the Molecular Bond

EMSL

SCIENTIFIC INNOVATION THROUGH INTEGRATION

October 2015

EMSL's Quiet Wing

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Hofmockel Joins EMSL

Orr an Inspiring Woman in STEM

Shedding Light on Soil Processes

New Models Could Improve Remediation

About the Cover

EMSL's Quiet Wing is among the most advanced quiet laboratories in the world for high-resolution imaging capabilities. Its design eliminates or reduces to a minimum the vibrations, acoustics and electromagnetic noise that can interfere with the resolution of ultrasensitive scientific instrumentation.

About *The Molecular Bond*

The Molecular Bond is EMSL's bimonthly newsletter for users, potential users and other interested individuals. EMSL Communications oversees the production of *The Molecular Bond*.

EMSL, the Environmental Molecular Sciences Laboratory, is a national scientific user facility sponsored by the Department of Energy's Office of Biological and Environmental Research in the Office of Science. Located at Pacific Northwest National Laboratory in Richland, Wash., EMSL offers an open, collaborative environment for scientific discovery to researchers around the world.

Its integrated computational and experimental resources enable researchers to realize important scientific insights and create new technologies. More information about EMSL is available at: www.emsl.pnnl.gov

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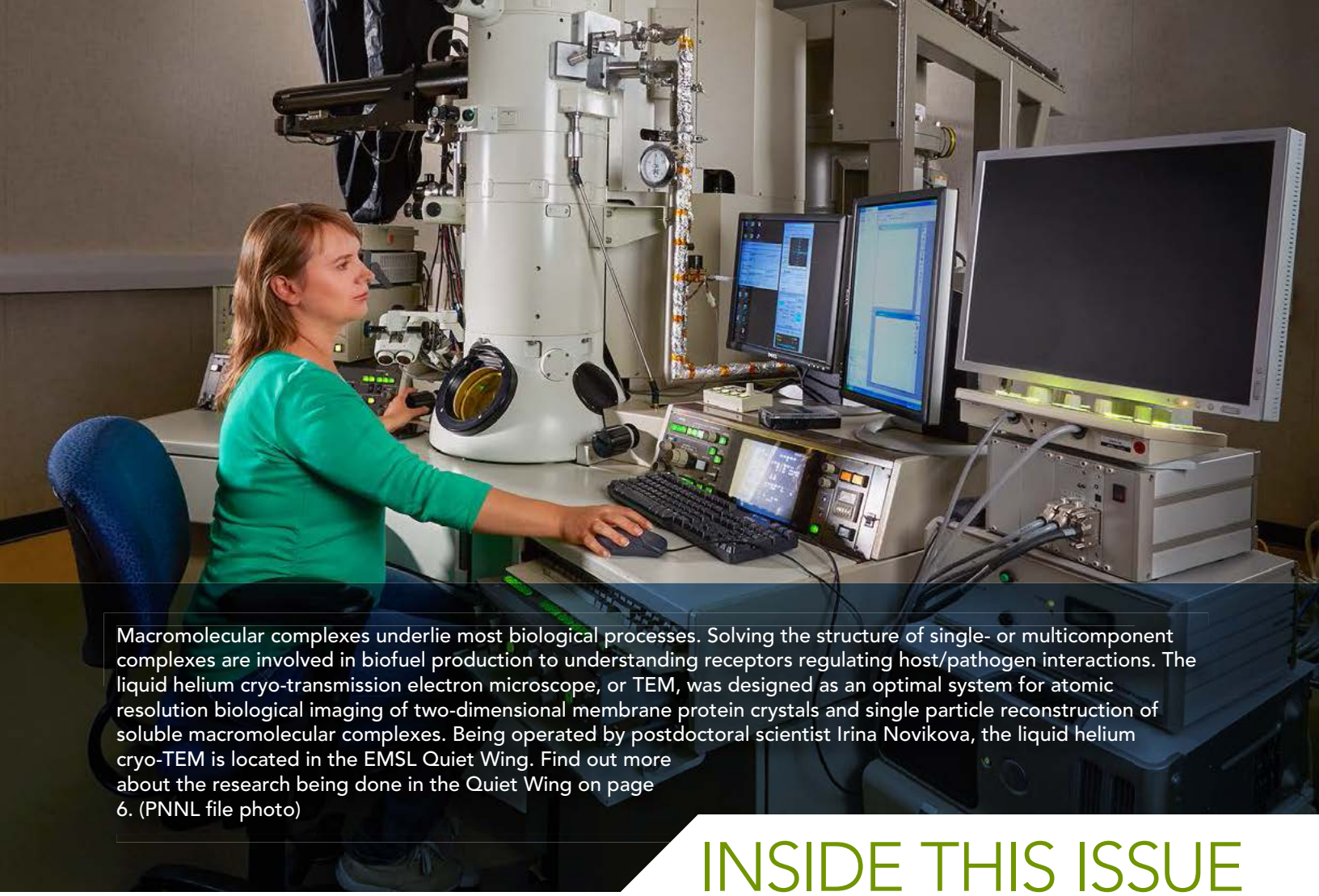

