EMSL Quarterly Highlights Report

1st Quarter, Fiscal Year 2009

(October 1, 2008, through

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EMSL Quarterly Highlights Report: 1st Quarter, Fiscal Year 2009

MA Showalter
LE Kathmann
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February 2008

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Pacific Northwest National Laboratory
Richland, Washington 99352

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

Atmospheric Aerosol Chemistry

Comparative Analysis of Urban Atmospheric Aerosol by Particle-Induced X-Ray Emission (PIXE), Proton Elastic Scattering Analysis (PESA), and Aerosol Mass Spectrometry (AMS)

KS Johnson[a],[b], *A Laskin*[c], *JL Jiminez*[d], *V Shutthanandan*[c], *LT Molina*[a],[e], *D Salcedo*[f], *K Dzepina*[d], *and MJ Molina*[a],[g]

(a) **Massachusetts Institute of Technology, Cambridge, Massachusetts**
(b) **Finnegan, Henderson, Farabow, Garrett, and Dunner, LLP, Washington, D.C.**
(c) **EMSL, Richland, Washington**
(d) **University of Colorado, Boulder, Colorado**
(e) **Molina Center for Energy and the Environment, La Jolla, California**
(f) **Universidad Autonoma del Estado de Morelos, Cuernavaca, Morelos, Mexico**
(g) **University of California, San Diego, La Jolla, California**

EMSL researchers and users have conducted the first comparison of data sets obtained from proton-induced X-ray emission (PIXE) and proton elastic scattering analysis (PESA) to aerosol mass spectrometry (AMS) aerosol measurements, constituting, to the researchers' knowledge, the first report of PESA hydrogen fraction measurements in urban organic aerosols. This multidisciplinary research can help researchers more accurately interpret data from large, expensive aerosol studies and is vital in devising strategies to reduce the impact of aerosols on the climate.

A multidisciplinary team from Massachusetts Institute of Technology, EMSL, University of Colorado, Molina Center for Energy and the Environment, and Universidad Autonoma del Estado de Morelos in Mexico published the first comparison of data sets obtained from proton-induced X-ray emission (PIXE) and proton elastic scattering analysis (PESA) to aerosol mass spectrometry (AMS) measurements. The team compared the results of PIXE and PESA, both at EMSL, with AMS results (Figure 1). PIXE, PESA, and AMS use different methods of analysis yet provided complementary data sets. By utilizing the strengths of each instrument, scientists can more accurately interpret the results of studies on air pollution, an important issue for human health and environmental protection.

As part of the novel study, the team found good agreement between the sulfur measurements from PIXE and AMS. This comparison will allow scientists to vet field results with laboratory measurements and vice versa. Also, they found discrepancies between the hydrogen mass fractions assessed from PESA and AMS measurements. The discrepancy was attributed to the presence of nonvolatile organic compounds in aerosol samples. These compounds were not vaporized in the PESA and therefore were detected by the PESA method, while AMS detects organic aerosols of relatively high volatility. The study highlights the fact that complementary aerosol analysis capabilities can be used in the same environmental setting to provide comprehensive information about the amount of volatile and nonvolatile particles in the air.

This research, funded by the Mexican Metropolitan Environmental Commission, National Science Foundation, Environmental Protection Agency, and DOE, was published in *Environmental Science and Technology*.

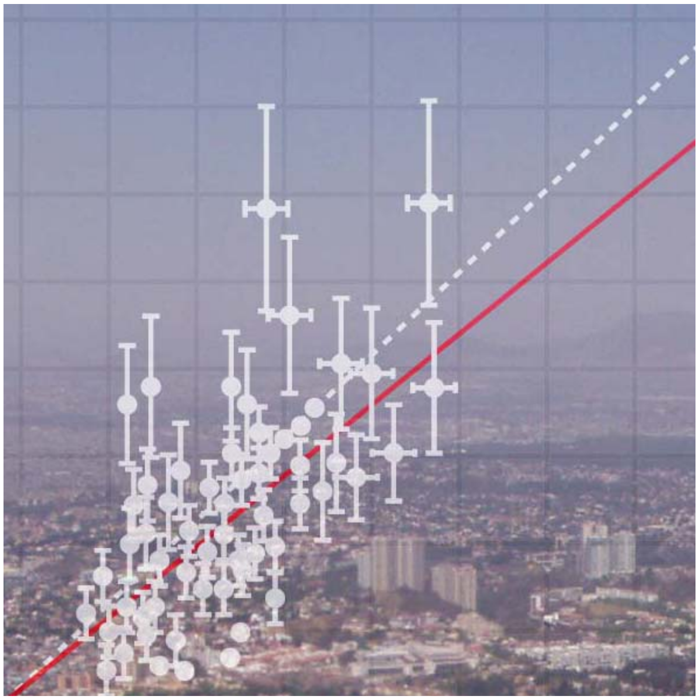


Figure 1. *Complementary capabilities of PIXE, PESA, and AMS measurements were used to provide comprehensive data for analysis of atmospheric aerosols in Mexico City.*

Citation

Johnson KS, A Laskin, JL Jiminez, V Shutthanandan, LT Molina, D Salcedo, K Dzepina, MJ Molina. 2008. "Comparative Analysis of Urban Atmospheric Aerosol by Particle-Induced X-ray Emission (PIXE), Proton Elastic Scattering Analysis (PESA), and Aerosol Mass Spectrometry (AMS)." *Environmental Science and Technology* 42(17):6619-6624 .

