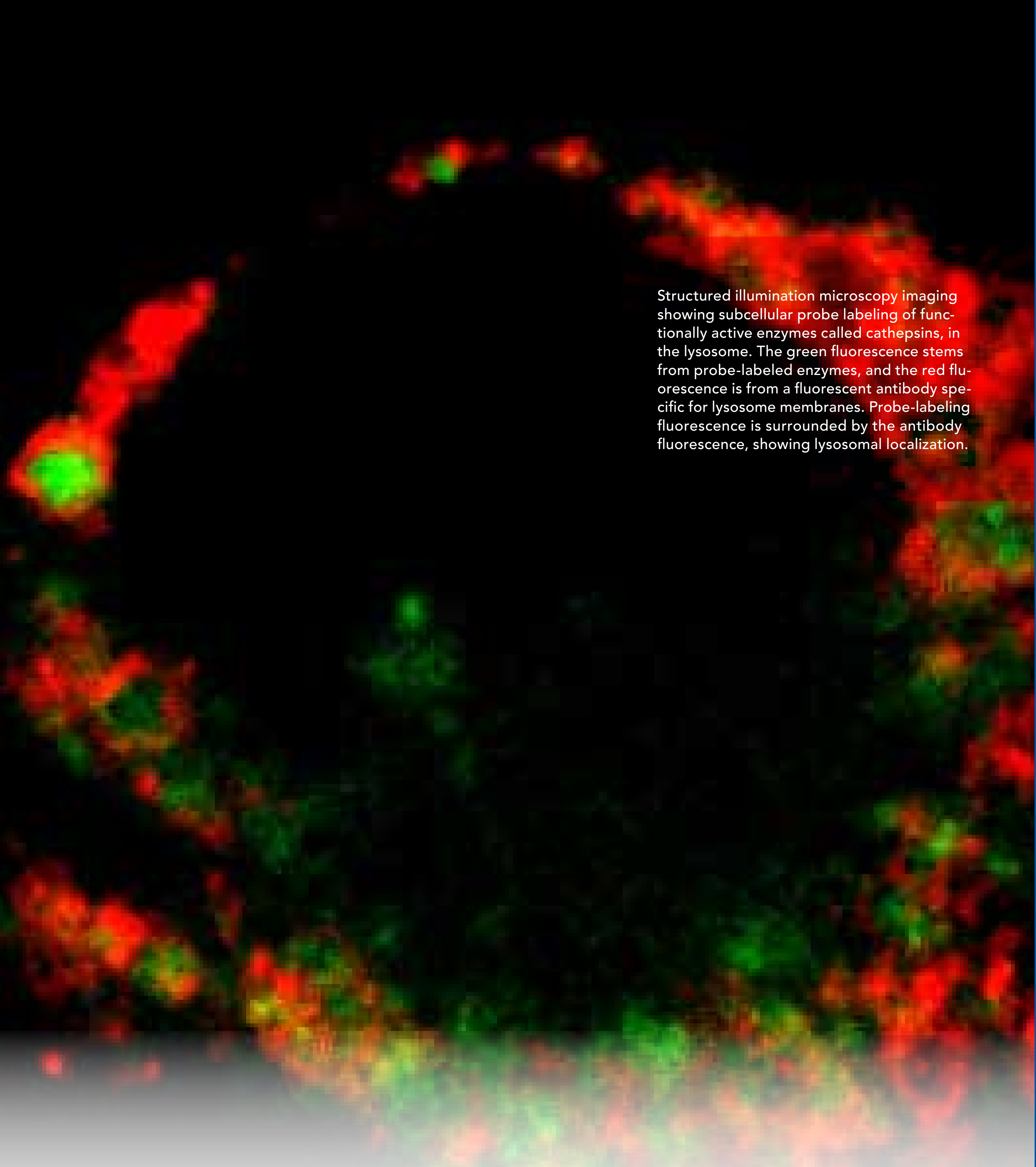


Understanding and successfully modeling flow over a surface characterized by spatially varying slip length, a phenomenon common in microfluidics, will help domain scientists and experimentalists generate future nano-device and lab-on-a-chip designs.

Pan W, J Bao and AM Tartakovsky. 2014. "Smoothed Particle Hydrodynamics-Continuous Boundary Force Method for Navier-Stokes Equations Subject to a Robin Boundary Condition." *Journal of Computational Physics* 259:242-259. DOI: 10.1016/j.jcp.2013.12.014.

Sponsor: DOE Office of Science, Office of Advanced Scientific Computing Research

BIOLOGICAL SYSTEMS SCIENCE



Structured illumination microscopy imaging showing subcellular probe labeling of functionally active enzymes called cathepsins, in the lysosome. The green fluorescence stems from probe-labeled enzymes, and the red fluorescence is from a fluorescent antibody specific for lysosome membranes. Probe-labeling fluorescence is surrounded by the antibody fluorescence, showing lysosomal localization.

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.

Cyanobacterial Consortia Shed New Light on Phototrophic Biofilm Assembly

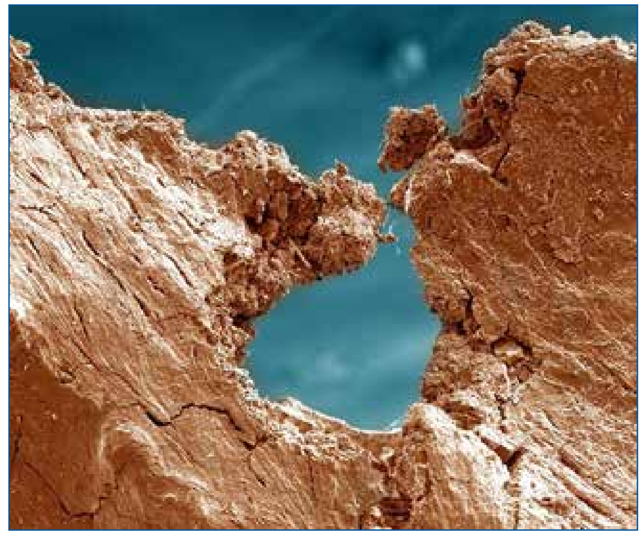
Microbial consortia are groupings of multiple microbial species interacting with one another. The communities are frequently found in nature, but few have been cultivated in the laboratory. As part of ongoing studies of the complex world of microbial communities, scientists at PNNL isolated two bacterial consortia from a microbial mat, a multi-layered sheet of microorganisms, in Hot Lake, located in north-central Washington State. They characterized each consortium's membership and metabolic function to identify the interactions thought to recruit and maintain genetic and functional diversity in the consortia over time. The team's results shed light on the principles needed for scientists to move closer to the goal of being able to predict, engineer and manipulate microbial communities of importance to global carbon and energy cycling.

"Primary production by microbial autotrophs and consumption by heterotrophs are occurring everywhere. If you don't understand the interactions, you can't predict how communities will respond to changing environmental conditions or engineer them to sustainably perform a useful function; for example, making them more productive—to generate more biomass for bioenergy applications—or resilient, so they recover quickly from environmental shocks. It's a big deal."

—Dr. Steve Lindemann, PNNL microbiologist

Cole JK, JR Hutchison, RS Renslow, YM Kim, WB Chrisler, HE Engelmann, A Dohnalkova, D Hu, TO Metz, JK Fredrickson and SR Lindemann. 2014. "Phototrophic Biofilm Assembly in Microbial-Mat-Derived Unicyanobacterial Consortia: Model Systems for the Study of Autotroph-Heterotroph Interactions." *Frontiers in Microbiology* 5:109. DOI: 10.3389/fmicb.2014.00109.

User Facility: EMSL
Sponsor: DOE Office of Science, Office of Biological and Environmental Research



Transmission electron microscopy image of a microbial mat. The mat was labeled with carbon-13, and a hole was drilled with a laser to get the molecular signature. PNNL scientists are studying microbial communities toward the goal of being able to predict, engineer and manipulate those of importance to global carbon and energy cycling.

Lost in Translation: Gene Expression Changes Don't Always Alter Protein Levels

The central dogma of biology is that DNA gives rise to messenger RNA (mRNA), which then gives rise to protein. It has been widely assumed that changes in specific mRNA levels are always accompanied by equal changes in the encoded proteins, and vice versa. To determine whether this is always the case, scientists at PNNL examined the metal-reducing bacteria *Shewanella oneidensis* MR-1 grown under steady conditions. In response to altering the oxygen levels, they found that changes in the expression of proteins were caused primarily by differences in the translational efficiency rather than changes in the mRNA levels. Interestingly, changes in translational efficiency were significantly correlated with the pattern of codons in genes that encode different amino acids. Because measurable transfer RNA pools, which read the codons, also changed in response to altered oxygen levels, this suggests that changes in the translational efficiency of genes are caused, in part, by alterations in the abundance of molecules that decode the mRNAs.

"To understand how microbes work together in communities, it's important to understand the functional state of their member species. Metagenomics analyses have provided important data on the functional potential of each community species, but their actual functions are highly dependent on their pattern of protein expression, which, in turn, is modulated by the local microenvironment of each cell."

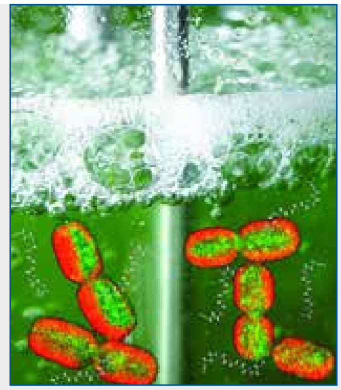
—Dr. Steven Wiley, PNNL Laboratory Fellow

Taylor RC, BJM Webb-Robertson, LM Markillie, MH Serres, BE Linggi, JT Aldrich, EA Hill, MF Romine, MS Lipton and HS Wiley. 2013. "Steady State Analysis of Integrated Proteomics and Transcriptomics Data Shows Changes in Translational Efficiency a Dominant Regulatory Mechanism in the Environmental Response of Bacteria." *Integrative Biology* 5(11):1393-1406. DOI: 10.1039/c3ib40120k.

User Facility: EMSL
Sponsor: DOE Office of Science, Office of Biological and Environmental Research

Scientists Capture "Redox Moments" in Living Cells

Scientists at PNNL have charted a significant signaling network in a tiny organism that's big in the world of biofuel research. Their findings about how a remarkably fast-growing organism conducts its metabolic business bolster scientists' ability to create biofuels using the hardy microbe *Synechococcus*, which turns sunlight into useful energy. The team glimpsed key chemical events, known as redox reactions, inside living cells of the organism by using a chemical probe they developed that allows live-cell labeling. They also developed an in vivo labeling and imaging strategy to identify proteins undergoing these reactions in the photoautotrophic cyanobacterium. Their publication marks the first time that redox activity has been observed in specific proteins within living cells.



Artistic rendition of cell-permeable chemical probes labeling redox-sensitive cysteine thiols in living *Synechococcus* PCC7002. The background depicts the photobioreactor used to culture the cyanobacteria. The probes and photobioreactor were developed at PNNL.

Sadler NC, MR Melnicki, M Serres, ED Merkley, WB Chrisler, EA Hill, MF Romine, S Kim, EM Zink, S Datta, RD Smith, AS Beliaev, A Konopka and AT Wright. 2014. "Chemical Profiling of Live Cell Temporal Redox Dynamics in a Photoautotrophic Cyanobacterium." *ACS Chemical Biology* 9(1):291-300. DOI: 10.1021/cb400769v.

User Facility: EMSL
Sponsor: DOE Office of Science, Office of Biological and Environmental Research

Eliminating a "Superbug"

Scanning electron micrograph of methicillin-resistant *Staphylococcus aureus* and human white blood cells. *Image credit: NIAID*

Antibiotics are designed to stamp out the microbes that make us sick, but their overuse has resulted in drug-resistant bacteria. These "superbugs" have modified their behavior to defy even the best medical efforts and are a growing public health concern. A team of researchers from Northeastern University, PNNL and Arietis Biotechnology developed a novel approach to treat and eliminate methicillin-resistant *Staphylococcus aureus* (MRSA). MRSA is a strong bacterium whose resistance to antibiotics has been unstoppable. The new work represents the culmination of more than a decade of research on a specialized class of cells produced by all pathogens called persisters. The team concluded that if they can kill these persisters, they may be able to attack chronic infections that are resistant to MRSA. They found that a drug called ADEP effectively wakes up the dormant cells and then initiates a self-destruct mechanism. The approach completely eradicated MRSA cells in a variety of laboratory experiments and, importantly, in a mouse model of chronic MRSA infection.

Conlon BP, ES Nakayasu, LE Fleck, MD LaFleur, VM Isabella, K Coleman, SN Leonard, RD Smith, JN Adkins and K Lewis. 2013. "Activated ClpP Kills Persisters and Eradicates a Chronic Biofilm Infection." *Nature* 503(7476):365-370. DOI: 10.1038/nature12790.

