



**EMSL Quarterly Highlights Report**  
**1<sup>st</sup> Quarter, Fiscal Year 2010**  
**(October 1, 2009, through**  
**December 31, 2009)**

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## **EMSL Quarterly Highlights Report, 1<sup>st</sup> Quarter, Fiscal Year 2010**

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EMSL—the Environmental Molecular Sciences Laboratory—is a U.S. Department of Energy (DOE) national scientific user facility located at Pacific Northwest National Laboratory (PNNL) in Richland, Washington. EMSL is operated by PNNL for the DOE Office of Biological and Environmental Research. At one location, EMSL offers a comprehensive array of leading-edge resources and expertise.

Access to the instrumentation and expertise is obtained on a peer-reviewed proposal basis. Users are participants on accepted proposals. Staff members work with users to expedite access. The EMSL Quarterly Highlights Report documents research and activities of EMSL staff and users.

## **Research Highlights**

### **Biological Interactions and Dynamics**

#### **A Seafloor Microbial Biome Hosted Within Incipient Ferromanganese Crusts**

***AS Templeton,<sup>(a)</sup> EJ Knowles,<sup>(a)</sup> KL Eldridge,<sup>(a)</sup> BW Arey,<sup>(b)</sup> AC Dohnalkova,<sup>(b)</sup> SM Webb,<sup>(c)</sup> BE Bailey,<sup>(d)</sup> BM Tebo,<sup>(e)</sup> and H Staudigel<sup>(d)</sup>***

*(a)* University of Colorado, Boulder, Colorado

*(b)* EMSL, Richland, Washington

*(c)* Stanford Synchrotron Radiation Lightsource, Menlo Park, California

*(d)* Scripps Institute of Oceanography, La Jolla, California

*(e)* Oregon Health and Sciences University, Beaverton, Oregon

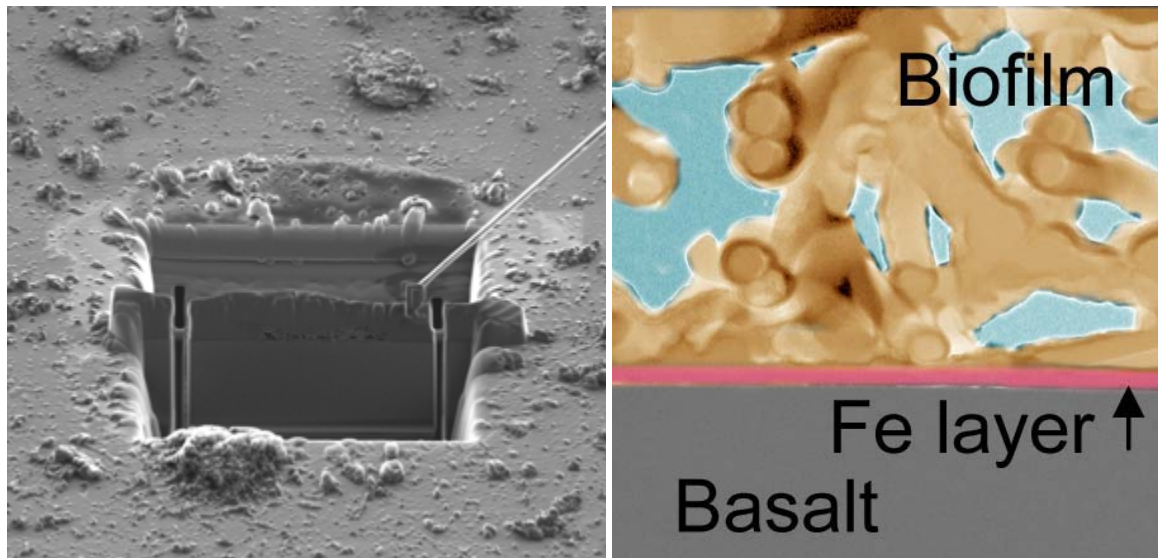
*Using resources at the Department of Energy's EMSL and the Stanford Synchrotron Radiation Lightsource, scientists found that very low concentrations of dissolved metals in seawater may be the energy source microbial communities use to colonize seafloor rocks, presenting insights into how microbial communities thrive in the Earth's crust. These insights into the real-time evolution of the biosphere show how the Earth and its environmental processes function.*

The current hypothesis is that these communities derive the energy needed to grow by dissolving and oxidizing volcanic-created basalt. The team began with samples of young pillow basalts from the Loihi seamount, an underwater volcano known as the youngest in the Hawaiian chain. They determined the chemical changes that occurred on the basalt surfaces as the microbes colonized and grew.

The analyses showed little evidence of basalt dissolution. Rather, biofilm growth was intimately tied to the oxidation of iron and manganese from the seawater, leading to the deposition of highly reactive Fe(III) and Mn(IV) oxide layer on the basalts surfaces. High-resolution imaging at EMSL on polished basalt glasses left near the volcano for a year also showed that volcanic glasses rapidly obtained an iron layer during biofilm growth. Over time, these mineral layers are likely to exert an enormous influence on the environmental chemistry of the seafloor. Microscopy experts at EMSL were significant contributors on the team from the University of Colorado at Boulder, SSRL, Scripps Institution of Oceanography, and the Oregon Health & Sciences University. This study was the first user project to apply EMSL's focused ion beam/scanning electron microscope.