Biological Interactions and Dynamics

De novo Sequencing of Unique Sequence Tags for Discovery of Post-Translational Modifications of Proteins

Y Shen[a], N Tolic[b], KK Hixson[b], SO Purvine[b], GA Anderson[a], and RD Smith[a]

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

(b) ***EMSL, Richland, Washington***

EMSL researchers and users have developed a unique strategy that allows for unambiguous and highly confident protein identifications, which can help better identify changes that signal disease, potentially improving techniques for early disease detection and monitoring changes in environmentally important organisms.

To improve proteomics studies of heart disease, cancer, neurodegenerative diseases, and diabetes, EMSL researchers and users developed a novel strategy that expands protein identifications beyond those predicted from genomic sequences. Their approach combines *de novo* sequencing and the UStag approach to discover post-translational modifications in proteins. *De novo* sequencing derives a peptide sequence without the help of a database of known protein sequences. The UStag approach uses a peptide sequence to unambiguously and uniquely identify a single protein.

The combined *de novo*—UStag approach, funded in part by EMSL's 2007 Intramural Research Program, allows scientists to discover protein posttranslational modifications, including complex multiple unknown/unexpected modifications on single protein sequences, and discover sequence mutations and genome-predicted database sequence errors. This research and other discoveries are advancing EMSL's goal of being able to predict biological functions from molecular and chemical data.

Figure 1. *A new approach that characterizes previously unknown protein modifications was featured on the cover of* Analytical Chemistry.

This research, which was funded by EMSL's Intramural Research Program, DOE's Office of Biological and Environmental Research, and the National Institutes of Health's National Center for Research Resources, was featured on the cover of the October 15, 2008, issue of *Analytical Chemistry* (Figure 1).

Citation

Shen Y, N Tolic, KK Hixson, SO Purvine, GA Anderson, and RD Smith. 2008. "*De novo* Sequencing of Unique Sequence Tags for Discovery of Post-Translational Modifications of Proteins." *Analytical Chemistry* 80(20):7742-7754.

The Effects of Aging on the Luminescence of P5EG-Coated Water-Soluble ZnO Nanoparticles Solutions

BK Woo[a], W Chen[a], AG Joly[b], and R Sammynaiken[c]

(a) ***University of Texas at Arlington, Arlington, Texas***
(b) ***Pacific Northwest National Laboratory, Richland, Washington***
(c) ***University of Saskatchewan, Saskatoon, Saskatchewan, Canada***

A team of EMSL users has conducted basic research that is furthering the understanding of the interactions of nanoparticles and their surroundings, and is providing insights into biomedical uses of nanoparticles, such as treating malignant tumors.

EMSL users from the University of Texas at Arlington, Pacific Northwest National Laboratory, and the University of Saskatchewan used EMSL expertise and instrumentation at to characterize the light-emitting properties of coated, water-soluble zinc oxide nanoparticles potentially useful in killing cancer cells. These particles could be targeted at malignant cells, followed by administration of X-rays that would cause the particles to glow. The light would activate a photosensitive chemical, also on the particles, that, in turn, would create energized oxygen that could destroy nearby cancer cells.

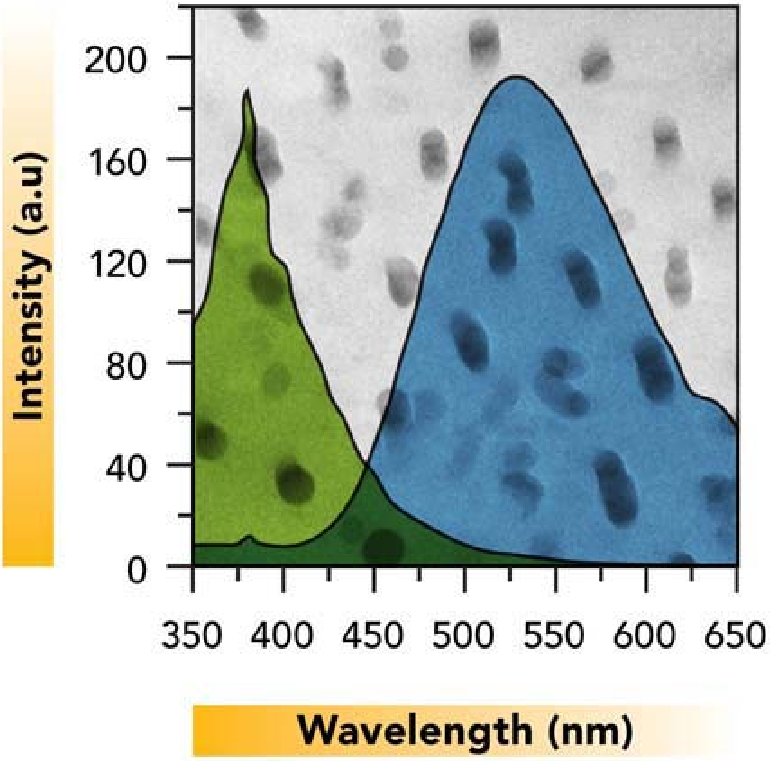


Figure 1. *The coating on the water-soluble zinc oxide particles allows them to deliver bright light for more than 7 weeks.*

The team found that the particles' coating of polyethylene glycol biscarboxymethyl increased the particles luminescence intensity over a period of 50+ days (Figure 1). The resulting nanoparticles displayed increased luminosity relative to the uncoated water-soluble particles. The uncoated particles luminesce because of defects on the surface. The coating fills in these defects, allowing the particles to rely on a different method of luminescence. This pathway is known as bandedge states. This characterization was done using the laser-based fluorescence spectrometer facilities at EMSL. The light from these particles can be used as part of an innovative treatment for deep tissue cancers, such as breast cancer.