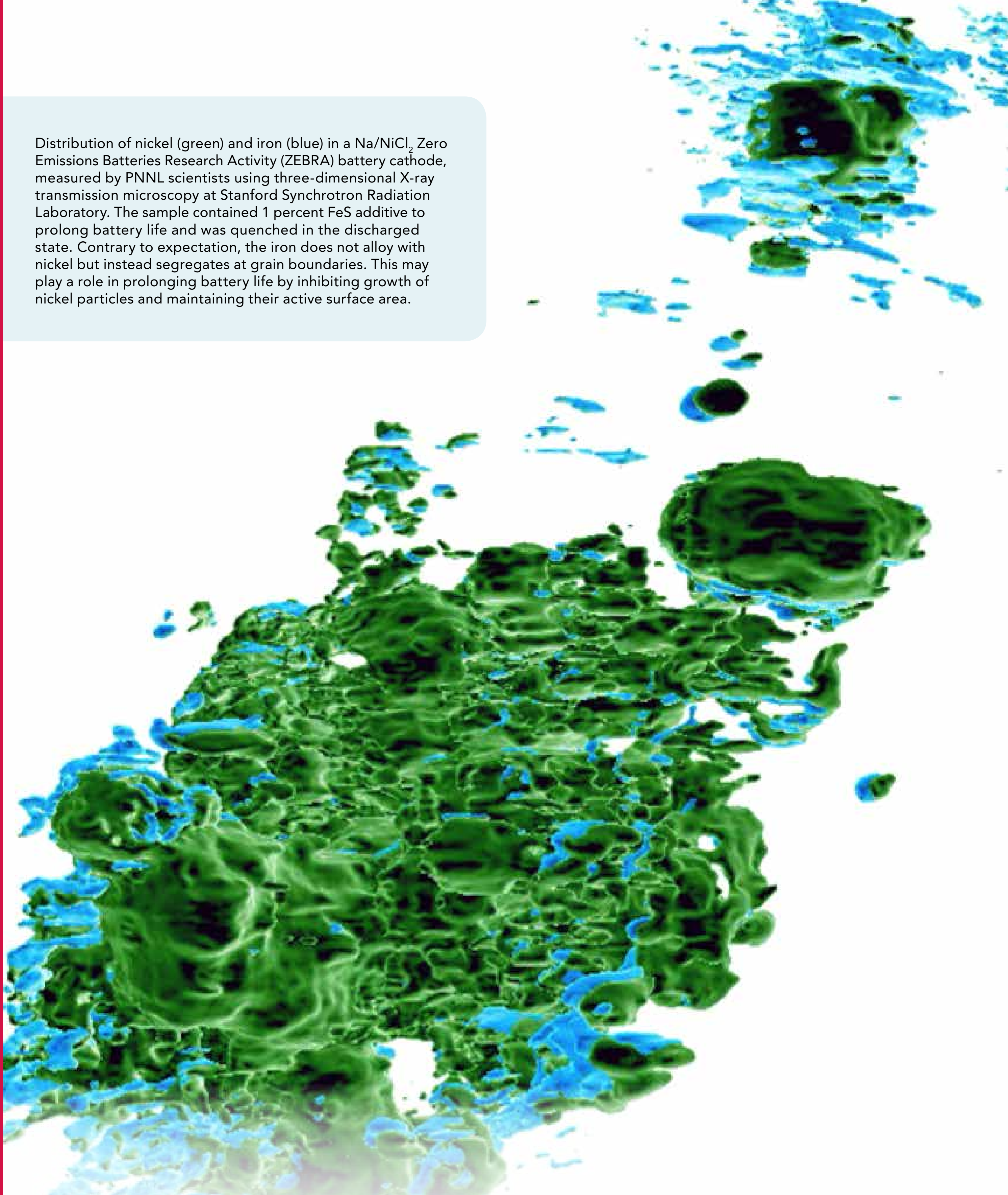
User Facility: EMSL
Sponsor: National Institutes of Heath

Resin-Assisted Method Is a Pitch-Perfect Improvement in Studying Influential Cysteine Thiols

In all organisms, reduction-oxidation—or "redox"—regulation is essential for many biological processes, including metabolism, gene expression, and environmental and stress responses. Key to understanding these processes is being able to determine how the post-translational modifications (PTMs) of proteins contribute to creating "redox switches" capable of regulating protein functions and protein-protein interactions. Researchers at PNNL developed an efficient method for enriching and quantitatively analyzing PTMs of cysteine residues of proteins using a commercially available resin. The team's innovative approach more quickly and efficiently reveals information about cysteine thiols and associated "reversible modifications," that affect protein activity, conformation, interaction and other characteristics. The team's advance will offer broad applications in biological studies by serving as a general enrichment strategy for multiple types of reversible cysteine modifications. Research has shown cysteine thiols in proteins frequently participate in changes that can significantly impact protein behavior and functioning. The PNNL-developed innovation is a key step toward more rapidly expanding knowledge in this field.

Guo J, MJ Gaffrey, D Su, T Liu, DG Camp II, RD Smith and WJ Qian. 2014. "Resin-Assisted Enrichment of Thiols as a General Strategy for Proteomic Profiling of Cysteine-Based Reversible Modifications." *Nature Protocols* 9(1):64-75. DOI: 10.1038/nprot.2013.161.

User Facility: EMSL
Sponsors: DOE Office of Science, Office of Biological and Environmental Research, National Institutes of Health

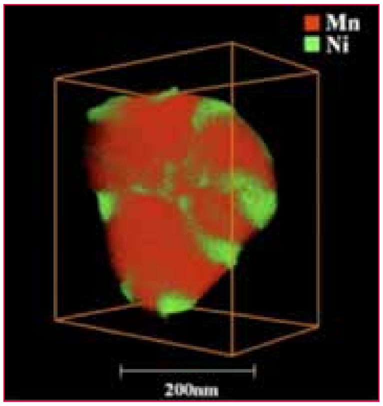


Distribution of nickel (green) and iron (blue) in a $Na/NiCl_2$ Zero Emissions Batteries Research Activity (ZEBRA) battery cathode, measured by PNNL scientists using three-dimensional X-ray transmission microscopy at Stanford Synchrotron Radiation Laboratory. The sample contained 1 percent FeS additive to prolong battery life and was quenched in the discharged state. Contrary to expectation, the iron does not alloy with nickel but instead segregates at grain boundaries. This may play a role in prolonging battery life by inhibiting growth of nickel particles and maintaining their active surface area.

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.

New Technique Efficiently Resolves Chemistry of Nanoparticles

A new technique developed at EMSL with the FEI Company lets scientists efficiently resolve elements' locations in three dimensions. The team's technique combines scanning transmission electron microscopy and X-ray energy dispersive spectrometry with a new detector arrangement and a brighter electron beam. The result is a three-dimensional map of the element's placement on a sample smaller than a single blood cell. The team applied this technique to a lithium-rich nickel-based material that could be part of tomorrow's batteries. They discovered how nickel was segregating away from other elements on the material's surface. The team's technique provides precise three-dimensional chemical images in hours, not days, and avoids the time and expense of reshaping samples and transporting them to other instruments. The information generated by this technique could help in the material design of longer-lasting, higher-capacity batteries.



A new technique combining scanning transmission electron microscopy and X-ray energy dispersive spectrometry showed this three-dimensional nanoparticle used as a cathode material in lithium-ion batteries. The technique enables clearer visualizations at much faster rates than currently used methods.

Genc A, L Kovarik, M Gu, H Cheng, P Plachinda, L Pullan, B Freitag and C Wang. 2013. "XEDS STEAM Tomography for 3D Chemical Characterization of Nanoscale Particles." *Ultramicroscopy* 131:24-32. DOI: 10.1016/j.ultramic.2013.03.023.

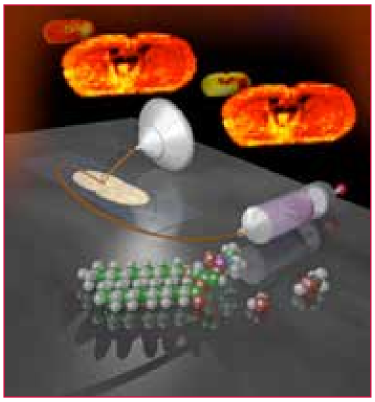
User Facility: EMSL
Sponsor: Chemical Imaging Initiative

New Imaging Approach Accurately Measures Molecules in Biological Samples

To understand how cells converse, scientists at PNNL and Oregon Health & Science University designed an approach that accurately determines the spatial location of molecules and quantifies lipids and metabolites in biological samples, providing valuable information for cost-effective production of biofuels and pharmaceuticals. It efficiently accounts for signal suppression—called a matrix effect—that may significantly alter molecule distributions obtained in mass spectrometry imaging experiments. The team compensated for matrix effects by adding two lipid standards to the solvent used in Nanospray Desorption Electrospray Ionization Mass Spectrometry, or nano-DESI, imaging.

"Our technique reflects what's in the sample. This is a new way of gathering and analyzing data that will feed into a lot of biological applications in the future."

—*Dr. Ingela Lanekoff, PNNL analytical chemist*



The team analyzed thin sections of the tissue sample using nano-DESI imaging, which allowed them to measure small quantities of materials with minimal sample preparation.

Lanekoff I, SL Stevens, MP Stenzel-Poore and J Laskin. 2014. "Matrix Effects in Biological Mass Spectrometry Imaging: Identification and Compensation." *Analyst* 139:3528-3532. DOI: 10.1039/C4AN00504J.

User Facility: EMSL
Sponsors: Chemical Imaging Initiative, National Institutes of Health

By Losing Their Shape, Materials Fail Batteries

Ubiquitous but frustrating, lithium-ion batteries fade because the materials lose their structure in response to charging and discharging. According to a multi-institutional team, including scientists at PNNL, this structural change is closely related to the formation of electron-rich regions within the electrode. Scientists used experiments and molecular simulations to show that the electron-rich region causes silicon bonds to break. The bond breakage transforms crystalline silicon into an amorphous alloy of lithium and silicon. This study's results could assist in designing longer-lasting materials for not just cell phones, but also for electric cars.

Wang Z, M Gu, Y Zhou, X Zu, JG Connell, J Xiao, D Perea, LJ Lauhon, J Bang, S Zhang, C Wang and F Gao. 2013. "Electron-Rich Driven Electrochemical Solid-State Amorphization in Li-Si Alloys." *Nano Letters* 13(9):4511-4516. DOI: 10.1021/nl402429a.

User Facility: EMSL
Sponsors: Chemical Imaging Initiative, National Science Foundation

In-Situ Chemical Imaging at the Sub-Biofilm Scale Now Possible

For the first time, a multi-disciplinary team at PNNL is able to demonstrate imaging of a biofilm's chemical components as they form in hydrated biological samples, rather than from frozen or dried samples. Using a surface technique called time-of-flight secondary ion mass spectrometry, scientists were able to study complex microbiological processes, such as chemical attachment of microbes to surfaces to form biofilms. Scientists study biofilms to understand how they grow and bond to surfaces—such as plaque on teeth or slippery scum on river rock—with implications for basic energy, industrial and biogeochemical research. The work will further the understanding of how natural microbial communities can influence larger biogeochemical processes in subsurface settings.

Hua X, XY Yu, Z Wang, L Yang, B Liu, Z Zhu, AE Tucker, WB Chrisler, EA Hill, S Thevuthasan, Y Lin, S Liu and MJ Marshall. 2014. "In Situ Molecular Imaging of Hydrated Biofilm in a Microfluidic Reactor by ToF-SIMS." *Analyst* 139(7):1609-1613. DOI: 10.1039/c3an02262e.

User Facility: EMSL
Sponsors: DOE Office of Science, Office of Basic Energy Sciences, Chemical Imaging Initiative, PNNL Technology Development Program

Superbright and Fast X-rays Image Single Layer of Proteins

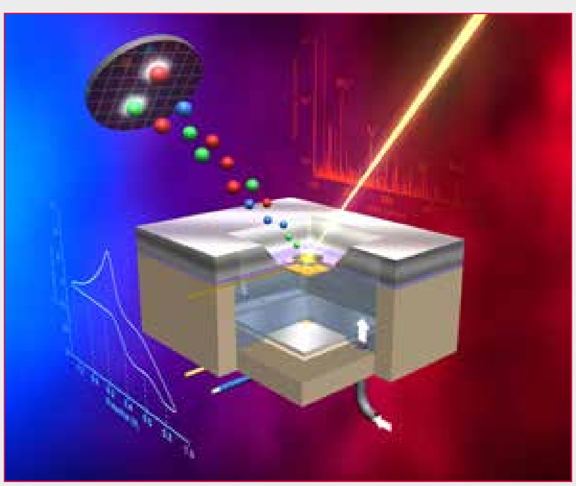
In biology, a protein's shape is key to understanding how it causes disease or toxicity. Researchers who use X-rays to take snapshots of proteins typically need a billion copies of the same protein stacked and packed into a neat crystal. Now, scientists at PNNL and Lawrence Livermore National Laboratory have found that by using exceptionally bright and fast X-rays, they can take a picture of a sheet of proteins just one protein layer thick. Using an X-ray free-electron laser, the technique opens the door to learning the structural details of almost 25 percent of known proteins, many of which have been overlooked because of their inability to stack properly.

Frank M, DB Carlson, M Hunter, GJ Williams, M Messerschmidt, NA Zatsepin, A Barty, H Benner, K Chu, A Graf, S Hau-Riege, R Kirian, C Padeste, T Pardini, B Pedrini, B Segelke, MM Seibert, JC Spence, CJ Tsai, SM Lane, XD Li, G Schertler, S Boutet, MA Coleman and JE Evans. 2014. "Femtosecond X-Ray Diffraction from Two-Dimensional Protein Crystals." *International Union of Crystallography Journal* 1:95-100. DOI: 10.1107/S2052252514001444.

Sponsors: University of California Office of the President Lab Fee Program, National Institutes of Health, National Science Foundation, Lawrence Livermore National Laboratory's Laboratory Directed Research and Development, Chemical Imaging Initiative

Microfluidic Probe Allows Real-Time Imaging of Electrode-Liquid Electrolyte Interface

A new imaging capability that allows direct probing of the solid-liquid interface, the most common interface in many important systems, now enables in-situ investigation of the surface and diffused layer regions in liquids using surface-sensitive techniques. Developed by scientists at PNNL, the electrochemical probe, or E probe, combines microfluidic, chemical physics, electrochemistry and sensitive surface techniques. Using this probe, scientists showed the molecular composition of the reaction products and intermediate species at different stages of the redox cycle in situ using—for the first time—time-of-flight secondary ion mass spectrometry, a surface imaging technique that operates in a vacuum.