This research offers a new hypothesis regarding the growth of microbial organisms in the ocean crust, and their key role in creating biominerals during dynamic biogeochemical processes in the seafloor ecosystem.

The research, funded by the National Science Foundation, the David and Lucille Packard Foundation, and a NASA Predoctoral Fellowship, was published in *Nature Geoscience*.



*Focused ion beam technology allows preparation of a precise cross-section into the basalt sample covered with a newly formed iron layer and biofilm. A thin section is used for imaging and analyses by transmission electron microscopy.*

**Citation:**

Templeton, AS, EJ Knowles, KL Eldridge, BW Arey, AC Dohnalkova, SM Webb, BE Bailey, BM Tebo, and H Staudigel. 2009. "A Seafloor Microbial Biome Hosted Within Incipient Ferromanganese Crusts." *Nature Geoscience*. DOI: 10.1038/NGE0696.

## Geochemistry/Biogeochemistry and Subsurface Science

### Uranium in Framboidal Pyrite from a Naturally Bioreduced Alluvial Sediment

*N Qafoku,<sup>(a)</sup> RK Kukkadapu,<sup>(b)</sup> JP McKinley,<sup>(a)</sup> BW Arey,<sup>(b)</sup> SD Kelly,<sup>(c)</sup> CM Wang,<sup>(b)</sup> CT Resch,<sup>(a)</sup> and PE Long<sup>(a)</sup>*

(a) Pacific Northwest National Laboratory, Richland, Washington

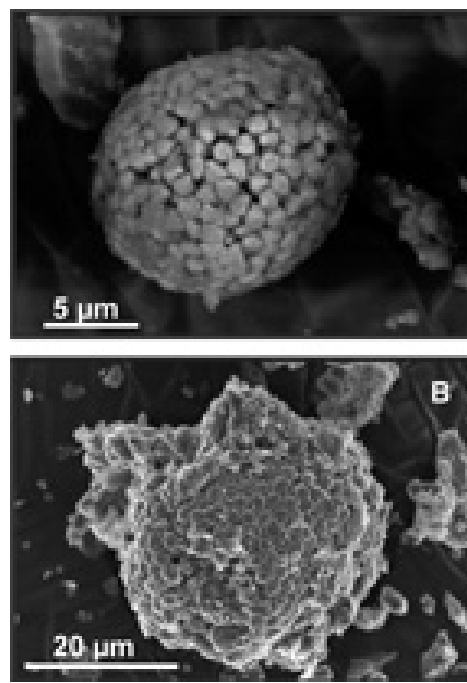
(b) EMSL, Richland, Washington

(c) Argonne National Laboratory, Argonne, Illinois

*Using microscopic and spectroscopic resources at the Department of Energy's EMSL, scientists determined that pyrites or fool's gold in bio-reduced alluvial sediments may initially sequester subsurface uranium and then serve as a long-term source under conditions of slow oxidation. Thus, microbially altered, unconsolidated sediment may contribute to the persistence of uranium in the groundwater at former uranium milling sites. These results may help in developing remediation measures for uranium-contaminated aquifers.*

At a number of sites around the country including former nuclear weapons sites, uranium has contaminated sediments and groundwater. For example, the subsurface at the Hanford Site in Washington State is estimated to hold 202,703 kilograms of uranium. Understanding how and when uranium migrates may aid in creating remediation approaches to extract or halt the radionuclide's progress.

In this research, small particles of framboidal pyrites ( $\text{FeS}_2$ ), from  $\sim 10\text{--}20\ \mu\text{m}$  in diameter, were abundant in the  $<53\text{-}\mu\text{m}$  fraction of the sediment from the saturated zone at the Integrated Field Challenge Site near the Colorado River near Rifle, Colorado. These particles were of varying microcrystal morphologies, degrees of surface weathering, and internal porosity. However, these pyrites were absent where microbial activity had not reduced the surrounding minerals. An array of spectroscopic techniques showed elevated uranium in both the oxidized and reduced states was present in framboidal pyrite. These characterizations were made possible by integrating spectroscopic and microscopic resources at EMSL. These resources included scanning electron microscopy combined with focused ion beam, high-resolution transmission electron microscopy combined with selected area electron diffraction and  $^{57}\text{Fe}$ -Mössbauer spectroscopy. Resources in laboratories at Pacific Northwest National Laboratory and Argonne National Laboratory (x-ray absorption spectroscopy) were also used.



*By integrating resources at EMSL, the team was to obtain extremely detailed views of the framboidal (French for raspberry) pyrites found in the sediment of interest. The top image is of a sphere-like structure and the bottom image is an irregular framboidal structure.*

This work, supported by DOE's Environmental Remediation Sciences Program within the Office of Biological and Environmental Research, was published in *Environmental Science & Technology*.

**Citation:**

Qafoku N, RK Kukkadapu, JP McKinley, BW Arey, SD Kelly, CM Wang, CT Resch, and PE Long. 2009. "Uranium in framboidal pyrite from a naturally bioreduced alluvial sediment." *Environmental Science & Technology* 43(22):8528-8534.