This research, supported by the University of Texas at Arlington, National Science Foundation, Department of Homeland Security, and Department of Defense, was featured in the *Journal of Physical Chemistry C.*

Citation

Woo BK, W Chen, AG Joly, and R Sammynaiken. 2008. "The Effects of Aging on the Luminescence of P5EG-Coated Water-Soluble ZnO Nanoparticles Solutions." *Journal of Physical Chemistry C* 112(37):14292-14296. doi: 10.1021/jp803649k

Automated Gain Control Ion Funnel Trap for Orthogonal Time-of-Flight Mass Spectrometry

YM Ibrahim[a]*, ME Belov*[a]*, AV Liyu*[b]*, and RD Smith*[a]

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

(b) ***EMSL, Richland, Washington***

EMSL users have developed improved mass spectrometry (MS) tools that detect peptides with ten times more sensitivity. Diverse applications of this new technology to environmental and biological research include early disease detection, identification of new pharmaceutical targets, and testing for agents that may threaten homeland security.

A research team comprised of scientists from Pacific Northwest National Laboratory and EMSL upped the ante for mass spectrometry (MS) by adding an electrodynamic ion funnel trap (IFT) with automated gain control (AGC) to a conventional time-of-flight (TOF) MS system, allowing for optimized ion control. The first step to MS analysis is to generate ions by electrospray ionization; ions are then fed to a TOF MS for mass and charge analysis. Because the MS is typically coupled with another analytical tool (reversed-phase capillary liquid chromatography), ions are not generated at a constant rate, and the concentrations of ions passed to a TOF MS from an ion trap may exceed the TOF MS optimal detection range. By adding IFT with AGC to a conventional TOF MS system, the team was able to control the concentration of ions, minimizing the possibility of TOF MS detector saturation. In addition, ion accumulation in the IFT with AGC drastically improved signal-to-noise ratios for low-concentration analytes as compared to conventional TOF MS analysis.

To test the effectiveness of the IFT AGC modification, the team analyzed the proteome of *Shewanella oneidensis*, a bacterium that can chemically modify and neutralize toxic metals without apparent harm to itself. Compared to conventional techniques, the team's new and improved MS tool gave rise to ten times more sensitivity and greater mass measurement accuracy for analysis of low-concentration samples, yielding five times as many *S. oneidensis* unique peptides with the AGC mode (383 peptides) than with the conventional continuous mode of operation (73 peptides) (Figure 1).

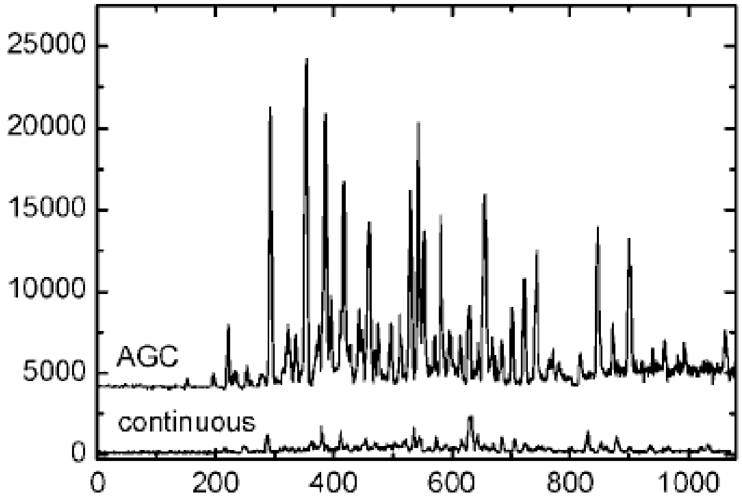


Figure 1. *Peak intensity for* S.oneidensis *MS measurements is greater in the AGC mode, demonstrating higher sensitivity of detection.*

The research is supported by the

DOE Office of Biological and Environmental Research's Genomes:GtL Program and the National Institutes of Health's National Center for Research Resources and National Institute of Allergy and Infectious Diseases. It was featured in *Analytical Chemistry*.

Citation

Ibrahim YM, ME Belov, AV Liyu, and RD Smith. 2008. "Automated Gain Control Ion Funnel Trap for Orthogonal Time-of-Flight Mass Spectrometry." *Analytical Chemistry* 80(14):5367-5376.

Geochemistry/Biogeochemistry and Subsurface Science

None reported.

Science of Interfacial Phenomena

Understanding How Surface Morphology and Hydrogen Dissolution Influence Ethylene Hydrogenation on Palladium

Z Dohnálek[(a)], J Kim[(a)], and BD Kay[(a)]

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

EMSL users have discovered that the arrangement of palladium atoms can improve the metal's ability to speed reactions. The team from Pacific Northwest National Laboratory designed a catalyst so that the palladium atoms on the catalyst surface had plenty of hydrogen atoms nearby but few other palladium atoms. When they tested the catalyst, it added hydrogen to 50 percent of the target hydrocarbons, an order-of-magnitude improvement over unmodified palladium.