The new microfluidic E probe, developed at PNNL, in position on a time-of-flight secondary ion mass spectrometry instrument.

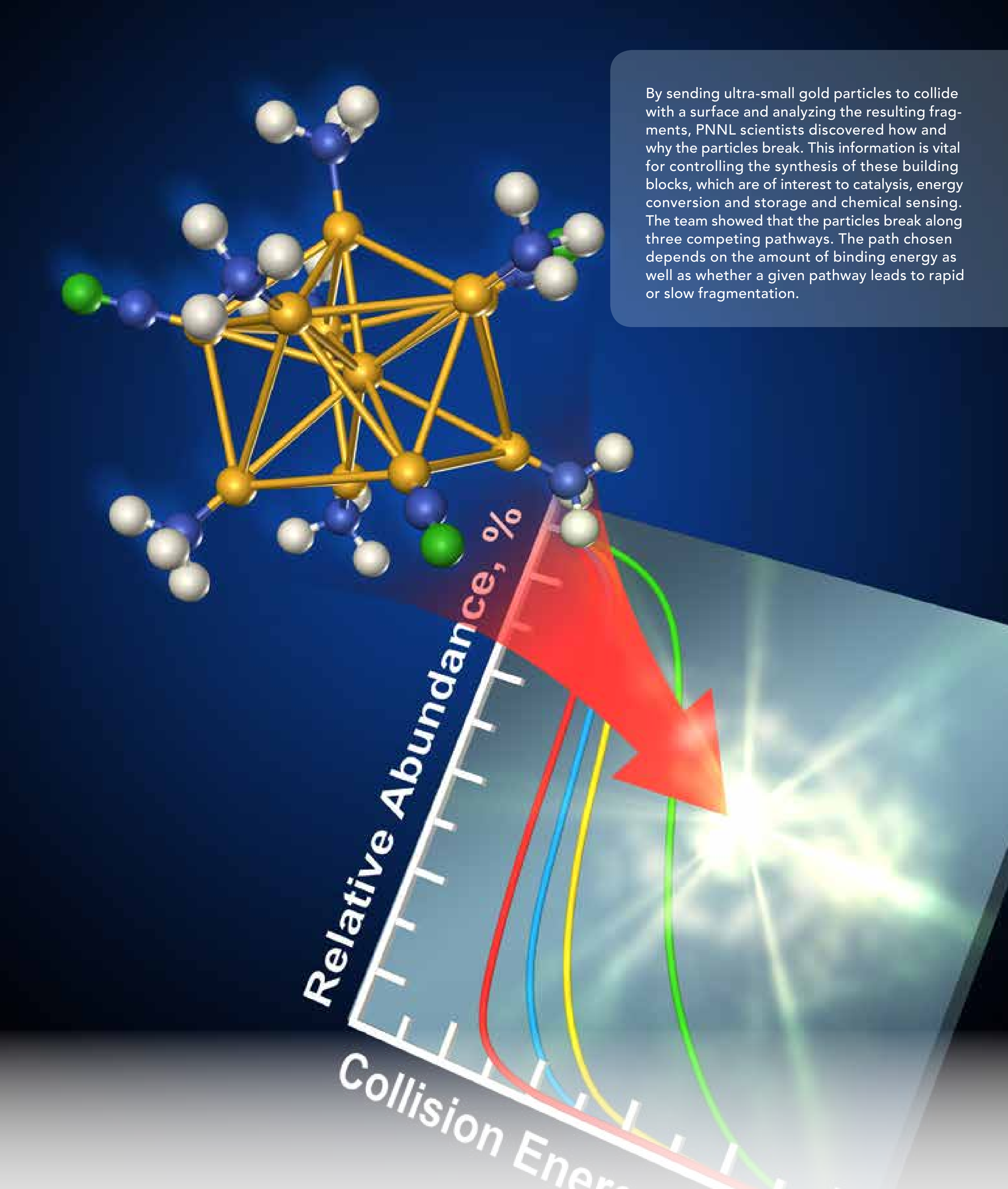
"This is a tremendous innovation for in-situ studies as a new means to interrogate the chemical language of microbial system interactions, as well as being relevant to the discovery and development of new electrode materials for energy storage. Moreover, this capability could be transformative for the study of chemical fluxes and effectiveness in advanced catalytic systems."

—Dr. Louis Terminello, PNNL Fundamental & Computational Sciences Chief Scientist

Liu B, XY Yu, Z Zhu, X Hua, L Yang and Z Wang. 2014. "In Situ Chemical Probing of the Electrode-Electrolyte Interface by ToF-SIMS." *Lab on a Chip* 14(5):855-859. DOI: 10.1039/C3LC50971K.

User Facility: EMSL
Sponsor: Chemical Imaging Initiative

CHEMISTRY & GEOCHEMISTRY



By sending ultra-small gold particles to collide with a surface and analyzing the resulting fragments, PNNL scientists discovered how and why the particles break. This information is vital for controlling the synthesis of these building blocks, which are of interest to catalysis, energy conversion and storage and chemical sensing. The team showed that the particles break along three competing pathways. The path chosen depends on the amount of binding energy as well as whether a given pathway leads to rapid or slow fragmentation.

Discoveries of how molecules, atoms, protons and electrons stand still, hop around or come apart are vital to understanding and controlling complex interactions that can solve national and international energy issues. At PNNL, scientists in collaboration with researchers from academia, other national labs and industry are making discoveries 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, bringing different scientific perspectives to our clients.

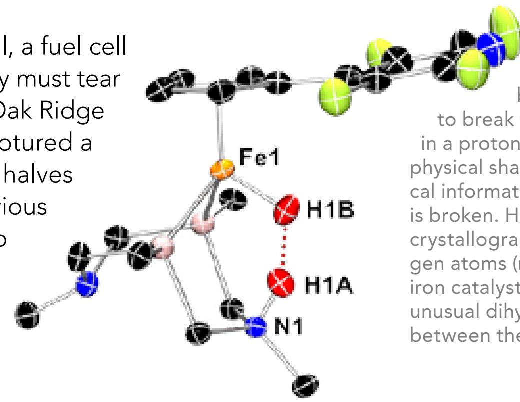
Halving Hydrogen

Like a hungry diner ripping open a dinner roll, a fuel cell catalyst that converts hydrogen into electricity must tear open a hydrogen molecule. Researchers at Oak Ridge National Laboratory and PNNL have now captured a view of such a catalyst holding onto the two halves of its hydrogen feast. The view confirms previous hypotheses and provides insight into how to make the catalyst work better for alternative energy uses.

This study is the first time scientists have shown precisely where the hydrogen halves end up in the structure of a molecular catalyst that breaks down hydrogen. The design of this catalyst was inspired by the innards of a natural protein called a hydrogenase enzyme.

Liu T, X Wang, C Hoffmann, DL DuBois and RM Bullock. 2014. "Heterolytic Cleavage of Hydrogen by an Iron Hydrogenase Model Investigated by Neutron Diffraction." *Angewandte Chemie International Edition* 53(21):5300-5304. DOI: 10.1002/anie.201402090.

Sponsor: Center for Molecular Electrocatalysis, an Energy Frontier Research Center funded by DOE Office of Science, Office of Basic Energy Sciences



An important step in breaking a hydrogen molecule so the bond's energy can be captured as electricity is to break the bond unevenly, resulting in a proton and a hydride. The catalyst's physical shape, along with electrochemical information, can reveal how the bond is broken. Here, scientists used neutron crystallography to locate the two hydrogen atoms (red spheres) gripped by the iron catalyst. This arrangement allows an unusual dihydrogen bond to form between the hydrogen atoms (dots).

"The catalyst shows us what likely happens in the natural hydrogenase system. The catalyst is where the action is, but the natural enzyme has a huge protein surrounding the catalytic site. It would be hard to see what we have seen with our catalyst because of the complexity of the protein."

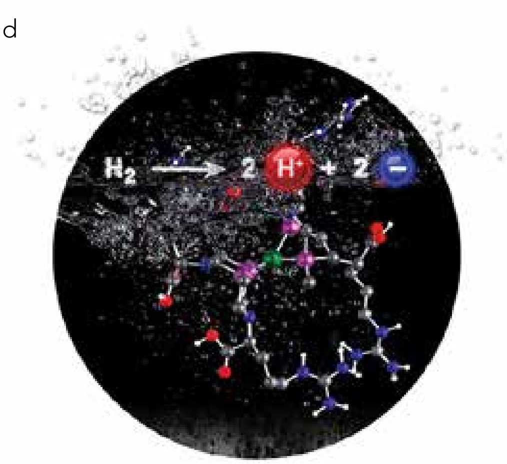
—Dr. Morris Bullock, PNNL Laboratory Fellow

Minor Adjustments Far from the Catalyst's Core

When it comes to making catalysts that quickly snap chemical bonds and free the stored energy, researchers often focus on the active site. However, small changes far from the active site can have a large impact. Taking a cue from enzymes, researchers at PNNL placed the amino acid arginine at the periphery of a hydrogen-splitting catalyst that cleaves hydrogen into protons and electrons. The arginine's carboxylic acid groups accelerated proton transfer and made the catalyst more energy efficient. At the same time, the arginine's guanidinium groups interacted to increase the rate of hydrogen binding and activation. With the appended arginine and a high concentration of hydrogen, this nature-inspired catalyst can split 144,000 molecules of hydrogen in a single second. Solar and wind energy could play a larger role if the energy they capture were to be stored in the chemical bonds of fuels such as hydrogen in fuel cells, then recovered later as electricity. Scientists are getting closer to enzymatic speed and energy efficiency—all with changes far from the active site and in a system that is much more stable than the enzyme under fuel cell conditions.

Dutta A, JAS Roberts and WJ Shaw. 2014. "Arginine Containing Ligands Enhance H_2 Oxidation Catalyst Performance." *Angewandte Chemie International Edition* 53:6487-6491. DOI: 10.1002/anie.201402304.

User Facility: EMSL
Sponsors: DOE Office of Science, Office of Basic Energy Sciences Early Career, Center for Molecular Electrocatalysis, an Energy Frontier Research Center funded by DOE Office of Science, Office of Basic Energy Sciences



Including an arginine in the ligand of a hydrogen oxidation catalyst results in water solubility, enhances proton movement through the carboxylic acid groups and alters that active site structure through intramolecular interactions.

"Here, we are incorporating minimal elements of natural enzymes into synthetic catalysts to understand their role and begin defining how much is necessary to make molecular catalysts as good as, or better than, the enzyme."

—Dr. Arnab Dutta, PNNL Postdoctoral Fellow

Hugging Hemes Help Electrons Hop

Researchers at PNNL and University College London simulating how certain bacteria run electrical current through tiny molecular wires have discovered a secret Mother Nature uses for electron travel. The results are key to understanding how the bacteria do chemistry in the ground, and will help researchers use them in microbial fuel cells, batteries or for turning waste into electricity. Within the bacteria's protein-based wire, molecular groups called hemes communicate with each other to allow electrons to hop along the chain-like stepping stones. The researchers found that evolution has set the protein up so that, generally, when the electron's drive to hop is high, the heme stepping stones are less tightly connected; when the drive to hop is low, the hemes are more closely connected. The outcome is an even electron flow along the wire. This is the first time scientists have seen this evolutionary design principle for electron transport.

"We were perplexed at how weak the thermodynamic driving force was between some of these hemes. But it turns out those pairs of hemes are essentially hugging each other. When the driving force is strong between hemes, they are only shaking hands. We've never seen this compensation scheme before."

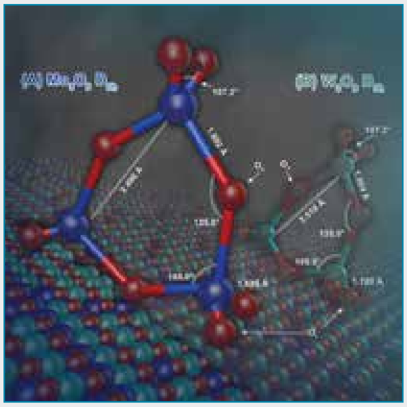
—Dr. Kevin Rosso, PNNL Laboratory Fellow

Breuer M, KM Rosso and J Blumberger. 2014. "Electron Flow in Multiheme Bacterial Cytochromes Is a Balancing Act Between Heme Electronic Interaction and Redox Potentials." *Proceedings of the National Academy of Sciences* 111(2):611-616. DOI: 10.1073/pnas.1316156111.

User Facility: EMSL
Sponsor: DOE Office of Science, Office of Biological and Environmental Research

Unified Picture of Alcohol's Interactions with Metal Oxide Catalysts

Based on 8 years of study, scientists at PNNL and the University of Alabama described in exquisite detail how alcohols behave on two early transition metal catalysts, molybdenum trioxide and tungsten trioxide. All the catalysts were prepared using an innovative method introduced at PNNL that prepares mono-dispersed catalytic clusters of identical size and structure. Such model systems can be used by scientists needing a structurally well-known material. The review provides a detailed discussion of the reaction mechanisms of these prepared catalysts for dehydration, dehydrogenation and condensation reactions of small aliphatic alcohols.



In the review article, the researchers discuss the characteristics and chemistry of catalytic cyclic $(WO_3)_3$ and $(MoO_3)_3$ clusters and the surfaces on which they react.

"We came up with a pretty simple picture of how these things work. We found the small changes in the molecular structure that determine whether the molybdenum or tungsten oxide catalyst is good for a reaction."