## **Characterization of an Electron Conduit between Bacteria and the Extracellular Environment**

***RS Hartshorne,<sup>(a)</sup> CL Reardon,<sup>(b)</sup> DE Ross,<sup>(c)</sup> J Nuester,<sup>(c)</sup> TA Clarke,<sup>(a)</sup> AJ Gates,<sup>(a)</sup> PC Mills,<sup>(a)</sup> JK Fredrickson,<sup>(b)</sup> JM Zachara,<sup>(b)</sup> L Shi,<sup>(b)</sup> AS Beliaev,<sup>(b)</sup> MJ Marshall,<sup>(b)</sup> M Tien,<sup>(c)</sup> L Brantley,<sup>(c)</sup> JN Butt,<sup>(a)</sup> and D Richardson<sup>(a)</sup>***

(a) University of East Anglia, Norwich, England

(b) Pacific Northwest National Laboratory, Richland, Washington

(c) Pennsylvania State University, University Park, Pennsylvania

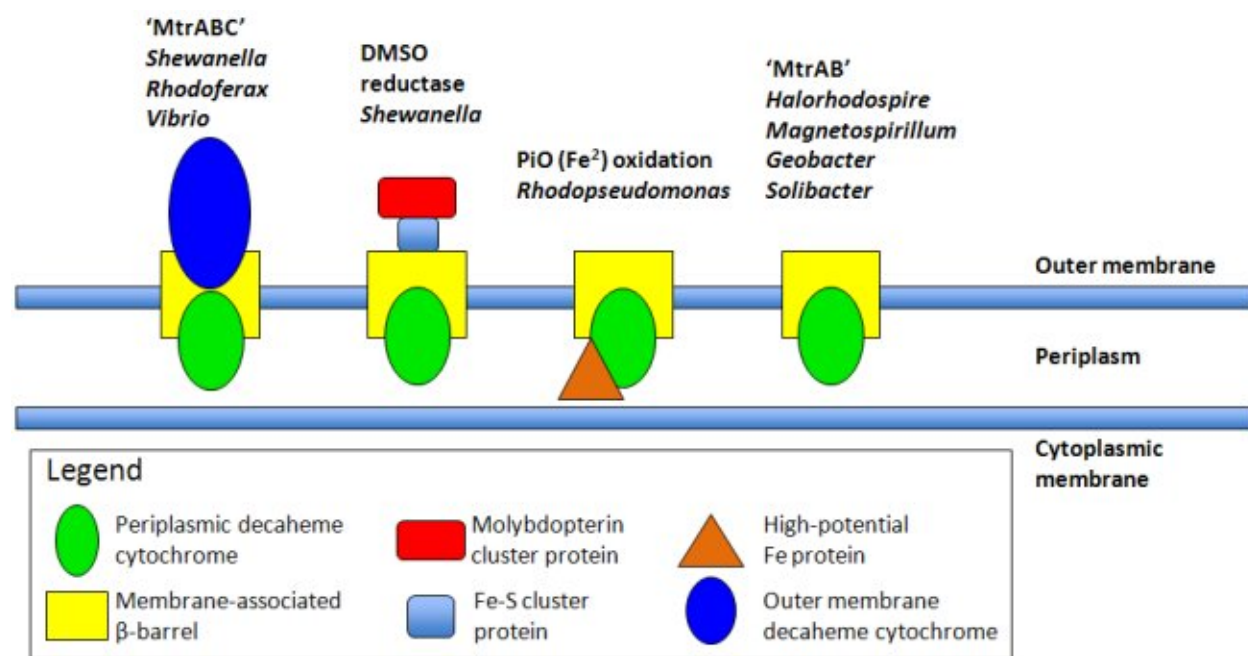
*Scientists at the University of East Anglia, Pacific Northwest National Laboratory, and Pennsylvania State University have demonstrated for the first time the mechanism by which some bacteria can transfer electrons across a membrane to the cell exterior, allowing them to "breathe" metals. These iron-respiring bacteria link the cycling of iron and carbon in subsurface and surface sediments and can catalyze the immobilization of subsurface contaminants such as uranium.*

In an article published in *Proceedings of the National Academy of Sciences*, the researchers described the protein complex—and its electrochemical properties—from *Shewanella oneidensis*, a bacterium renowned for its diverse metabolism and ability to immobilize certain radioactive contaminants. This research demonstrated a novel outer membrane-spanning electron transfer system that enables the proteins MtrA (inward facing) and MtrC (outward facing) to embed sufficiently within a third transmembrane protein, MtrB, to allow electron transfer to take place between them.

Iron respiration is one of the most ancient respiratory processes for microorganisms. It is among the most common in oxygen-free habitats and therefore has wide environmental significance. In species of *Shewanella* and other metal-reducing bacteria, some electron transfer proteins, called cytochromes, are positioned at the extracellular face of the bacterium's outer membrane where they can interact with insoluble substrates such as iron oxides. To transfer electrons onto these substrates to gain energy for growth and metabolism, these proteins must be charged by the cell's electron transfer system much of which resides at the inner membrane. The electron transfer reaction results in an oxidation state change (reduction) in electron acceptors such as iron minerals that are external to the cell. The electron delivery to these proteins requires that electrons originating from the inner membrane be transferred across the outer membrane. The biochemical basis for this has not previously been understood.