Palladium (Figure 1, palladium surface) is an expensive industrial catalyst, costing about $180 an ounce. Designing the catalyst so that it performs better could mean less palladium is needed and more of the desired products are generated. This atom-by-atom design of the catalyst could open doors for controlling the physical and chemical properties of this important material.

At EMSL, the team began by depositing palladium atoms at -420 Fahrenheit. To deposit the atoms, they placed a substrate at an oblique angle to make an extremely porous palladium film. They characterized the surface morphology using a combination of scanning electron microscopy and low-temperature physisorption techniques afforded by EMSL's suite of state-of-the-art instrumentation. The team saw that the deposition caused the atoms to be arranged in peaks and valleys.

They tested the catalyst with a hydrogenation reaction, converting ethylene to ethane by adding hydrogen. They discovered that the tailored catalyst was more efficient than previous studies suggested. Typically, when palladium catalyzes the hydrogenation reaction, less than 1 percent of the ethylene is converted. Now, 50 percent of the ethylene was converted.

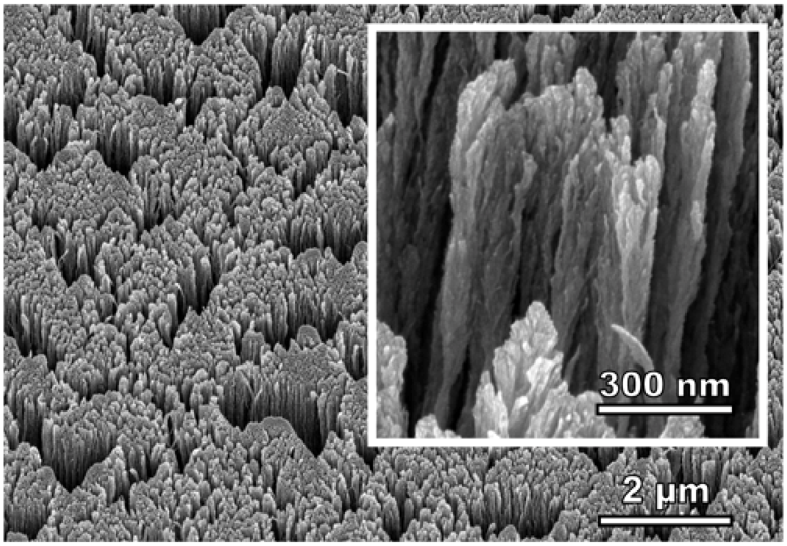


***Figure 1**. Palladium surface.*

Based on their observations of high catalytic activity, the team embarked on additional experiments. They grew thin layers of palladium on a nonporous substrate, creating a smooth surface. Then, they added a few extra palladium atoms on top.

Again, the researchers noted the catalyst's improved efficiency. They analyzed the results and determined the catalyst worked for two reasons. First, the palladium atoms on the surface were unencumbered by nearby palladium atoms. Second, the thin films prevented the hydrogen atoms from diffusing into the bulk of the material. The thin films kept the hydrogen at the surface, where it could be used. Past studies did not see these results because thicker crystals soaked up the hydrogen.

The researchers are now continuing to provide new insights into the behavior of catalysts that are of value to industrial and energy applications.

This research, funded by DOE's Office of Basic Energy Sciences, Chemical Sciences Division and which is part of PNNL's Institute for Interfacial Catalysis, was featured in the *Journal of Physical Chemistry C.*

Citation

Dohnálek Z, J Kim, and BD Kay. 2008. "Understanding How Surface Morphology and Hydrogen Dissolution Influence Ethylene Hydrogenation on Palladium." *Journal of Physical Chemistry C* 112(40):15796-15801.

Vacancy-Assisted Diffusion of Alcoxy Species on Rutile TiO$_2$(110)

Z Zhang[a], R Rousseau[a], J Gong[b], SC Li[b], BD Kay[a], Q Ge[c], and Z Dohnálek[a]

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

(b) ***University of Texas at Austin, Austin, Texas***

(c) ***Southern Illinois University, Carbondale, Illinois***

This study is the first to show how the vacancies on the surface of a titanium dioxide catalyst can aid in moving molecules. Learning how atoms behave on the surface of the catalyst could help tailor molecular delivery systems. For example, scientists could design a vacancy-rich system to lead the desired portions of an alcohol to sites where they are converted into hydrogen fuel and carbon dioxide. In addition, this atom-by-atom understanding can help in designing or refining technologies that use titanium dioxide, such as water purifiers, self-cleaning glass, and air purifiers.