—Dr. Roger Rousseau, PNNL computational scientist

Rousseau R, DA Dixon, BD Kay and Z Dohnálek. 2014. "Dehydration, Dehydrogenation, and Condensation of Alcohols on Supported Oxide Catalysts Based on Cyclic $(WO_3)_3$ and $(MoO_3)_3$ Clusters." *Chemical Society Review.* Advance article. DOI: 10.1039/C3CS60445D.

Sponsors: DOE Office of Science, Office of Basic Energy Sciences, Robert Ramsay Endowment of the University of Alabama

Satisfying Metals' Thirst Vital for High-Capacity Batteries

Imagine a cell phone battery that worked for days between charges. At PNNL, scientists are answering basic science questions about replacing traditional lithium with metals that can carry multiple charges as a way to potentially double or triple the amount of charge that could be held in a battery. A roadblock to this future is understanding how to keep multiply charged ions stable with respect to hydrolysis channels.

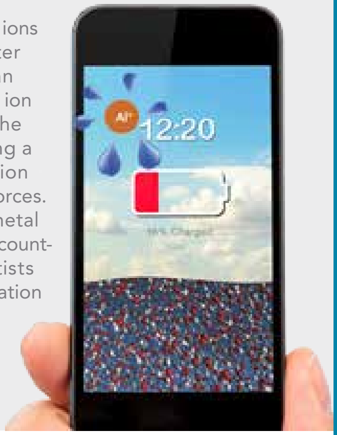
PNNL scientists determined the paths that lead to either the hydrolysis of water or the creation of stable metal ion clusters surrounded by water. It comes down to the pH of the solution, the number of water molecules nearby and the energy needed to remove electrons from the metal, known as the ionization potential.

Miliordos E, and SS Xantheas. 2014. "Elucidating the Mechanism Behind the Stabilization of Multi-Charged Metal Cations in Water: A Case Study of the Electronic States of Microhydrated Mg^{2+}, Ca^{2+} and Al^{3+}." *Physical Chemistry Chemical Physics* 16:6886-6892. DOI: 10.1039/C3CP53636J.

Miliordos E, and SS Xantheas. 2014. "Unimolecular and Hydrolysis Channels for the Detachment of Water from Microsolvated Alkaline Earth Dication (Mg^{2+}, Ca^{2+}, Sr^{2+}, Ba^{2+}) Clusters." *Theoretical Chemistry Accounts* 133:1450. DOI: 10.1007/s00214-014-1450-4.

Sponsor: DOE Office of Science, Office of Basic Energy Sciences

When multiple charged ions encounter a single water molecule, the result can be explosive. The metal ion rips an electron from the water molecule, causing a molecular-level explosion caused by Coulombic forces. But multiply charged metal cations exist in water in countless ways. PNNL scientists found out why—information that could be critical to replacing lithium-ion batteries with ones that last longer.



Pollution can decrease Earth's daily temperature range via larger high clouds left after a thunderstorm, spreading out across the sky and looking like anvils. These clouds cast shadows and cool the Earth during the day, but trap heat like a blanket at night. For late afternoon thunderstorms in summer, pollution can cause clouds to last long into the night rather than dissipate, causing warmer nights. Accounting for pollution's effects on storm clouds could affect the ultimate amount of warming predicted for the Earth in the next few decades. PNNL researchers are focusing on how human-caused pollution, natural emissions and the mix of both affect convection, deep clouds and precipitation.

How do human activities and natural systems interact to affect the Earth's climate? Ultimately, that is the challenge for scientists at PNNL. 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 molecular to global scales.

Cooler Days, Warmer Nights

A team led by PNNL scientists revealed how pollution causes thunderstorms to leave behind larger, deeper, longer-lasting clouds and affects climate warming. Researchers had thought that pollution causes larger and longer-lasting storm clouds by making thunderheads draftier through a process known as convection. The team showed that instead, pollution makes clouds linger by decreasing the sizes of water and ice particles. The difference will affect how scientists represent clouds in climate models. Accounting for how pollution affects storm clouds could impact the ultimate amount of warming predicted for the Earth in the next few decades.

"This study reconciles what we see in real life to what computer models show us. Observations consistently show taller and bigger anvil-shaped clouds in storm systems with pollution, but the models don't always show stronger convection. Now we know why."

—Dr. Jiwen Fan, PNNL atmospheric scientist

Fan J, LR Leung, D Rosenfeld, Q Chena, Z Lid, J Zhang and H Yan. 2013. "Microphysical Effects Determine Macrophysical Response for Aerosol Impacts on Deep Convective Clouds." *Proceedings of the National Academy of Sciences* 110(48):E4581-E4590. DOI: 10.1073/pnas.1316830110.

User Facility: ARM Climate Research Facility

Sponsor: DOE Office of Science, Office of Biological and Environmental Research

Water Woes Projected in U.S. Southwest

Water in the soil, streams and groundwater is critical for Earth ecosystems and food and energy production. Understanding and projecting how water availability is going to change in the future is a major science challenge with important societal implications. New research from scientists at PNNL identified a trajectory of spring drying that will alter water availability across the U.S. Southwest. To describe the net change in water, they calculated the water gained through precipitation and subtracted the water lost through evaporation and transpiration in an ensemble of regional and global simulations. Their findings indicate future challenges for regional water resource managers and agricultural production.

Gao Y, LR Leung, J Lu, Y Liu, M Huang and Y Qian. 2014. "Robust Spring Drying in the Southwestern U.S. and Seasonal Migration of Wet/Dry Patterns in a Warmer Climate." *Geophysical Research Letters* 41(5):1745-1751. DOI: 10.1002/2014GL059562.

Sponsor: DOE Office of Science, Office of Biological and Environmental Research

A dry irrigation canal illustrates one challenge presented by large shifts in spring wet and dry periods across the U.S. Southwest—reductions in water availability.

Global Natural Gas Boom Alone Won't Slow Climate Change

Expanding the current bounty of cheap natural gas alone will not help to reduce greenhouse gas emissions worldwide, according to an analysis of global energy use, economics and the climate by researchers at PNNL working at the Joint Global Change Research Institute in Maryland. Though natural gas produces half the amount of carbon dioxide as coal, the research found that the flood of natural gas in the market replaces both high and low emission fuels, erasing its advantage in lowering carbon emissions. The study shows that an abundance of competitively priced natural gas globally would displace all energy sources—including coal, nuclear and relatively more-expensive renewable energy technologies such as wind and solar—as well as accelerate economic growth that would expand overall energy use.

"Abundant natural gas alone will do little to slow climate change."

—Dr. Haewon McJeon, PNNL atmospheric scientist

McJeon H, J Edmonds, N Bauer, L Clarke, B Fisher, BP Flannery, J Hilaire, V Krew, G Marangoni, R Mi, K Riahi, H Rogner and M Tavoni. 2014. "Limited Impact on Decadal-Scale Climate Change from Increased Use of Natural Gas." *Nature*, October 2014. DOI: 10.1038/nature13837

Sponsor: The Global Technology Strategy Project

Natural gas power plants emit half the amount of carbon dioxide into the atmosphere as coal-fired plants. Recent advances in gas production technology have led to bountiful natural gas and a technology revolution in energy production. But due to lower costs, natural gas would also replace some low-carbon energy, such as renewables or nuclear energy. *Photo courtesy of Scott_Butner@charter.net.*

Water-Stressed World Will Face Increased Thirst

By the end of the century, an increased demand for fresh water will hit certain regions harder than others, according to PNNL researchers. Projections analyzed by the team show that the Middle East and India, already dealing with water scarcity, will face even more water stress. The team included sectoral water requirements for the first time in a prominent, complex model specifically designed to link economic, energy, land-use and climate systems to reveal future fresh water requirements from the energy, agricultural and municipal sectors of the economy. The study indicates that water conservation technologies and practices likely will have an increasingly important and unavoidable role in water-use planning.

To address the impact of climate change on water's availability, this study indicates the increasing importance of water conservation technologies and strategies, especially in already water-stressed regions.

Hejazi MI, J Edmonds, L Clarke, P Kyle, E Davies, V Chaturvedi, M Wise, P Patel, J Eom, K Calvin, R Moss and S Kim. 2014. "Long-Term Global Water Use Projections Using Six Socioeconomic Scenarios in an Integrated Assessment Modeling Framework." *Technological Forecasting and Social Change* 81(2014):205-226. DOI: 10.1016/j.techfore.2013.05.006.

Sponsor: DOE Office of Science, Office of Biological and Environmental Research

Distant Desert Dust Increases Snowpack in California

Overseas dust influences the Sierra Nevada Mountain snowpack far more than home-produced pollution, according to scientists at PNNL. By modeling two cloud conditions during a field experiment, results showed that dust blown in possibly from Asia and Africa increases snow in winter clouds over California and increases precipitation by 10 to 20 percent. However, local pollution exerts a very small impact on snowfall. Its influence on rain from warm clouds heavily depends on cloud conditions and the strength of a low-level jet that blows parallel to the Sierra Nevada Mountains. Understanding the complex factors that impact precipitation and mountain snowpack will help improve regional climate predictions and far-reaching effects on populations and food supply.

Fan J, LR Leung, PJ DeMott, JM Comstock, B Singh, D Rosenfeld, JM Tomlinson, A White, KA Prather, P Minnis, JK Ayers and Q Min. 2014. "Aerosol Impacts on California Winter Clouds and Precipitation during CalWater 2011: Local Pollution versus Long-Range Transported Dust." *Atmospheric Chemistry and Physics* 14:81-101. DOI: 10.5194/acp-14-81-2014.

User Facility: ARM Climate Research Facility
Sponsors: California Energy Commission, DOE Office of Science, Office of Biological and Environmental Research

Testing a Land Model's Water Cycle Simulation Skills

Scientists at PNNL and Oak Ridge National Laboratory applied a computational technique to systematically evaluate the relative importance of key parameters for climate prediction and water resources management. Scientists are working to nail down the uncertainties. Using the new technique, researchers found that the most uncertain parameters are those associated with deep subsurface processes. Droughts, floods, superstorms and changing weather patterns are reminders of our vulnerability to uncertain future water resources. With improved predictions of water cycle fluctuation, land-use managers and policy-makers will have increased understanding for future planning.

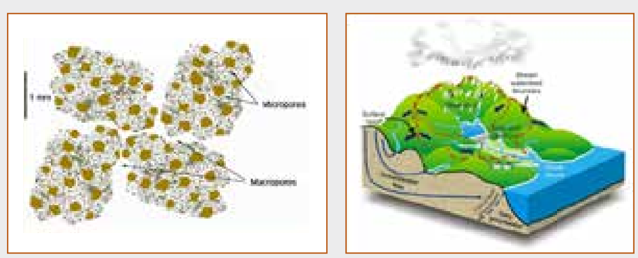
Huang M, Z Hou, LR Leung, Y Ke, Y Liu, Z Fang and Y Sun. 2013. "Uncertainty Analysis of Runoff Simulations and Parameter Identifiability in the Community Land Model: Evidence from MOPEX Basins." *Journal of Hydrometeorology* 14(6):1754-1772. DOI: 10.1175/JHM-D-12-0138.1.

Hou Z, M Huang, LR Leung, G Lin and DM Ricciuto. 2012. "Sensitivity of Surface Flux Simulations to Hydrologic Parameters Based on an Uncertainty Quantification Framework Applied to the Community Land Model." *Journal of Geophysical Research* 117(D15108). DOI: 10.1029/2012JD017521.

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

Several Faces of Physics Become One

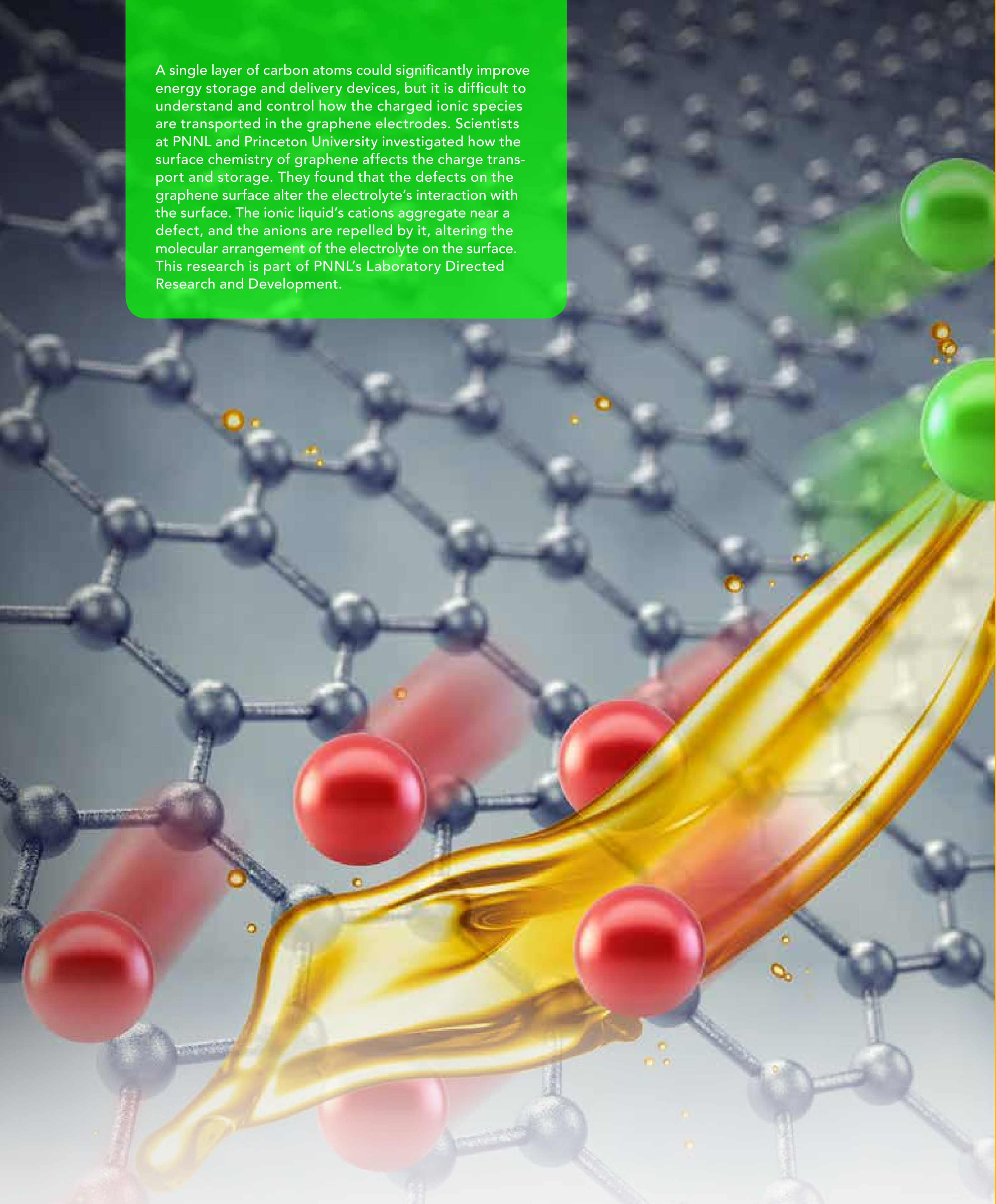
Water moves through multi-faceted physical boundaries. This poses a significant challenge for scientists who must simulate water flow across many domains. Scientists at PNNL conquered this barrier by merging different physical laws. The researchers developed a new approach that eliminates the repeated calculations at the domain interfaces, significantly simplifying water flow simulations for ecosystems. The new approach can describe any type of water flow in soils and the terrestrial ecosystem, in soil pores, streams, lakes, rivers and oceans and in mixed media of pores and solids for soil and aquifer. The versatile properties of the new approach allow cross-domain simulation of water flow at different scales.