The research team used proteoliposomes—lipid vesicles containing proteins—and the redox dye methyl viologen to demonstrate electron transfer across a membrane. They then used protein film voltammetry to measure the electrochemical properties of the proteins, individually and as a complex.

According to the PNNL team, this is the first demonstration of protein complex that catalyzes such an important reaction. The authors also noted that similar MtrA-MtrB modules are present in many other types of bacteria, possibly for different reactions that require electron transfer to, or possibly from, the cell surface.



*MtrAB* homologues in a range of phyla and outer membrane electron transport systems. The 'MtrAB' electron transfer module could be a solution to electron exchange across the outer membrane in a range of respiratory systems and bacterial phyla. For example, *Shewanella* can respire extracellular forms of DMSO by localizing the catalytic subunits (*DmsAB*) to the outside of the cell. The genes encoding the catalytic subunits cluster with *dmsE* and *dmsF* that encode homologues of *MtrA* and *MtrB*, suggesting a similar mechanism for moving electrons across the outer membrane. Homologues of *MtrA* and *MtrB* (*PioA* and *PioB*) are also associated with phototropic Fe(II) oxidation in *Rhodopseudomonas palustris*. In this case, electrons could be moving into the cell from extracellular Fe(II).

The next steps in this research involve obtaining high-resolution structures for each of the proteins as well as the entire complex to use the structural information in concert with protein interaction data to establish precisely how electrons enter, traverse, and then exit the protein complex. The discovery and functional understanding of protein modules capable of electron transfer across membranes may also be of use in synthetic biology; for example, in bioenergy applications.

This work was funded by EMSL's Biogeochemistry Grand Challenge and the Subsurface Science Scientific Focus Area of DOE's Environmental Remediation Sciences Program.

**Citation:**

Hartshorne RS, CL Reardon, DE Ross, J Nuester, TA Clarke, AJ Gates, PC Mills, JK Fredrickson, JM Zachara, L Shi, AS Beliaev, MJ Marshall, M Tien, SL Brantley, JN Butt, and D Richardson. 2009. "Characterization of an Electron Conduit between Bacteria and the Extracellular Environment." *Proceedings of the National Academy of Sciences of the United States of America* 106 (52):22169-22174.

## Geophysical Monitoring of Coupled Microbial and Geochemical Processes during Stimulated Subsurface Bioremediation

*KH Williams,<sup>(a)</sup> A Kemna,<sup>(b)</sup> MJ Wilkins,<sup>(c)</sup> J Druhan,<sup>(d)</sup> E Arntzen,<sup>(c)</sup> AL N'Guessan,<sup>(c)</sup> PE Long,<sup>(c)</sup> SS Hubbard<sup>(d)</sup> and JF Banfield<sup>(d)</sup>*

(a) Lawrence Berkeley National Laboratory, Berkeley, California

(b) University of Bonn

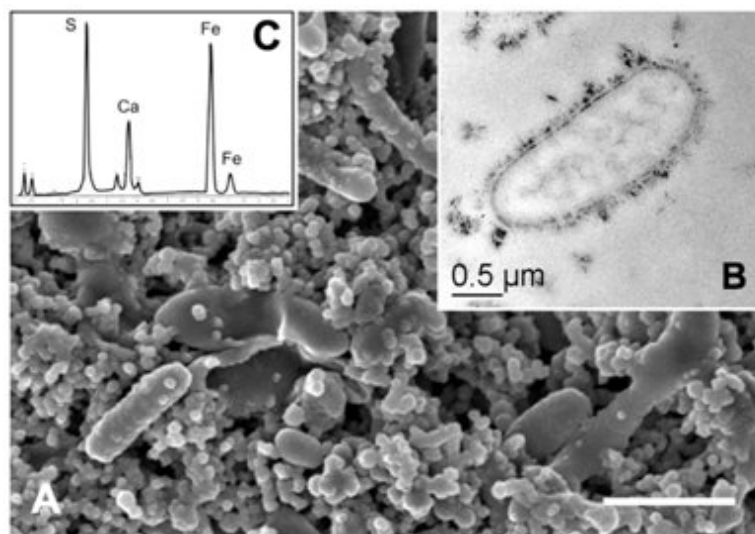
(c) Pacific Northwest National Laboratory, Richland, Washington

(d) University of California, Berkeley, California

*Scientists as superheroes? Well, maybe, at least in their ability to "see" through subsurface soil and rock, by using a new technique for monitoring groundwater contamination that eliminates the need to drill wells. Scientists recently performed the first field demonstration of a minimally invasive monitoring approach for tracking subsurface biogeochemical changes accompanying the bioreduction of a uranium-contaminated aquifer. Their results showed that the approach, called surface spectral-induced polarization (SSIP), is both feasible and practical for remote monitoring of microbial activity stimulated during microbiological reduction.*

The SSIP approach lets scientists track geochemical and mineralogical changes that occur when electron donors, such as acetate, are added to groundwater to stimulate subsurface microbial activity. SSIP was developed by scientists from Lawrence Berkeley National Laboratory, Pacific Northwest National Laboratory, the University of Bonn in Germany, and the University of California, Berkeley. The field demonstration took place at a former uranium mill tailings site near Rifle, Colorado.