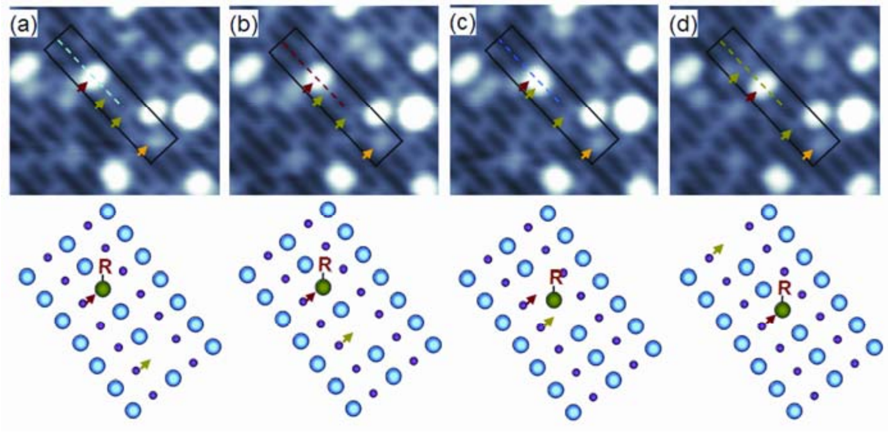


Figure 1. *Images from a scanning electron microscope (top) and a simple model show how the oxygen from the alcohol (green with R on top) diffuses on the surface of titanium dioxide (the oxygen is represented by the blue spheres and the titanium by the purple).*

On the surface of a common catalyst, alcohol molecules do the unexpected: they hop with the help of defects, according to a team of EMSL users from the Pacific Northwest National Laboratory, University of Texas at Austin, and Southern Illinois University. The catalyst's surface has holes or vacancies where an oxygen atom should be, but isn't. Instead of ignoring these vacancies, the alcohol discards the hydrogen from its only oxygen and jumps into the vacancy. Then, the molecule hops from one vacancy to the next as they come nearby.

The researchers combined experiment and theory at EMSL to study the behavior of alcohol on rutile titanium dioxide (Figure 1). For the experiments, they used imperfect titanium dioxide with holes or vacancies on the surface where oxygen atoms should be. Then, they added a 4-carbon alcohol, called 2-butanol.

Using a state-of-the-art scanning tunneling microscope, they found that the alcohol did not behave as expected. The alcohol shed its hydroxyl hydrogen (see sidebar), leaving the oxygen exposed. The oxygen, still attached to the alcohol's carbons and hydrogens, jumped into the nearest hole. But, the oxygen did not stay put for long. It hopped from vacancy to vacancy as the vacancies came nearby.

Next, the team analyzed these results with detailed theoretical calculations. They found that this travelling behavior at low temperatures required less energy than the other route: breaking off the whole hydroxyl group and moving the hydrocarbon along the surface. To confirm these results, the team studied a range of alcohols, one to eight carbons in length. They found the same pattern of movement.

The team is now moving on to determine how other molecules would break and diffuse on more active oxides, such as tungsten trioxide.

The research was supported by DOE's Office of Basic Energy Sciences, Chemical and Material Sciences Division, the Robert A. Welch Foundation, the National Science Foundation, and PNNL's Summer Research Institute. Results were featured in *Physical Review Letters.*

Citation

Zhang Z, R Rousseau, J Gong, SC Li, BD Kay, Q Ge, and Z Dohnálek. 2008. "Vacancy-assisted Diffusion of Alkoxy Species on Rutile TiO_2(110)." *Physical Review Letters* 101:156103.

Self-Assembly of Cerium Oxide Nanostructures in Ice Molds

AS Karakoti[a], SVNT Kuchibhatla[a],[b], DR Baer[b], S Thevuthasan[b], DC Sayle[c], and S Seal[a]

(a) ***University of Central Florida, Orlando, Florida***
(b) ***EMSL, Richland, Washington***
(c) ***Defence Academy of the United Kingdom, Swindon, United Kingdom***

Defining the conditions under which nanoparticles can be made to self-assemble into desired geometries opens new doors for nanomaterials research. In addition, many existing processes to manufacture nanomaterials use high molecular weight surfactants and solvents such as toluene, often generating chemical waste. EMSL staff and collaborators have demonstrated a new method to produce nanostructures that minimizes harm to the environment in a cost-effective manner. Nanomaterials produced with the research teams' new water-based method are less expensive and could drive technological advancements in a variety of nano-fields.

EMSL researchers and their collaborators have tested a new way to build nanostructures that is "green" and elegantly simple. Taking a cue from nature, collaborators from EMSL, the University of Central Florida, and Defence Academy of the United Kingdom grew cerium oxide nanostructures inside the tiny voids that form in aqueous solutions upon freezing. By controlling solution freezing rate, nanoparticle concentration, and storage temperature, the team's ice mold method may be used to produce nanostructures with tailored shapes and sizes that have a myriad of applications – from biology to electronics.

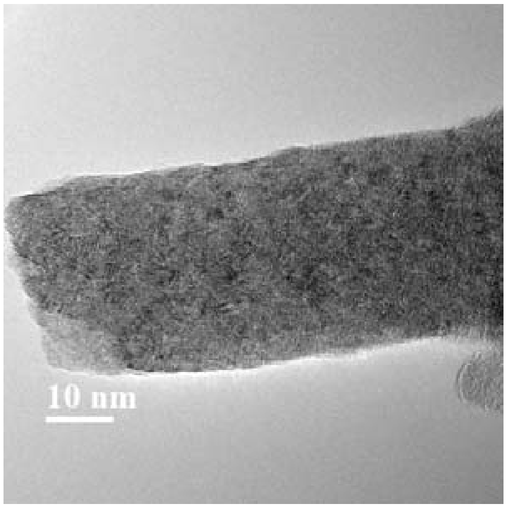


Figure 1. *Transmission electron microscopy image of a cerium oxide nanorod formed in an ice channel.*

The team's green chemical method was made possible by two natural phenomena: solute rejection and self-assembly. Upon freezing, aqueous solutions force out, or reject, impurities because they cannot be accommodated in the rigid lattice structure of ice. Depending on the freezing conditions, ice does not form a perfect lattice throughout. Rather, it has tiny pockets and channels. It is into these voids that impurities, in this case cerium oxide nanoparticles, become trapped together and can self-assemble.