The unified multi-scale model developed at PNNL couples water transport equations in such a way that this one model can represent transport at both pore (left) and watershed (right) scales.

Yang X, C Liu, J Shang, Y Fang and VL Bailey. 2014. "A Unified Multi-Scale Model for Pore-Scale Flow Simulations in Soils." *Soil Science Society of America Journal* 78(1):108-118. DOI: 10.2136/sssaj2013.05.0190.

User Facility: EMSL
Sponsor: DOE Office of Science, Office of Biological and Environmental Research



A single layer of carbon atoms could significantly improve energy storage and delivery devices, but it is difficult to understand and control how the charged ionic species are transported in the graphene electrodes. Scientists at PNNL and Princeton University investigated how the surface chemistry of graphene affects the charge transport and storage. They found that the defects on the graphene surface alter the electrolyte's interaction with the surface. The ionic liquid's cations aggregate near a defect, and the anions are repelled by it, altering the molecular arrangement of the electrolyte on the surface. This research is part of PNNL's Laboratory Directed Research and Development.

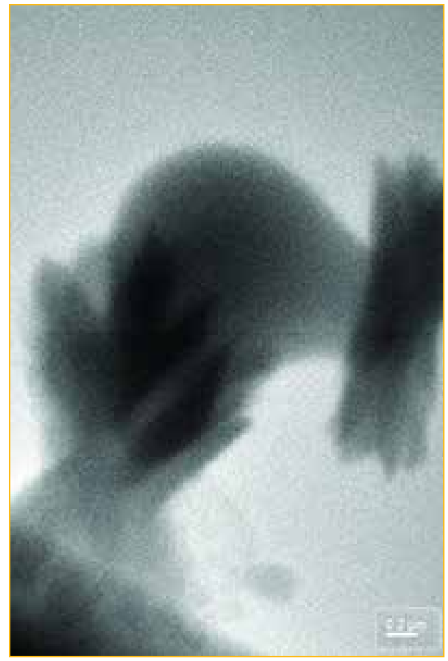
Revolutionary materials are needed to produce, use and store domestically produced energy. These materials are unlikely to be discovered via trial and error, as such an approach is too slow and costly. At PNNL, our research focuses on making, measuring and modeling materials and then scaling that knowledge to tailor materials to specific situations. Understanding materials often involves understanding how defects and interfaces form and affect the material's behavior.

Creation of a Material

One of the most important molecules on earth, calcium carbonate crystallizes into chalk, shells and minerals. In a study led by PNNL, researchers used a powerful microscope that allows them to see the creation of crystals in real time, giving them a peek at how different calcium carbonate crystals form. The results might help scientists understand how to lock carbon dioxide out of the atmosphere as well as how to better reconstruct ancient climates. When carbon resides within calcium carbonate, it is not hanging out in the atmosphere as carbon dioxide, warming the world. Understanding how calcium carbonate turns into various minerals could help scientists control its formation to keep carbon dioxide from getting into the atmosphere.

"For a decade, we've been studying the formation pathways of carbonates using high-powered microscopes, but we hadn't had the tools to watch the crystals form in real time. Now we know the pathways are far more complicated than envisioned in the models established in the 20th century."

—Dr. James De Yoreo, PNNL materials scientist



These crystals of aragonite, with the characteristic "sheaf of wheat" form, grew on the surface of a particle of amorphous calcium carbonate.

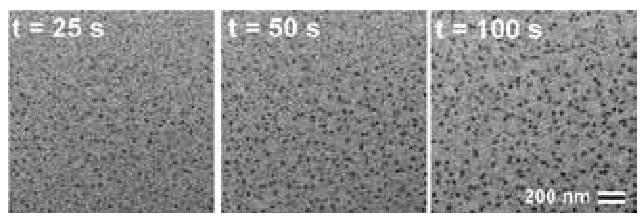
Nielsen MH, S Aloni and JJ De Yoreo. 2014. "In Situ TEM Imaging of $CaCO_3$ Nucleation Reveals Coexistence of Direct and Indirect Pathways." *Science* 345(6201):1158-1162. DOI: 10.1126/science.1254051.

Sponsors: DOE Office of Science, Office of Basic Energy Sciences, U.S. Department of Defense, Air Force Office of Scientific Research, National Defense Science and Engineering Graduate Fellowship, National Science Foundation

Watching Nanoparticles Grow

Whether storing renewable energy for later use or designing longer lasting batteries for electric-powered vehicles, many of today's energy problems will not be solved with today's materials. The key to avoiding time-consuming trial-and-error research is to tightly control nanoparticle growth to build the materials needed, from the bottom up. Scientists at PNNL, the University of California, Davis and Florida State University discovered that individual silver nanoparticles in solutions typically grow through single atom attachment, but importantly, when they reach a certain size they can link with other particles. This seemingly simple result has shifted a long-held scientific paradigm that did not consider kinetic models when explaining how nanoparticle ensembles formed.

Conventional methods have either been limited to "post-mortem" analysis long after the growth subsided, "cherry picked" the particles being examined, thereby missing the mesoscale implications, or only analyzed the population average and missed the individual particle variances. Now, by considering the kinetics of the average growth rate and the distribution of particle sizes, the team explains why scientists see what they see when nanoparticle ensembles form via non-classical mechanisms.



By considering the kinetics of the average growth rate and the distribution of particle sizes, scientists can explain what they see when nanoparticle ensembles form via non-classical mechanisms.

The team's findings shed light on previously unexplained observations of aggregative nanoparticle growth. Such understanding of mesoscale interactions provides more precision in material synthesis, bringing us closer to tailored materials for catalysis, energy storage and other uses.

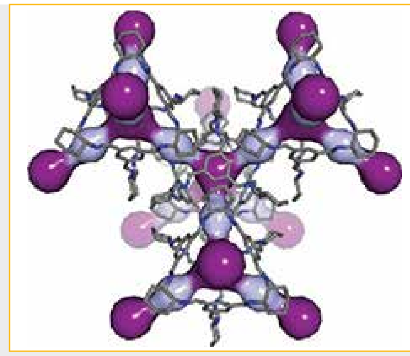
Woehl TJ, C Park, JE Evans, I Arslan, WD Ristenpart and ND Browning. 2014. "Direct Observation of Aggregative Nanoparticle Growth: Kinetic Modeling of the Size Distribution and Growth Rate." *Nano Letters* 14(1):373-378. DOI: 10.1021/nl4043328.

User Facility: EMSL
Sponsors: DOE Office of Science, Office of Basic Energy Sciences, National Institutes of Health, National Science Foundation, Chemical Imaging Initiative

MATERIALS SCIENCES

A Noble Gas Cage

When nuclear fuel gets recycled, the process releases radioactive krypton and xenon gases. A new porous material called CC3 effectively traps these gases, and researchers show how: by breathing enough to let the gases in but not out. Scientists from the University of Liverpool, PNNL, Newcastle University and Aix-Marseille Université performed simulations and laboratory experiments to determine how—and how well—CC3 might separate these gases from exhaust or waste. The CC3 material could be helpful in removing unwanted or hazardous radioactive elements from nuclear fuel or air in buildings and also in recycling useful elements from the nuclear fuel cycle. CC3 is much more selective in trapping these gases compared to other experimental materials. Also, CC3 will likely use less energy to recover elements than conventional treatments.



In this computer simulation, light and dark purple highlight the cavities within the three-dimensional pore structure of CC3.

"Xenon, krypton and radon are noble gases, which are chemically inert. That makes it difficult to find materials that can trap them. So we were happily surprised at how easily CC3 removed them from the gas stream."

—Dr. Praveen Thallapally, PNNL materials scientist

Chen L, PS Reiss, SY Chong, D Holden, KE Jelfs, T Hasell, MA Little, A Kewley, ME Briggs, A Stephenson, KM Thomas, JA Armstrong, J Bell, J Busto, R Noel, J Liu, DM Strachan, PK Thallapally and AI Cooper. 2014. "Separation of Rare Gases and Chiral Molecules by Selective Binding in Porous Organic Cages." *Nature Materials*. Advance article. DOI: 10.1038/nmat4035.

Sponsors: Engineering and Physical Sciences Research Council, European Research Council, DOE Office of Nuclear Energy

Chromium's Bonding Angles Let Oxygen Move Quickly

By taking advantage of the natural tendency of chromium atoms to avoid certain bonding environments, scientists have generated a material that allows oxygen to move through it very efficiently, and at relatively low temperatures. Using a combination of experimental and theoretical methods, scientists at PNNL probed the properties of ultra-pure crystalline films. They used molecular beam epitaxy to prepare the films. To characterize the films, they used scanning transmission electron microscopy, electron energy loss spectroscopy, X-ray diffraction, X-ray and ultraviolet photoemission, optical absorption and electrical transport. They used first-principles modeling to determine the structural transformations and oxygen anion diffusion kinetics. Specifically, they found that their attempts to make metallic $SrCrO_3$ led instead to the formation of semiconducting $SrCrO_{2.8}$. Because chromium as an ion with a charge of +4 does not like to form 90-degree bonds with oxygen, as it must in $SrCrO_3$, $SrCrO_{2.8}$ forms instead with a completely different crystal structure. This material contains oxygen-deficient planes through which oxygen can diffuse very easily. This work represents an important scientific advancement relevant to increasing the efficiency of solid oxide fuel cells, which require oxides capable of absorbing and transmitting oxygen anions at low temperature.

"If oxygen vacancies are present at high enough concentrations, they can aggregate and form new *ordered* structures. The ordered structures can create novel, mesoscale crystals."

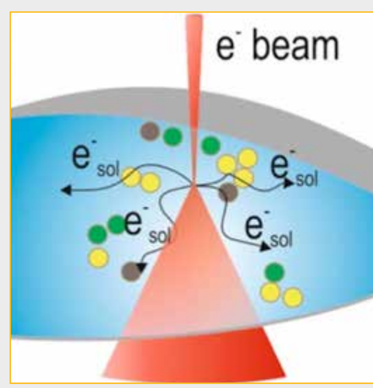
—Dr. Scott Chambers, PNNL Laboratory Fellow

Zhang H, Y Du, PV Sushko, ME Bowden, RJ Colby and SA Chambers. 2014. "Reversible Nano-Structuring of $SrCrO_{3-\delta}$ through Oxidation and Reduction at Low Temperatures." *Nature Communications* 5, Article number 4669. DOI: 10.1038/ncomms5669.

User Facility: EMSL
Sponsors: DOE Office of Science, Office of Basic Energy Sciences, EMSL postdoctoral fellowship, PNNL Laboratory Directed Research and Development

Degradation Mechanisms Uncovered in Lithium-Ion Battery Electrolytes

To develop new battery technologies, novel electrolytes with increased electrochemical stability are needed. A team led by PNNL characterized the stability and interconnected degradation mechanisms in electrolytes commonly used for lithium-ion batteries via an environmental liquid stage in a scanning transmission electron microscope (STEM). The results match with those from previous experiments achieved during battery operation, and the breakdown products and mechanisms agree with known mechanisms. The analysis indicates that liquid-stage STEM can provide insights into electrolyte behavior to winnow the library of candidate solutions for further characterization and reduce the experimental time spent on less-effective electrolytes.



Electrons in the solvent and other electron-beam-induced radical species interact through secondary chemical reactions with a lithium salt and solvent to degrade the battery electrolytes.