Groundwater contamination by industry and nuclear weapons programs has spurred research into the use of microorganisms to facilitate remediation by isolating aqueous metals and radionuclides in forms in which they can't move. Much of the research has focused on microorganisms capable of immobilizing contaminants, such as uranium, after introducing organic carbon compounds, such as acetate, lactate and ethanol.



*Scanning electron microscope image of filter residue obtained from groundwater pumped from a Rifle well. (B) High-resolution TEM image of individual cell and surface-associated precipitates. (C) Energy dispersive X-ray spectrum of precipitates in (A).*



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

The research team used SSIP to monitor stimulated microbial activity in the Rifle aquifer while acetate is added. They injected variable frequency currents into the ground and measured resulting voltage potentials using electrodes embedded in the ground surface. The electrical response was dependent upon the predominant metabolic processes active in the subsurface at a given point in time.

The accumulation of mineral precipitates, such as iron sulfide, and electroactive ions, such as ferrous and hydrogen sulfide) altered the ability of fluids in the subsurface pore spaces to conduct electrical charge. This accounted for the anomalous electrical response and revealed the usefulness of such measurements for monitoring mineralogical and geochemical changes accompanying subsurface bioremediation.

SSIP may also be used to extend geochemical data from a few boreholes that provide valuable information about remediation effectiveness over large areas. This will thus require less monitoring while providing a high level of assurance that the remedial process is working as intended.

Future work will focus on collecting SSIP over a much wider range of frequencies (e.g. 0.05-500 Hz), testing the method for detecting naturally occurring zones of bioreduction, and specifying system requirements for widespread application.

Kenneth Williams, LBNL, leads geophysical monitoring research for the Rifle Integrated Field Research Challenge, which is part of the Environmental Remediation Science Program within DOE's Office of Biological and Environmental Research. The research was featured in *Environmental Science & Technology*.

**Citation:**

Williams KH, A Kemna, MJ Wilkins, J Druhan, E Arntzen, AL N'Guessan, PE Long, SS Hubbard and JF Banfield. 2009. "Geophysical monitoring of coupled microbial and geochemical processes during stimulated subsurface bioremediation." *Environmental Science & Technology* 43(17):6717-6723 DOI: 10.1021/es900855j.

## **Science of Interfacial Phenomena**

### **Evaluating Regional Cloud-Permitting Simulations of the WRF Model for the Tropical Warm Pool International Cloud Experiment (TWP-ICE), Darwin, 2006**

***Y Wang,<sup>(a)</sup> CN Long,<sup>(a)</sup> LR Leung,<sup>(a)</sup> J Dudhia,<sup>(b)</sup> SA McFarlane,<sup>(a)</sup> JH Mather,<sup>(a)</sup> SJ Ghan,<sup>(a)</sup> and X Liu<sup>(c)</sup>***

*(a)* Pacific Northwest National Laboratory, Richland, Washington

*(b)* National Center for Atmospheric Research, Boulder, Colorado

*(c)* Chinese Academy of Sciences, Beijing, China

*Enabled in part by the Department of Energy's EMSL, computer simulations of thunderstorms using data from a field campaign in Australia confirm that the "ice-phase" cloud processes in climate models contribute most to the wide discrepancy between model results and actual cloud measurements. The study revealed the most effective tool for detecting when current schemes within climate models do not work well enough: evaluating the simplified representations of these clouds in climate models using actual measurements from field campaigns.*

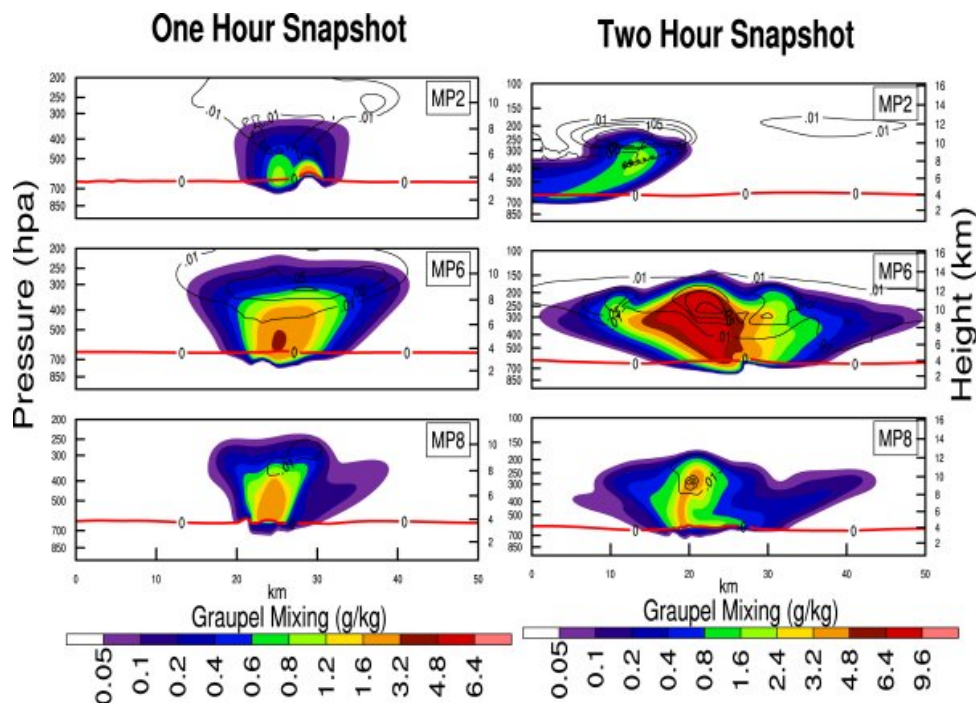
This finding highlights the importance of representing ice clouds properly in models, which is important to the success of the next generation of climate models and their ability to predict future climate. As high performance computing resources and technology advance, the next generation of climate models will run at much finer spatial resolutions (less than 10 km). This finer resolution permits the representation of cloud-sized phenomenon such as thunderstorms. At such high resolutions, the information gained from traditional larger-scale climate model resolutions may be invalid. These next-generation climate models will rely heavily on newer, more sophisticated means of representing clouds.