Upon freezing cerium oxide nanoparticles in solution at different temperatures and rates and storing the frozen solution for days to weeks, the research team used transmission electron microscopy and other tools to characterize the resulting nanostructures (Figure 1). They observed that cerium oxide nanoparticles trapped in channels in the ice formed nanorods, and those trapped in larger voids formed octahedral superstructures. The team's experimental observations were consistent with molecular dynamics simulations of nanoparticle behavior under geometrically constrained conditions.

This research, supported by the National Science Foundation, was featured in *Small*.

Citation

Karakoti AS, SVNT Kuchibhatla, DR Baer, S Thevuthasan, DC Sayle, and S Seal. 2008. "Self-Assembly of Cerium Oxide Nanostructures in Ice Molds." *Small* doi:10.1002/smll.200800219. The work was also highlighted in *Nature Nanotechnology*, doi:10.1038/nnano.2008.259.

Intrinsic Diffusion of Hydrogen on Rutile TiO_2(110)

***SC Li*[a]*, Z Zhang*[b]*, D Sheppard*[a]*, BD Kay*[b]*, JM White*[a]*, Y Du*[c]*, I Lyubinetsky*[c]*, G Henkelman*[a]*, and Z Dohnálek*[b]**

(a) ***University of Texas at Austin, Austin, Texas***
(b) ***Pacific Northwest National Laboratory, Richland, Washington***
(c) ***EMSL, Richland, Washington***

Understanding what happens on the surface of rutile titanium dioxide could help researchers tailor this material to use sunlight to speed the reaction that splits water into hydrogen and oxygen. The resulting hydrogen can be used to power fuel cells that could replace gasoline-powered engines in cars and trucks.

When water breaks apart on a well-known catalyst, the once-close hydrogen atoms quickly part company in a complicated process, according to scientists at Pacific Northwest National Laboratory and the University of Texas at Austin. Their detailed study shows the hydrogen atoms are slightly repelled by each other on the surface of the rutile titanium dioxide catalyst. The atoms move apart by first sliding an electron over to their new home. Then, the rest of the atom follows.

The research team took a two-prong approach to studying hydrogen movement or diffusion. They began with experimental studies and followed up with theoretical calculations. For the experiments, they used temperature-dependent measurements to track hydrogen movement on the catalyst's surface. They performed these measurements using one of EMSL's scanning tunneling microscopes that can resolve single atoms on a surface (Figure 1). For the theoretical studies, they used density functional theory calculations and other models.

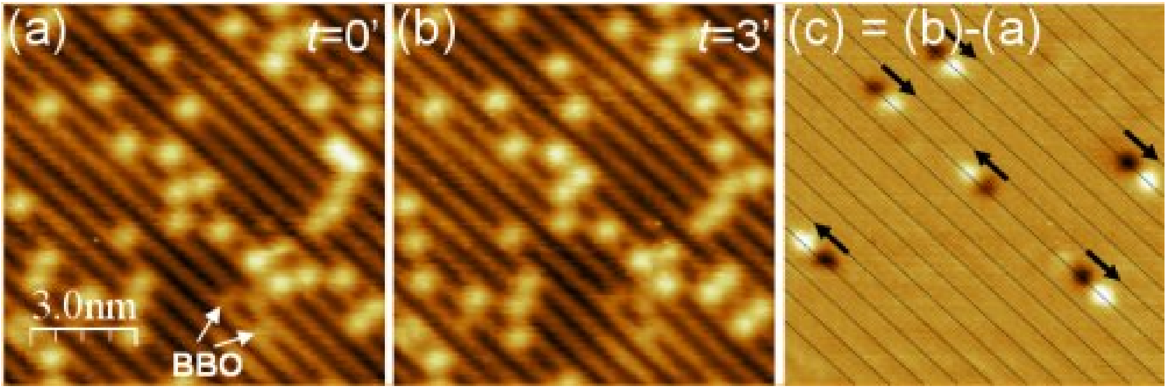


Figure 1. *Hydrogen movement shown by the scanning tunneling microscope. By taking snapshots before (left) and after (middle) of the motion of the hydrogen atoms on the catalyst, the scientists can determine where and how fast the atoms moved (final).*

The results from the experimental and theoretical studies did not agree. While both show hydrogen diffusing across the surface at the same rates, the underlying parameters controlling the rates differed.

The researchers believed the differing results were because of how the hydrogen moves. They speculated that the hydrogen diffused via a two-step process. A hydrogen atom has two parts: a positive nucleus and a negative electron. In diffusion, the lone electron nimbly hops over to the new location first. Then, the larger nucleus hefts itself to the new location. The first step, the electron moving, is not accounted for in the theoretical calculations.

The team is continuing to study water on rutile titanium dioxide, focusing on its reactions with oxygen to get one step closer to understanding titanium dioxide as a water splitting catalyst.