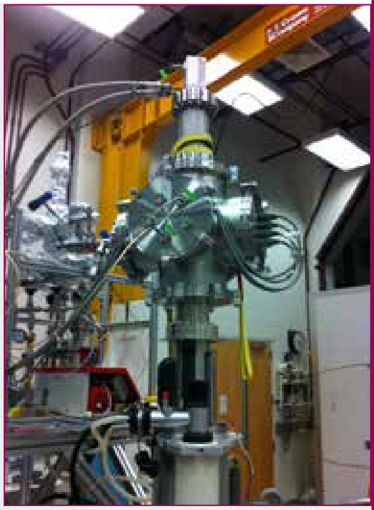
Abellan P, BL Mehdi, LR Parent, M Gu, C Park, W Xu, Y Zhang, I Arslan, J Zhang, CM Wang, JE Evans and ND Browning. 2014. "Probing the Degradation Mechanisms in Electrolyte Solutions for Li-Ion Batteries by In Situ Transmission Electron Microscopy." *Nano Letters* 14(3):1293-1299. DOI: 10.1021/nl404271k.

User Facility: EMSL
Sponsors: Chemical Imaging Initiative, Joint Center for Energy Storage Research

Installation of U.S.-made detector modules into Belle II Experiment at KEK Laboratory, Japan. PNNL is leading the U.S. contribution to the Belle II experiment. This international collaboration of more than 600 researchers from 23 countries is working to address why the universe contains matter, but is nearly void of antimatter.

Particle physics is the study of the fundamental constituents of matter and the forces of nature. PNNL is advancing the frontiers of nuclear and particle physics through the design and construction of cathedral-sized detector systems, novel materials and high-performance computer systems. The particle physics program at PNNL is built from a foundation in low background materials, precision assays, radiochemistry, detector design, microwave detection, remote handling, irradiation testing and data-intensive, high-performance computing. PNNL scientists and engineers are eager to apply this experience and technology to address today's key scientific questions in nuclear and particle physics.

Project 8: A Novel Approach to Probe the Neutrino Mass Scale



Project 8 prototype experiment.

Despite remarkable progress in understanding the fundamental properties of neutrinos, the scale of neutrino masses remains an open question. Knowledge of this scale will have significant impact on our understanding of both particle physics and cosmology, and hence it is the subject of inquiry for a number of experimental endeavors. Oscillation experiments conducted over the past 40 years have firmly concluded that neutrinos must possess a non-zero mass; yet, the mass scale itself remains elusive to experimental determination.

Project 8—a collaboration between PNNL, University of Washington, Massachusetts Institute of Technology and University of California at Santa Barbara—recently established a new technique to measure the neutrino mass scale based on detecting cyclotron radiation emitted by magnetically trapped electrons that holds the promise of 50 times the sensitivity of the current limits.

In addition to full engagement in the scientific effort, PNNL is providing computing for data processing and analysis, and enabling expertise in radiofrequency and microwave engineering to Project 8.

An Ultra-Rare Nuclear Decay with Massive Implications

With a half-life more than a quadrillion times longer than the age of the universe, one would be forgiven for thinking neutrinoless double beta decay could have little impact on the cosmic scale. And yet if nuclei can decay without the emission of neutrinos in the well known double beta decay process, it would signal that neutrinos are their own antiparticle—fundamentally different than all of the other elementary particles of the Standard Model. This situation could pave the way to understanding why the universe is predominately filled with matter. Our naïve theoretical notions of the Big Bang suggest a matter-dominated universe is unexpected. Curiously, the measurement of a decay process that fails to emit neutrinos also provides a window into the mass scale of the neutrinos (not) participating in this process. The neutrino's mass is another unknown wrinkle in the Standard Model of particle physics. PNNL scientists are collaborating on the construction of the Majorana Demonstrator, which looks toward the ultimate ton-scale experiment required to fully test the implications of neutrinoless double beta decay. Seeking to measure this ultra-rare nuclear process will help shed light on a rich set of scientific questions about the nature of the cosmos.

International Matter and Antimatter Experiment

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 collection of several million channels of precise radiation sensors that recorded the debris from electron-positron collisions at near 10 GeV center-of-mass energy from 1999 to 2010. These data are used for rare decay studies, exotic particle searches and precise measurements of B and D mesons and tau leptons and have resulted in nearly 400 publications in physics journals.

Alongside more than 600 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 KEK-B accelerator that will lead to a 50-fold increase in data available for precision studies and discovery science.

PNNL provides high-performance computational capabilities to support Belle and Belle II scientists in data management and analysis. Since July 2011, a high-performance computing capability for Belle has been available at PNNL with a storage footprint of about a petabyte. 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 trans-Pacific network bandwidth requirements."

—Dr. David Asner, PNNL Laboratory Fellow

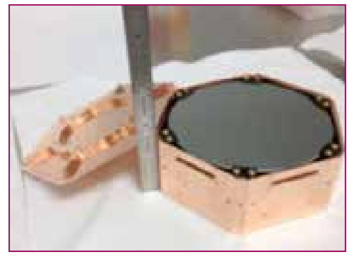
Dark Matter: A New Sector of Particles

Although invisible to our telescopes, dark matter is known by its gravitational effects throughout the universe. The nature of dark matter is unknown, but the consensus of the astrophysics and particle physics communities is that the dark matter is composed of new fundamental particles associated with an unknown sector of physics. PNNL is involved in the search for signals from dark matter particle interactions in the SuperCDMS, PICO and MiniCLEAN experiments. These experiments involve extremely low-background radiation detectors in deep underground laboratories.

Inner vessel of the MiniCLEAN detector deployed at SNOLAB.

SuperCDMS uses unique germanium detectors to search for dark matter interactions and cryogenic bolometry to identify background events. A new SuperCDMS project in the SNOLAB laboratory in Sudbury, Ontario, was recently selected as a second-generation dark matter project by DOE.

PICO has revived the bubble chamber technique that is extremely sensitive to low-energy nuclear interactions indicative of dark matter. PICO has the world's best sensitivity to dark matter interactions that depend on nuclear spin.



SuperCDMS prototype detector mounted inside a copper housing.

MiniCLEAN uses a novel approach to dark matter detection using 500 kg of liquid argon as the target material. The scintillation light of liquid argon fundamentally contains information on the nature of the particle interaction. Although MiniCLEAN is a large dark matter detector, it is a small, but critical, demonstration for the envisioned third-generation experiment, a high priority in the long-term strategy of the high energy physics community.

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, uranium and thorium assay and detector assembly are helping these experiments make order-of-magnitude improvements in sensitivity.

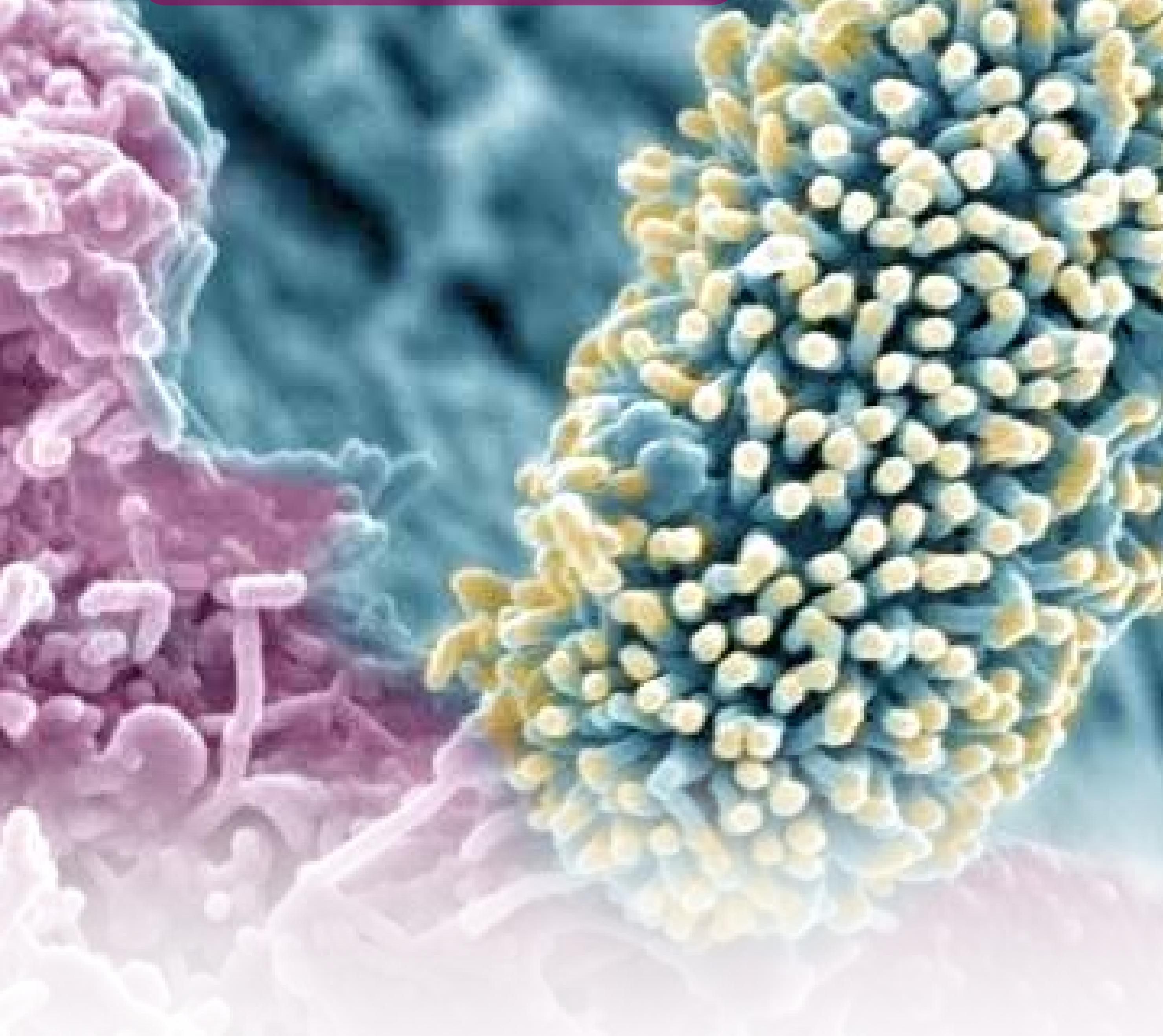
Exploring the Unknown in the Universe

Unique capabilities in ultra-low-background radiation detection and exploration of dark matter research contribute to PNNL's growing expertise in high energy physics to 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 DarkSide collaboration effort to purify low-activity argon extracted from underground sources engages PNNL in another leading dark matter effort and allows us to use this unique resource of low-activity argon for national security projects and in advancing age dating for environmental science. A supply of low-activity argon gas depleted in the radioactive isotope ^{39}Ar is essential for third-generation dark matter experiments but also benefits measurements for environmental science and security applications.
- Our computing and physics capabilities are contributing to the science case and detector optimization for experiments at the proposed international linear collider particle accelerator, which has a planned collision energy of 500 GeV and a possible upgrade to 1000 GeV (1 TeV).
- PNNL is working with the research physics community to understand the needs and requirements for low-background materials and their assay for next-generation dark matter and neutrinoless double beta decay experiments. Chemists and material scientists have much of the expertise required to identify and control primordial radioactivity in experimental instruments.
- PNNL is a founding member of the RaDIATE collaboration (Radiation Damage In Accelerator Target Environments) that seeks to understand and predict the radiation response of structural window and target materials used in the uniquely challenging radiation environment of high-power accelerators relevant to nuclear and particle physics applications. PNNL brings its expertise in fission and fusion reactor materials and post-irradiation examination to the collaboration.
- Detector development for future high energy and nuclear 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 2012.

Sponsors: PNNL Laboratory Directed Research and Development, DOE Offices of High Energy Physics and Nuclear Physics and U.S.-Japan Collaboration in High Energy Physics

There is a growing realization that the physiology of higher organisms is strongly impacted by the associated microflora. This is also true of plants where microbes aid nutrient acquisition and environmental tolerance. A multi-institutional group of scientists is studying the role and impact of microbial communities in the rhizosphere using multiple capabilities. This work is specifically focused on understanding how carbon allocation to the root environment impacts the diversity and size of the rhizosphere community. As is the case for most environmental microbial communities, many of the organisms present are unculturable, but new genomic methods allow their identification. This soil bacterium, shown attached to the plant root surface, was imaged using the Helios Nanolab dual-beam focused ion beam/scanning electron microscope 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.

Research Hones Pore-Scale Models

The physical and chemical processes that occur at the scale of individual soil particles dictate the way fluids flow underground over much larger scales. To more accurately predict how plumes of subsurface fluids, such as those harboring contaminants, will spread underground, scientists design numerical models that simulate flow at the pore scale. However, linking these numerical models to tangible experimental data has been challenging. Numerical simulations are required not only to model the way fluids move at the pore scale, but also to extrapolate to areas more expansive by several orders of magnitude, such as CO_2 sequestration sites, oil and gas reservoirs or contaminated mining or nuclear disposal sites. This study, the first of three learning challenges for the modeling community, allowed scientists from multiple institutions to hone their models on experimental data produced in EMSL's microfluidics laboratory, thus improving the predictive power of such models.

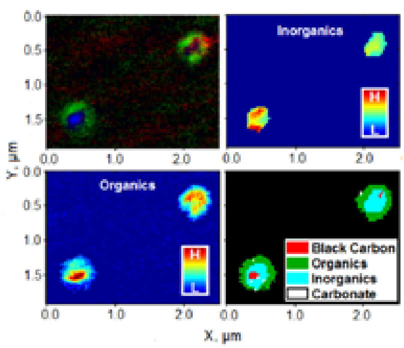
Modelers from eight institutions used different simulations to predict the simplest kind of flow: nonreactive transport. In this scenario, only one type of fluid flowed through the chamber and did not chemically react with the pore material. This way, researchers could focus on tweaking the physical properties that alter fluid movement, such as the flow rate, size and distribution of pores.