The tropics are the so called "heat engine" of the atmosphere. The clouds in the tropics have a large impact on climate, global water and energy cycles, and weather patterns by affecting the amount of solar energy that reaches the Earth's surface. A better understanding of tropical clouds and their interactions with the environment will help scientists develop better climate models.

The team used data collected from the 2006 Tropical Warm Pool-International Cloud Experiment (TWP-ICE)—a DOE Atmospheric Radiation Measurement (ARM) Program-sponsored field campaign, which took place at the ARM Climate Research Facility site in Darwin, Australia. The team conducted a suite of evaluations for three different ice-cloud-producing schemes in one of the more sophisticated of current models: the Weather Research and Forecasting model. The evaluations consisted of comparing the TWP-ICE data to corresponding model results for each of the three different ways that the model produces ice clouds.

To ensure that only the different ways that ice clouds are represented and interact with other predicted physical quantities in the models, all other possible influences and processes were treated the same during the model runs for this study. The team's evaluations using a simulated thunderstorm especially illustrated the wide discrepancy of the ice-phase-cloud microphysics in tropical clouds.

The team is working to improve the model simulation of high-layer cirrus clouds during the monsoon periods of TWP-ICE when there were clouds but not widespread rainfall. The results will be compared with TWP-ICE and satellite observations from NASA.



Thunderstorms in the tropics generate widespread cirrus clouds that are important in reflecting and absorbing energy. These mixing ratios for granular snow pellets (also called “soft hail”) (shades) and cloud ice (contours) from comparison testing of thunderstorm clouds in the tropics illustrate the wide discrepancy of the ice-phase cloud microphysics in current models. The melting line is marked as a thicker, red line. These types of discrepancies must be resolved for models to more accurately predict cloud influence on climate change.

The research, supported by DOE's Biological and Environmental Sciences as part of the ARM Program, was published in the *Journal of Geophysical Research*.

**Citation:**

Wang, Y., C.N. Long, L.R. Leung, J. Dudhia, S.A. McFarlane, J.H. Mather, S.J. Ghan, and X. Liu. 2009. "Evaluating Regional Cloud-Permitting Simulations of the WRF Model for the Tropical Warm Pool International Cloud Experiment (TWP-ICE), Darwin, 2006." *Journal of Geophysical Research* 114, D21203, doi: 10.1029/2009JD012729.

## Enhanced Activity and Stability of Pt Catalysts on Functionalized Graphene Sheets for Electrocatalytic Oxygen Reduction

*R Kou,<sup>(a)</sup> Y Shao,<sup>(a)</sup> D Wang,<sup>(a)</sup> MH Engelhard,<sup>(b)</sup> JH Kwak,<sup>(a)</sup> J Wang,<sup>(a)</sup> VV Viswanathan,<sup>(a)</sup> C Wang,<sup>(b)</sup> Y Lin,<sup>(a)</sup> Y Wang,<sup>(a)</sup> IA Aksay,<sup>(c)</sup> and J Liu<sup>(a)</sup>*

(a) Pacific Northwest National Laboratory, Richland, Washington

(b) EMSL, Richland, Washington

(c) Princeton University, Princeton, New Jersey

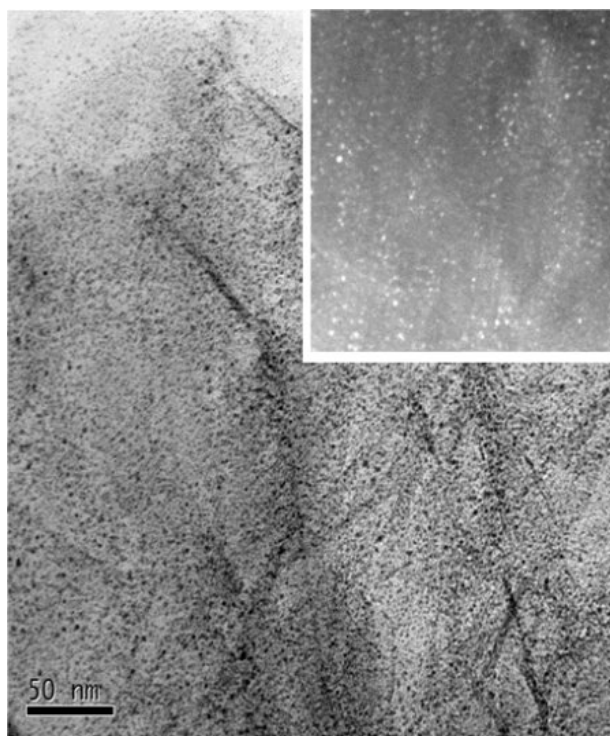
*A new carbon support that greatly increases the durability of proton-exchange membrane fuel cells has been developed by EMSL users from Pacific Northwest National Laboratory and Princeton University. This new material significantly improves the stability of the fuel cell catalyst and will potentially lower the cost of these fuel cells. This breakthrough research hit number one on the most-downloaded list of Electrochemistry Communications articles this fall.*