The research was funding by DOE's Office of Basic Energy Sciences, Chemical Sciences; the Robert A. Welch Foundation; and National Science Foundation. It was featured in the *Journal of the American Chemical Society*.

Citation

Li SC, Z Zhang, D Sheppard, BD Kay, JM White, Y Du, I Lyubinetsky, G Henkelman, and Z Dohnálek. 2008. "Intrinsic Diffusion of Hydrogen on Rutile $TiO_2(110)$." *Journal of the American Chemical Society* 130(28):9080-9088.

Photoelectron Spectroscopic and Theoretical Study of B_{16}^- and B_{16}^{2-}: An All-Boron Naphthalene

AP Sergeeva[a]*, DY Zubarev*[a]*, HJ Zhai*[b][c]*, AI Boldyrev*[a]*, and LS Wang*[b][d]

(a) *Utah State University, Logan, Utah*

(b) *Washington State University-Tri-Cities, Richland, Washington*

(c) *EMSL, Richland, Washington*

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

Engineering technologies to solve energy or security issues benefit from knowledge of the atomic-level structure of materials such as highly reactive boron. Researchers from Utah State University, Washington State University, and Pacific Northwest National Laboratory have discovered the atomic structure of two boron clusters: B_{16}^- *and* B_{16}^{2-}.

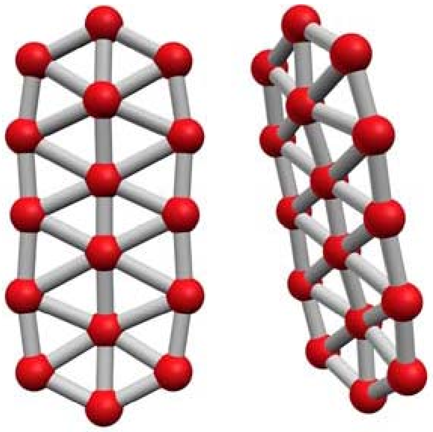


Figure 1. *The structures of two 16-atom boron clusters were recently discovered by EMSL users. The* B_{16}^{2-} *structure (right) has 10 π electrons and a π bonding pattern similar to naphthalene.*

Using EMSL's laser vaporization and time-of-flight mass spectrometry capabilities, a researcher team from Utah State University, Washington State University, and Pacific Northwest National Laboratory produced B_{16} clusters and examined them using photoelectron spectroscopy. They did theoretical calculations to compare with the experimental data and determined the cluster's structure and chemical bonding. Molecular orbital analysis indicated that B_{16}^{2-} possesses 10 π electrons and a π bonding pattern similar to naphthalene, and it can be viewed as an all-boron version of the aromatic organic molecule used in mothballs (Figure 1).

This research provides detailed knowledge about the structure and chemical bonding in B_{16} clusters, information that was not known previously. This work furthers the scientific basis for the development of novel boron nanostructures. In addition, fundamental insights into the structure of highly reactive boron clusters provide foundational information that other researchers can build on. This information could help the design of new boron-based nanomaterials for energy or security applications.

The research, supported by the National Science Foundation, was published in the *Journal of the American Chemical Society*.

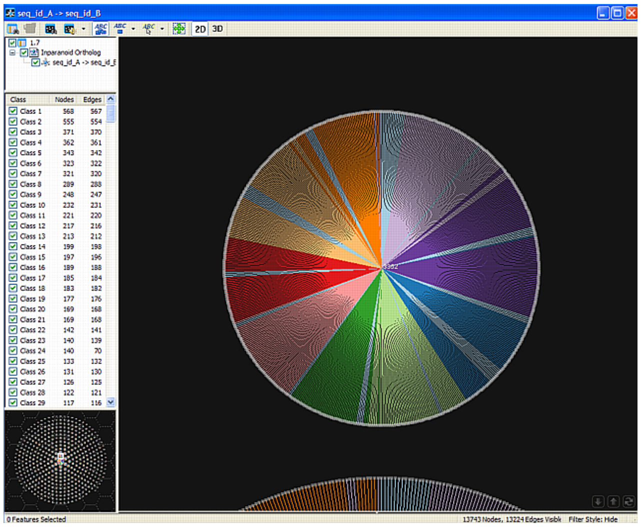
Citation

Sergeeva AP, DY Zubarev, HJ Zhai, AI Boldyrev, and LS Wang. 2008. "Photoelectron Spectroscopic and Theoretical Study of B_{16}^- and B_{16}^{2-}: An All-Boron Naphthalene." *Journal of the American Chemical Society* 130(23):7244-7246.

Awards and Recognition

Rosso selected as Virginia Tech Outstanding Alumnus. EMSL user Kevin Rosso (Pacific Northwest National Laboratory) was honored by Virginia Tech for his outstanding research and contributions to the scientific community. Each year the university's alumni association selects, from each academic college, a gifted person who has graduated in the past decade. Rosso received the award from the College of Science, where he earned a doctoral degree in geochemistry in 1998. Rosso leads internationally recognized research in environmental spectroscopy and biogeochemistry. He is an expert in mineral-water interface geochemistry, combining scanning probe microscopy and *ab initio* molecular modeling. He is known for his insightful models of electron transfer kinetics in environmental systems. His recent studies illuminate the relationship between bacteria and environmental metals, such as iron and uranium. Rosso has written or co-written more than80 peer-reviewed journal articles, including a recent article in *Science*. He is frequently invited to lecture at universities and symposia, in the United States and abroad. In addition, he is a life fellow of the Mineralogical Society of America, and he served for two years as an associate editor for *American Mineralogist*. He is a member of the American Chemical Society and has organized topical symposia for the society's national meetings.