Oostrom M, Y Mehmani, P Romero-Gomez, Y Tang, H Liu, H Yoon, Q Kang, V Joekar-Niasar, MT Balhoff, T Dewers, GD Tartakovsky, EA Leist, NJ Hess, WA Perkins, CL Rakowski, MC Richmond, JA Serkowski, CJ Werth, AJ Valocchi, TW Wietsma and C Zhang. 2014. "Pore-Scale and Continuum Simulations of Solute Transport Micromodel Benchmark Experiments." *Computational Geosciences.* DOI 10.1007/s10596-014-9424-0.

Sponsors: DOE Office of Science, Offices of Biological and Environmental Research and Basic Energy Sciences, PNNL Laboratory Directed Research and Development

Forecast Calls for Better Models

Predicting how atmospheric aerosols influence cloud formation and the resulting feedback to climate is a challenge that limits the accuracy of atmospheric models. This is especially true in the Arctic, where both ice- and liquid-based clouds are frequently observed, but the processes that determine their composition are poorly understood. To obtain a closer look at what makes up Arctic clouds, scientists characterized cloud droplets and ice crystals collected at the North Slope of Alaska. The chemical composition, mixing state and size of individual particles and cloud droplet/ice residuals from Arctic clouds were characterized using a combination of scanning and transmission electron microscopy, X-ray analysis and spectroscopy at EMSL and the Advanced Light Source. The work differentiated particles that serve as cloud condensation nuclei and ice nuclei from those that do not, revealing compositional differences. The team found carbonate has a chemical advantage for Arctic mixed-phase cloud nucleation over other aerosol components.



Scanning transmission X-ray microscopy images of individual residues from Alaskan clouds.

Hiranuma N, SD Brooks, RC Moffet, A Glen, A Laskin, MK Gilles, P Liu, AM MacDonald, JW Strapp and GM McFarquhar. 2013. "Chemical Characterization of Individual Particles and Residuals of Cloud Droplets and Ice Crystals Collected on Board Research Aircraft in the ISDAC 2008 Study." *Journal of Geophysical Research: Atmospheres* 118(12):6564-6579. DOI: 10.1002/jgrd.50484.

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

How a Plant Beckons Bacteria

A common plant puts out a welcome mat to bacteria seeking to invade, and scientists have discovered the mat's molecular mix. The research examines a key moment in the relationship between microbe and host, when a microbe recognizes a host as a potential target and employs its molecular machinery to pierce it, injecting its contents into the plant's cells—a crucial step in infecting an organism. The study reveals new targets during the battle between microbe and host that researchers can exploit to protect plants. The humble and oft-studied plant *Arabidopsis* puts out a molecular signal that invites an attack from a pathogen. The findings come from a collaborative effort between scientists at the University of Missouri, PNNL and EMSL.

"This signaling system triggers a structure in bacteria that actually looks a lot like a syringe, which is used to inject virulence proteins into its target. It's exciting to learn that metabolites excreted by the host can play a role in triggering this system in bacteria."

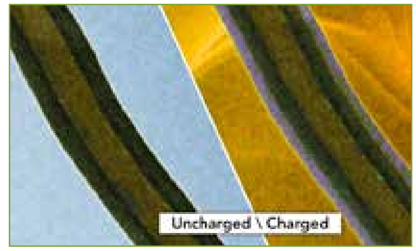
—Dr. Thomas Metz, PNNL chemist

Anderson JC, Y Wan, YM Kim, L Pasă-Tolić, TO Metz and SC Peck. 2014. "Decreased Abundance of Type III Secretion System-Inducing Signals in *Arabidopsis* mkp1 Enhances Resistance Against *Pseudomonas syringae*." *Proceedings of the National Academy of Sciences* 111(18):6846-6851. DOI: 10.1073/pnas.1403248111.

Sponsors: National Science Foundation, DOE Office of Science, Office of Biological and Environmental Research, EMSL

Batteries as They are Meant to Be Seen

Researchers at a host of national laboratories and universities have developed a wet battery cell in a transmission electron microscope at EMSL to microscopically view battery electrodes while they are bathed in wet electrolytes. This view mimics realistic conditions inside actual batteries. While life sciences researchers regularly use transmission electron microscopy to study wet environments, this time scientists have applied it successfully to rechargeable battery research. The work showed that many aspects can be studied under dry conditions, which are much easier to use. However, wet conditions are needed to study the hard-to-find solid electrolyte interphase layer, a coating that accumulates on the electrode's surface and dramatically influences battery performance.



Images from EMSL's transmission electron microscopy show the electrode transformation during the uncharged/charged process.

"The liquid cell gave us global information about how the electrodes behave in a battery environment, and it will help us find the solid electrolyte layer. It has been hard to directly visualize in sufficient detail."

—Dr. Chongmin Wang, EMSL senior research scientist

Gu M, LR Parent, BL Mehdi, RR Unocic, MT McDowell, RL Sacci, W Xu, JG Connell, P Xu, P Abellan, X Chen, Y Zhang, DE Perea, JE Evans, LJ Lauhon, JG Zhang, J Liu, ND Browning, Y Cui, I Arslan and CM Wang. 2013. "Demonstration of an Electrochemical Liquid Cell for Operando Transmission Electron Microscopy Observation of the Lithiation/Delithiation Behavior of Si Nanowire Battery Anodes." *Nano Letters* 13(12):6106-6112. DOI: 10.1021/nl403402q.

Sponsors: Joint Center for Energy Storage Research, DOE Office of Science, Office of Basic Energy Sciences, Chemical Imaging Initiative, DOE Assistant Secretary for Energy Efficiency and Renewable Energy, DOE Office of Vehicle Technologies, PNNL Laboratory Directed Research and Development, EMSL

Oxidative Corrosion of Uraninite Surfaces

Uraninite (UO_2) is the most abundant uranium ore mineral. UO_2 is the primary component of most nuclear fuels, and can be a major phase in bio-remediated uranium-contaminated soils and aquifers. Understanding the mechanisms of UO_2 surface oxidation and corrosion is essential to predicting its stability in the environment throughout the nuclear fuel cycle. The research team's earlier studies characterized uranium in oxidized surface films on the faces of single crystals of UO_2 using crystal truncation rod (CTR) X-ray diffraction. CTR shows the structural changes associated with the oxidation process, but does not yield direct information on oxidation state. Consequently, the team used X-ray photoelectron spectroscopy in EMSL's Radiochemistry Annex to measure oxidation states and found the presence of both U(V) and U(VI) in the oxidized layer, consistent with the team's computational results. The CTR measurements indicated development of a complex, oscillatory oxidation front that is distinct from a classical diffusion profile. This anomalous type of diffusion/oxidation has not been observed before and may be relevant to other fluorite structures, including plutonium dioxide.

Stubbs JE, AM Chaka, ES Ilton, CA Biwer, JR Bargar and PJ Eng. 2014, "Oxidative Corrosion of Uraninite (UO_2) Surfaces." (In preparation)

Sponsors: DOE Office of Science, Offices of Basic Energy Sciences and Biological and Environmental Research, National Science Foundation

Biofuel Breakdown: Freeing Plant Sugars in Lignin

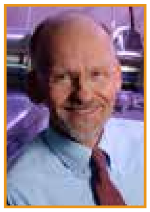
Biofuels made from plant materials—also known as lignocellulosic biofuels—are promising as sustainable alternative fuels thanks to soil bacterium known as *Enterobacter lignolyticus* SCF1. SCF1 degrades lignin and decomposes plant cell walls, allowing access to the cellulose sugars plants use for energy. Much remains to be learned about the processes and functions of SCF1 in breaking down lignin for use in biofuels. Using EMSL capabilities, this study reveals key insights, including that SCF1 is the first soil bacterium to demonstrate the dual ability to degrade lignin both as a food source and for breathing. Lignocellulose is a renewable and abundant energy source with sufficient national supply to make lignocellulosic biofuels sustainable and economically feasible. Furthermore, lignocellulose is not used for food and therefore does not take food out of the supply chain. However, lignocellulose is one of the more difficult biomass materials to break down and transform for biofuel use. This work moves scientists one step further toward that goal.

DeAngelis KM, D Sharma, R Varney, B Simmons, NG Isern, LM Markilllie, C Nicora, AD Norbeck, RC Taylor, JT Aldrich and EW Robinson. 2013. "Evidence Supporting Dissimilatory and Assimilatory Lignin Degradation in *Enterobacter lignolyticus* SCF1." *Frontiers in Microbiology.* DOI: 10.3389/fmicb.2013.00280.

Sponsors: University of Massachusetts, DOE Office of Science, Office of Biological and Environmental Research, Joint BioEnergy Institute

DICK SMITH

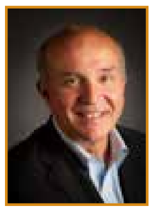
CDC Board



Battelle Fellow **Dick Smith** is serving on the Board of Scientific Counselors, Office of Public Health Preparedness and Response of the Centers for Disease Control and Prevention (CDC) through September 2017. He was invited for his knowledge of new technologies and their applications to study, measure and monitor biological systems. He is internationally known for development of advanced analytical methods and instrumentation, with emphasis on high-resolution separations and mass spectrometry, and their applications in biological and biomedical research.

JOHANNES LERCHER

Francois Gault Lectureship



Director of PNNL's Institute for Integrated Catalysis **Johannes Lercher** received the 2013 Francois Gault Lectureship Award, Europe's highest honor in catalysis. He was recognized for his groundbreaking contributions in understanding molecular interactions in solid catalysts through elegant combinations of physicochemical and kinetic analyses. As recipient, he will give plenary lectures across Europe.

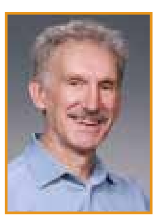
MORRIS BULLOCK

Royal Society of Chemistry Fellow

Laboratory Fellow **Morris Bullock** was named a fellow of the Royal Society of Chemistry, the largest organization in Europe for advancing the chemical sciences. He was recognized for his scientific contributions and for winning the Society's 2013 Homogeneous Catalysis award.

PHIL RASCH

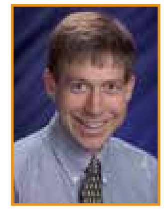
Climate Modeling Achievement Award



Chief Scientist for climate science at PNNL, **Phil Rasch** was awarded the 2013 Community Earth System Model (CESM) Distinguished Achievement Award by the CESM advisory board. He was honored for his contributions to the growth and prominence of the model, in development for over 30 years. Scientists use CESM for global climate studies as the model provides state-of-the-art simulations of the Earth's past, present and future climate states.

SCOTT BAKER

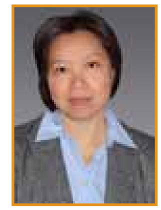
SIMB President-Elect



EMSL Biosystem Dynamics and Design Science Theme lead **Scott Baker** was chosen to be president-elect for the Society for Industrial Microbiology and Biotechnology. This international association advances microbiological sciences, especially as they apply to industrial products, biotechnology, materials and processes. Baker was chosen, in part, for his work using genetic, genomic and proteomic strategies to understand important fungal biology problems.

RUBY LEUNG

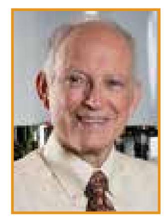
AGU Fellow



Laboratory Fellow **Ruby Leung** joined the American Geophysical Union (AGU) as a fellow. She is an internationally recognized leader in regional climate modeling. Her innovative research on modeling regional climate change and its impacts guide national policy-makers on decisions related to water, agriculture, energy, public health and national security.

DON BAER

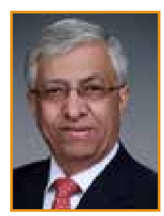
ASTM International Award of Merit



Laboratory Fellow and EMSL Science Theme lead Don Baer was selected to receive the 2014 ASTM Award of Merit. The award and its accompanying title of fellow are ASTM's highest organizational recognition for individual contributions to standards activities.

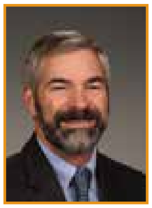
GHASSEM ASRAR

AGU Ambassador



Director of the Joint Global Change Research Institute **Ghassem Asrar** was named a 2014 Ambassador for the American Geophysical Union. He is one of five honorees recognized for outstanding contributions in the areas of societal impact, service to the Earth and space community, scientific leadership and promotion of talent.

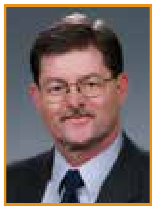
JIM DE YOREO



Materials Research Society Fellow

Jim De Yoreo, Chief Scientist of PNNL's Materials Synthesis and Simulation across Scales Initiative, was selected as a Materials Research Society Fellow. He was chosen for his pioneering research in the field of bio-inspired materials science and engineering along with his distinguished leadership and service to the materials community.

JAY GRATE



Electrochemical Society Fellow

Named a fellow in the Electrochemical Society, Laboratory Fellow **Jay Grate** was chosen for his contributions to chemical sensors and the scientific community. He is known for pioneering a systematic understanding of vapor-polymer interactions critical to the selectivity of polymer-coated vapor sensors.

BORA AKYOL

IEEE Senior Member

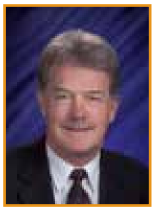
Computational scientist **Bora Akyol** was named an Institute of Electrical and Electronics Engineers (IEEE) senior member, the highest grade for IEEE members. He demonstrated significant performance in network security, information sharing protocols and the Smart Grid, earning recognition from his peers for technical and professional excellence.

DANIEL CHAVARRÍA-MIRANDA

ACM Senior Member

Computational scientist **Daniel Chavarría-Miranda** was named an Association for Computing Machinery senior member. He was chosen for his expertise in the areas spanning parallel and distributed systems, compilers for high-performance and parallel computing, programming languages and interactions of architectural features with software systems.