Currently, proton-exchange membrane fuel cells are not widely used because of the high manufacturing cost and relatively low endurance. To be commercially viable, the cost needs to be dramatically reduced. These new carbon supports might do just that.

Inside today's fuel cell, platinum catalyzes the reaction. The conditions inside the fuel cell are pretty harsh: high pressure, high temperature. Under these conditions, some of the platinum particles fly off the support, making them unavailable to speed the reactions. Some of the particles clump together. When this happens, the particles present less surface area. And, it is on the surface where the reaction happens. So, less surface area, less catalysis. The team investigated a new type of support.

For this study, they sliced graphite, similar to the carbon in a pencil, into single atomic layers to form dense wrinkled sheets called functionalized graphene sheets.

Then, they treated these sheets with the platinum catalyst. Using a transmission electron microscope, they saw the difference in how the catalysts particles were attached to the graphene sheets and a commercial support. The images clearly showed a uniform distribution of much smaller platinum



*Transmission electron microscopic image of small platinum catalyst particles supported on a functionalized graphene sheet.*

nanoparticles on the graphene. Using an X-ray photoelectron spectrometer, they proved the graphene has more functional groups available to bind the platinum catalyst compared to the commercial support. Both of these instruments are at EMSL.

Their conclusion was that the graphene sheets have a stronger metal-support interaction and produced smaller catalysts particles that were more resistant to degradation. Functionalized graphene sheets could potentially lead to a more stable, efficient, and lower-cost fuel cell.

This study lays the foundation for future work with this promising carbon material. Future research will focus on increasing the efficiency of the material fabrication and the durability of the graphene sheets. This research, funded by DOE's U.S. Department of Energy's Office of Energy Efficiency & Renewable Energy, was featured in *Electrochemistry Communications*.

**Citation:**

R Kou, Y Shao, D Wang, MH Engelhard, JH Kwak, J Wang, VV Viswanathan, C Wang, Y Lin, Y Wang, IA Aksay, and J Liu. 2009. "Enhanced activity and stability of Pt catalysts on functionalized graphene sheets for electrocatalytic oxygen reduction." *Electrochemistry Communications*, Volume 11, Issue 5, May 2009, Pages 954-957.

## **The Reorientation Mechanism of Hydroxide Ions in Water: A Molecular Dynamics Study**

***X Sun,<sup>(a)</sup> S Yoo,<sup>(a)</sup> SS Xantheas,<sup>(a)</sup> and LX Dang<sup>(a)</sup>***

**(a) Pacific Northwest National Laboratory, Richland, Washington**

*Whole water molecules form complex shapes around hydroxide ions, simple negatively charged particles, according to a recent study by EMSL users from Pacific Northwest National Laboratory. The shapes are the result of hydrogen bonds between the ions and the molecules. This research answers the question, debated in scientific circles for more than 70 years, of how hydroxide ions get oriented in water. This work graced the cover of the October 19, 2009, issue of Chemical Physics Letters.*

Knowing how hydroxide ions are arranged in water could aid scientists in fine-tuning current industrial processes, such as manufacturing biodiesel, making processes more efficient or less wasteful. Further, it could assist in developing future industrial processes, such as turning poplar trees and other vegetation into automotive fuel.

The theoretical chemistry team built and ran simulations of how hydroxide ions and water molecules moved based on the basic principles of physics. These simulations took into account the mutable shape of the electron clouds around each atom. These models are called classic molecular dynamics simulations with a polarizable force field

Studying the ions in water, the team found the hydroxide ion can form two different structures. In the most common motif, created about 57% of the time, hydroxide's oxygen atoms bonded with the hydrogen atoms on 4 water molecules while the hydroxide's hydrogen bonded to the oxygen atom on another water molecule. The structure looks like a pyramid with a square base. In the other motif, formed about 38% of the time, hydroxide's hydrogen atom refused to bond to any water molecules.

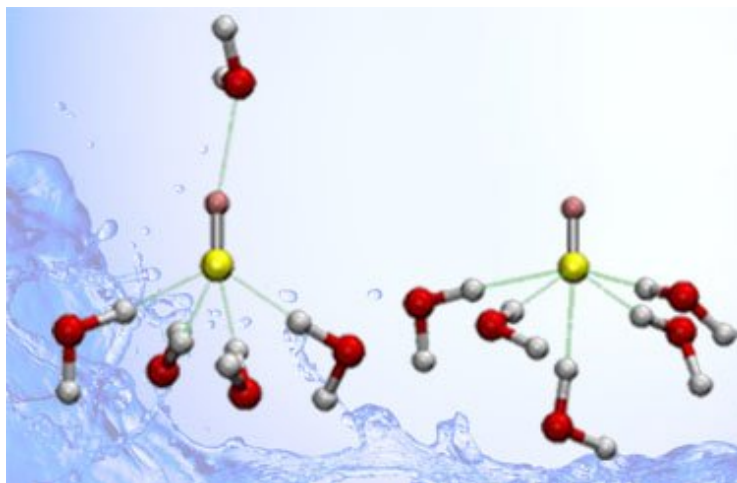
The researchers determined that the structures are created via a two-step process. First, the water molecules around the hydroxide ion bounced around, positioning and creating hydrogen bonds with the hydroxide. Once the structure was formed, the hydroxide ion relaxed to the minimum energy configuration.