Kevin Rosso



Class	Nodes	Edges
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☑ Class 2	555	554
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☑ Class 5	343	342
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☑ Class 7	321	320
☑ Class 8	289	288
☑ Class 9	248	247
☑ Class 10	232	231
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☑ Class 21	169	168
☑ Class 22	142	141
☑ Class 23	140	139
☑ Class 24	140	70
☑ Class 25	133	132
☑ Class 26	131	130
☑ Class 27	126	125
☑ Class 28	122	121
☑ Class 29	117	116

0 Features Selected

13743 Nodes, 13224 Edges Visibl Filter Style: Hide

A computer program developed by EMSL users with help of EMSL computational resources shows that a graphical cluster compares 42,000 unknown proteins from 10 species of Shewanella *against a single known protein at the center of the pie. The user has zoomed in on this cluster from the panoply of clusters at the bottom left of the screen.*

EMSL users earn top honors at Supercomputing 08. DNA sequencing is easier than ever, but the amount of data to be analyzed is piling up. An award-winning computer program now shows that genome sequence analysis can be made interactive and intuitive, helping researchers find hidden relationships in massive amounts of data.

Researchers from the Pacific Northwest National Laboratory captured "Best Overall" for their entry at the Supercomputing '08 High Performance Computing Analytics Challenge in Austin, Texas, on November 20.

In the competition, scientists were judged on solving real world problems using comprehensive computational approaches, large data sets, and high-end visualization technology to display results -- which means it had to look good and be easy to use.

PNNL's Chris Oehmen led a multidisciplinary team composed of Scott Dowson, Chandrika Sivaramakrishnan, Justin Almquist, Lee Ann McCue, Bobbie-Jo Webb-Robertson, and Jason McDermott to the win. Resources the team used included computing capabilities housed in EMSL to develop the interactive program.

For more information, see the EurekaAlert press release at http://www.eurekalert.org/pub_releases/2008-12/dnnl-pre120208.php and a video demonstration of the program at http://www.pnl.gov/science/highlights/highlight.asp?id=516.

Don Baer

Baer named Reviews Editor for journal. Don Baer, EMSL Lead Scientist for Interfacial Chemistry, was selected to serve as the Reviews Editor for *Surface and Interface Analysis*. This international, refereed journal is devoted to publishing papers on developing and applying techniques for characterizing surfaces, interfaces, and thin films. As the Reviews Editor, Baer will work with world-leading scientists to obtain articles on topics of interest to the journal's audience of materials scientists, physicists, physical chemists, and others. In addition to traditional review articles, he will encourage leading scientists to prepare perspectives on current research directions and technology advances and tutorial articles. Baer is internationally known for applying surface analysis methods to examine the reactive properties of oxides and mineral surfaces, determining behaviors of nanostructured materials, and understanding corrosion processes. He specializes in using surface sensitive techniques to study surface interphase reactions and materials surface chemistry. He has authored or co-authored more than 200 peer-reviewed articles, edited books and special journal issues, and lectured at major conferences. He is a member of the American Association for the Advancement of Science, American Physical Society, and the Electrochemical Society, among others. He has served as an associate editor on *Surface Science Spectra* since 1991. In addition, he serves on the *Surface and Interface Analysis* publication's advisory board.

Dave Koppenaal

Koppenaal invited to serve on journal international advisory board. David Koppenaal, EMSL's Chief Technology Officer, was invited to serve a 3-year term on the International Advisory Board for the new journal *Metallomics: Integrated Biometal Science*. The journal is a Royal Society of Chemistry publication that will be launched in January 2009. Metallomics is the integrated study of metals and metal species and their interactions, transformations, and functions in biological systems. The subject is receiving attention as a new frontier in the investigation of trace elements in biology. Metallomics is expected to develop as an interdisciplinary science complementary to metabolomics and proteomics. At EMSL, Koppenaal leads numerous biological studies. His research is primarily focused on characterizing inorganic compounds and isotopes with innovative mass spectrometry and other analytical techniques. For example, Koppenaal and his colleagues at Pacific Northwest National Laboratory pioneered the application of inductively coupled plasma/mass spectrometry as a powerful and relevant radioanalytical tool and demonstrated its use for radioactive waste characterization, ultra-trace nuclear forensics, and, most recently, metallomics applications. He is also responsible for leading the development of world-leading capabilities for EMSL, such as a current collaboration with the National High-Field Magnetic Laboratory to develop a 21-Tesla magnet that will lead to the highest resolving power and mass accuracy possible in mass spectrometry. His more than 75 publications include several invited review articles, and he is a frequent keynote and plenary lecturer at major conferences. Koppenaal recently completed a 7-year term as Editorial Board member for the RSC publication *Journal of Analytical and Atomic Spectrometry*. Koppenaal is a fellow of the American Association for the Advancement of Science and the

Royal Society of Chemistry. He is a member of the American Chemistry Society and the American Society for Mass Spectrometry.

Visitors and Users

During the first quarter of Fiscal Year 2009, a total of 367 users benefited from EMSL capabilities and expertise. This total included 238 onsite users and 129 remote users.

Publications

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