DAVE KOPPENAAL



Chemical Instrumentation Award

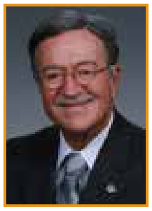
EMSL's Chief Technology Officer **Dave Koppenaal** was named the American Chemical Society's recipient of the Division of Analytical Chemistry Award in Chemical Instrumentation. He was honored for his work in developing unique plasma-source mass spectrometry instrumentation, which has pushed the frontiers of environmental and nonproliferation analysis and detection.

KIM HIXSON

Graduate Student Award

EMSL research scientist **Kim Hixson** was honored by the American Chemical Society's Withycombe-Charalambous Graduate Student Symposium Award. She was recognized for her work altering the enzyme composition of arogenate dehydratase in plants to reduce lignin levels and to study the systems-level effects of such changes using multi-omics technology.

JEAN FUTRELL



International Conference Dedication

The high-resolution mass analysis session at the Innovations in Mass Spectrometry Instrumentation 2013 Conference was dedicated in honor of Battelle Fellow **Jean Futrell's** 80th birthday. The conference was co-sponsored by the United States and Russia to promote the exchange of ideas and information among academia, industry and others that rely on mass spectrometry. He was chosen for his work in the theory and practice of mass spectroscopy.

JANET JANSSON

President of International Society for Microbial Ecology

Director of Biological Sciences **Janet Jansson** was installed as president of the International Society for Microbial Ecology (ISME). She will serve as president through 2016, and will preside during the period leading up to the 2018 symposium in Montreal, Canada. She has served as president-elect since the 2012 symposium. ISME is the principal scientific society for the burgeoning field of microbial ecology and its related disciplines.

KATRINA WATERS

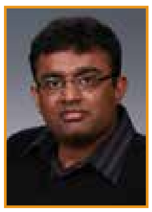
New National Academies Committee


Katrina Waters

Deputy Director of Biological Sciences **Katrina Waters** has been appointed to a new National Academies Study on Predictive-Toxicology Approaches. The study committee will evaluate modern toxicology approaches for use by the Department of Defense to predict toxicity, in efforts to prevent debilitating acute exposures to deployed personnel.

ABHINAV VISHNU, GEORGE CHIN, SUTANAY CHOUDHURY

Scientists Take Lead at ParLearning 2014


Abhinav Vishnu


George Chin


Sutanay Choudhury

Abhinav Vishnu, George Chin and **Sutanay Choudhury** led efforts involved in the Workshop on Parallel and Distributed Computing for Large Scale Machine Learning and Big Data Analytics, or ParLearning 2014. The workshop focused on the potential of parallel and distributed computing to deal with the massive data sets generated by today's computing platforms. ParLearning 2014 was another example of PNNL's leadership position in the big data research area.

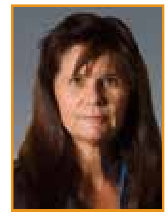
RESEARCH PLAYS KEY ROLE IN IPCC CONCLUSIONS

Groundbreaking research from PNNL provided scientific insights for the Intergovernmental Panel on Climate Change (IPCC) Fifth Assessment Report's new lower bound estimate of the climate's sensitivity to increasing carbon dioxide concentrations. With contributions from thousands of experts around the world, the report—the first of three working group contributions to the Fifth Assessment—prominently cited PNNL's work in several of its key conclusions on the causes and physical consequences of climate change. PNNL contributions to the report are evidenced by citations of 17 PNNL lead-authored papers and more than 50 papers with PNNL authors cited.

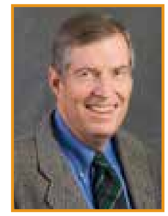
RICHARD MOSS, KATHY HIBBARD, JAMES EDMONDS, ALLISON THOMSON

Contribute to National Climate Assessment


Richard Moss

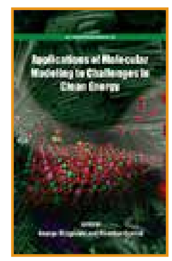

Kathy Hibbard


Allison Thomson


James Edmonds

Atmospheric scientists **Richard Moss, Kathy Hibbard, James Edmonds** and **Allison Thomson** were key contributors to the third National Climate Assessment. The report presents an analysis of the best science and information from U.S. agencies, institutes, national laboratories and universities to understand the implications of climate and global change.

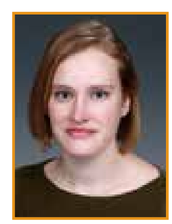
BOOK ON ANSWERING CLEAN ENERGY CHALLENGES

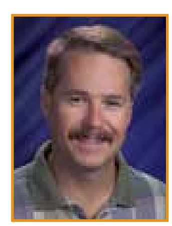


Scientists at PNNL contributed to *Applications of Molecular Modeling to Challenges in Clean Energy*, which was based on invited talks at an American Chemical Society symposium. The book focuses on using computational modeling to answer basic questions in catalysis, biofuels and other sustainable solutions. PNNL contributors were **Niranjan Govind, Vanda Glezakou, B. Peter McGrail, H. Todd Schaef, Yeohoon Yoon, Ming-Hsun Ho, Shentan Chen, Roger Rousseau, Michel Dupuis, Morris Bullock** and **Simone Raugei.**

SUSAN CROWELL, JUSTIN TEEGUARDEN

Best Risk Assessment Paper Honors


Susan Crowell


Justin Teeguarden

Contributions to two papers by **Susan Crowell** and **Justin Teeguarden** led to "Best Papers Published in 2013 Demonstrating Application of Risk Assessment" honors by the Risk Assessment Specialty Section of the Society of Toxicology, the major scientific society focusing on the acquisition and use of knowledge in toxicology to aid in the protection of human health. They each were the primary authors of their respective papers.

SRIRAM KRISHNAMOORTHY

Three SC14 Papers Prove HPC Matters

Computational scientist **Sriram Krishnamoorthy** is making a notable impact at this year's International Conference for High Performance Computing (HPC), Networking, Storage and Analysis, or SC14, as co-author of three accepted papers—two of which are up for best paper awards. The SC14 conference accepted only 84 out of 392 paper submissions, which includes 8 best paper and 6 best student paper finalists.

MAHANTESH HALAPPANAVAR

Best Paper for Homeland Security

Homeland Security Affairs released a supplement showcasing the top five "best papers" resulting from the 2013 Institute of Electrical and Electronics Engineers International Conference on Technologies for Homeland Security. Among the chosen best was PNNL's preliminary research involving effective reconstitution approaches for cyber systems, authored by **Pradeep Ramuhalli, Mahantesh Halappanavar** (pictured), **Jamie Coble** and **Mukul Dixit**.

PATRICIA ABELLAN

Best Ph.D. Thesis in Materials Science

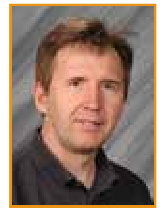
Patricia Abellan received the international Best Ph.D. Thesis in Material Science award from the Microscopy Society of Spain. At the Autonomous University of Barcelona, she studied how strain state and interface structure in oxide nanostructured materials grown by a solution route changed the material's superconductivity, magnetism and other properties. She also discovered a novel mechanism for lattice parameter relaxation.

CENTER FOR MOLECULAR ELECTROCATALYSIS RENEWED

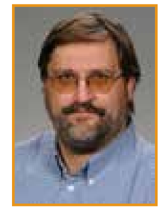
Directed by PNNL chemist **Morris Bullock**, the Center for Molecular Electrocatalysis was renewed and will receive $3.5 million a year for four years from DOE's Office of Science. Since 2009, researchers at the center have been studying catalysts that convert electrical energy into chemical bonds and back again. These reactions are at the core of technologies such as solar energy and fuel cells.

MARAT VALIEV, KAROL KOWALSKI

Best 80 Papers in 80 Years



Marat Valiev

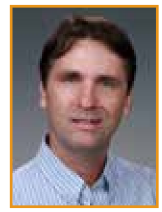


Karol Kowalski

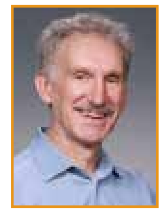
The *Journal of Chemical Physics* selected an article by EMSL senior research scientists **Marat Valiev** and **Karol Kowalski** as one of the best 80 papers in the journal's 80 years. The paper, "Hybrid Coupled Cluster and Molecular Dynamics Approach: Application to the Excitation Spectrum of Cytosine in the Native DNA Environment," was published in the journal's 2006 issue.

ALEX GUENTHER, PHIL RASCH, YUEHE LIN

Researchers Named Most Cited



Alex Guenther



Phil Rasch

Yuehe Lin

Researcher **Alex Guenther, Phil Rasch,** and **Yuehe Lin** have been named to a comprehensive list of the world's most referenced scientists in Thomson Reuters' Highly Cited Researchers 2014. The list includes more than 3,200 researchers whose scientific publications were in the top 1 percent of papers receiving the most references. Only 250 researchers in each field were selected based on total citations to their papers published during this period.

XIAO-YING YU, MARTIN IEDEMA, BINGWEN LIU, ZIHUA ZHU, MATTHEW MARSHALL

R&D 100 Award

A team of research scientists developed the System for Analysis at the Liquid Vacuum Interface, or SALVI, that for the first time allows instruments to image liquid samples in real-time and space. R&D Magazine honored SALVI's research team with an R&D 100 award. R&D Magazine selects the 100 most innovative scientific and technological breakthroughs of the year from nominations spanning private, academic and government institutions. With SALVI, scientists can gain new insights about nanoparticles, bacteria, batteries and more. The team recognized for developing SALVI includes **Xiao-Ying Yu, Martin Iedema, Bingwen Liu, Zihua Zhu,** and **Matthew Marshall**. The team developed SALVI in collaboration with scientists at EMSL.

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 4,300 staff, has an annual budget of $936 million, and has been managed by Ohio-based Battelle since the Laboratory's inception in 1965.

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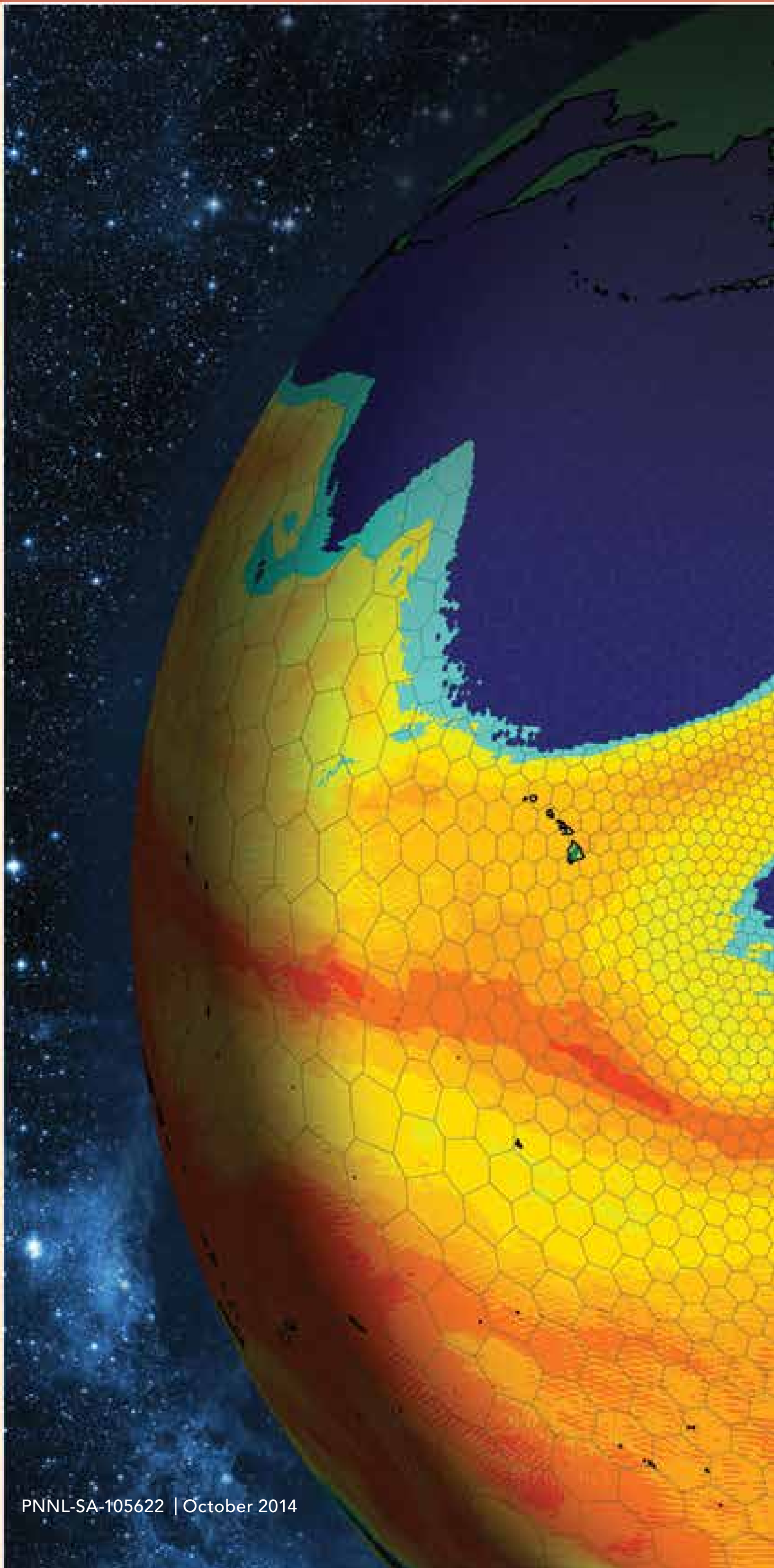
▶ **www.pnnl.gov/science**



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