The scientists continue to examine the behavior of hydroxide ions at the water/air interfaces with molecular dynamics simulations and other approaches. The knowledge they gain will help control complex chemical processes.

This research was funded by DOE's Office of Basic Energy Sciences.

**Citation:**

Sun X, S Yoo, SS Xantheas, and LX Dang. 2009. "The Reorientation Mechanism of Hydroxide Ions in Water: A Molecular Dynamics Study." *Chemical Physics Letters* 481(2009):9-16.



*Studying hydroxide ions in water, the team found that the ion (center) can form two different structures: one with five hydrogen bonds (left) and the other with four.*

### ***Awards and Recognition***

#### **Wysocki selected for Distinguished Contribution in Mass Spectrometry Award.**

EMSL user Professor **Vicki Wysocki** (University of Arizona) won the American Society for Mass Spectrometry's Award for Distinguished Contribution. This annual award recognizes a focused, singular achievement in fundamental or applied mass spectrometry. Wysocki, jointly with Professor Simon Gaskell of the University of Manchester, was chosen for her contributions to creating the mobile proton model. Wysocki and her team created a model that helps unify different observations from real-world collision-induced peptide fragmentation, which is vital in environmental and health studies. The model provides specific predictions regarding peptide fragmentation and enables spectra to be interpreted and simulated. The model serves as the foundation for other scientists in the area of peptide mass spectrometry to build more advanced models of fragmentation. Further, it underpins increasingly sophisticated database search algorithms. A collaborative part of this research utilized a large dataset of peptide fragmentation spectra provided by Richard Smith and Ljiljana Pasa-Tolic at EMSL. Wysocki received the award at the annual American Society for Mass Spectrometry conference, held in June 2009 in Philadelphia, Pennsylvania.



*Wysocki*

#### **Smith receives HUPO Award for advancements in proteomics technologies.**

EMSL user Dick Smith (PNNL) received the 2009 Human Proteome Organisation (HUPO) Discovery Award for Proteomic Sciences. The award is for a single discovery in the field and consists of a plaque and \$3000. Smith was honored at the HUPO 8<sup>th</sup> Annual World Congress September 26-30 in Toronto, where he presented a major lecture on some of the proteomics developments that earned him this recognition. HUPO is an international scientific organization representing and promoting proteomics through international cooperation and collaborations. Smith is a member of the HUPO Board of Directors.



*Smith*

## Visitors and Users

Year to date in Fiscal Year 2010, a total of 437 users benefited from EMSL capabilities and expertise. This total included 276 onsite users and 161 remote users.

## Publications

### Book Section

Buchko, G. W. (2009). Pentapeptide Repeat Proteins and Cyanobacteria. Handbook on Cyanobacteria: Biochemistry, Biotechnology and Applications. P. M. Gault and H. J. Marler. Hauppauge, NY, Nova Science Publishers: 233-257.

### Conference Paper

Buck, E. C. and R. S. Wittman (2009). The Formation and Modeling of Colloids from the Corrosion of Nuclear Waste Forms. Materials Research Society Symposium Proceedings: Scientific Basis for Nuclear Waste Management XXXII. Warrendale, PA, Materials Research Society. **1124**: 509-518.

### Journal Article

Andzelm, J., B. C. Rinderspacher, et al. (2009). "Performance of DFT Methods in the Calculation of Optical Spectra of TCF-Chromophores." Journal of Chemical Theory and Computation **5**(10): 2835-2846.

Bai, J., C. Liu, et al. (2009). "Study of sorption-retarded U(VI) diffusion in Hanford silt/clay material." Environmental Science & Technology **43**(20): 7706-7711.

Cort, J. R. and H. M. Cho (2009). "1H and 13C NMR Chemical Shift Assignments and Conformational Analysis for the Two Diastereomers of the Vitamin K Epoxide Reductase Inhibitor Brodifacoum." Magnetic Resonance in Chemistry **47**(10): 897-901.

Cross, E., T. B. Onasch, et al. (2009). "Single particle characterization using a light scattering module coupled to a time-of-flight aerosol mass spectrometer." Atmospheric Chemistry and Physics **9**(20): 7769-7793.

Jiang, W., H. Wang, et al. (2009). "Response of Nanocrystalline 3C Silicon Carbide to Heavy-Ion Irradiation." Physical Review. B, Condensed Matter **80**(16): Art. No.161301(R).

Joly, A. G., K. M. Beck, et al. (2009). "Photodesorption of excited iodine atoms from KI (100)." Journal of Chemical Physics **131**(14): 144509-144501/144506.

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