Macromolecular complexes underlie most biological processes. Solving the structure of single- or multicomponent complexes are involved in biofuel production to understanding receptors regulating host/pathogen interactions. The liquid helium cryo-transmission electron microscope, or TEM, was designed as an optimal system for atomic resolution biological imaging of two-dimensional membrane protein crystals and single particle reconstruction of soluble macromolecular complexes. Being operated by postdoctoral scientist Irina Novikova, the liquid helium cryo-TEM is located in the EMSL Quiet Wing. Find out more about the research being done in the Quiet Wing on page 6. (PNNL file photo)

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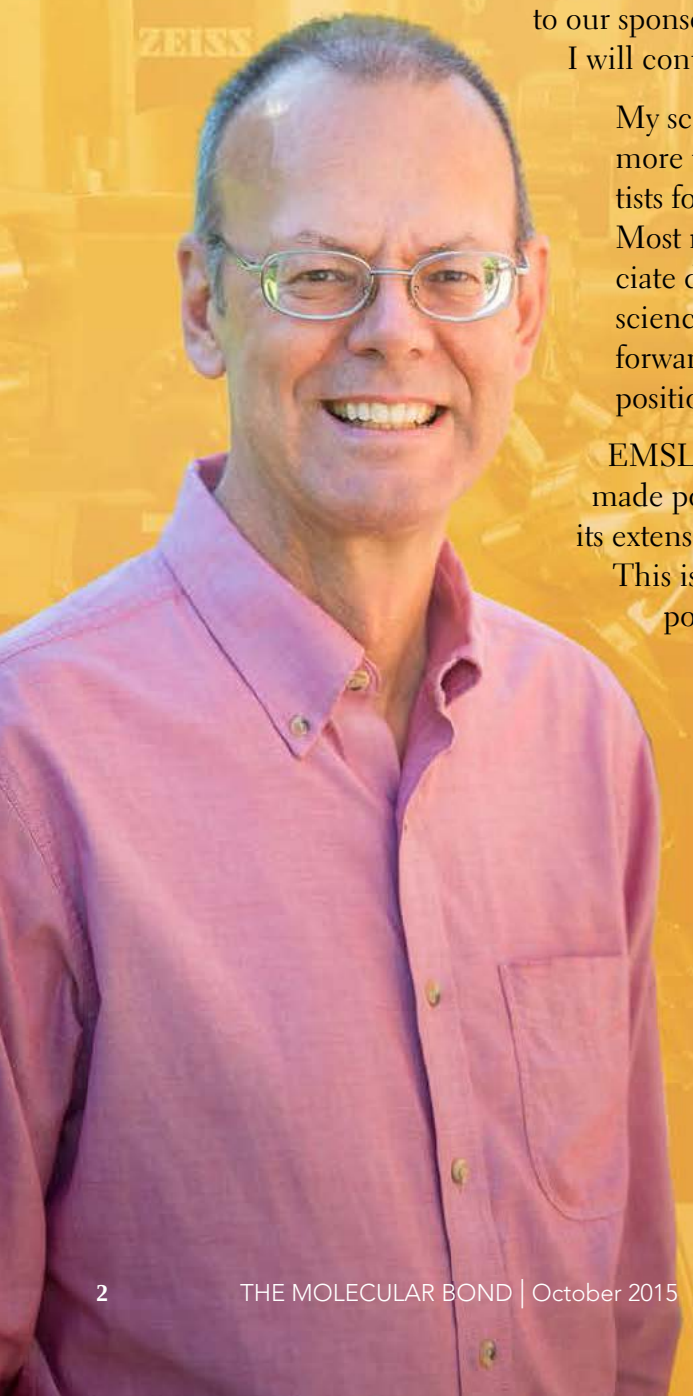
FROM THE DIRECTOR

Harvey Bolton



First let me say how honored I am to serve as interim EMSL director. Following Allison Campbell, who was EMSL's director for more than a decade, is a bit daunting – she leaves a great legacy.

During my time in this role, one of my goals will be to maintain the momentum of EMSL's scientific vision and continue our emphasis on raising our impact to our sponsor, DOE's Office of Biological and Environmental Research. I will continue EMSL's tradition of scientific achievement.

My scientific background is environmental microbiology. I have more than 25 years' experience leading projects and teams of scientists focused on research supporting the mission of the DOE BER. Most recently, I have served for a little over a year as EMSL's associate director, and before that I was a division director of biological sciences at Pacific Northwest National Laboratory. I am looking forward to the new opportunities and challenges of my new position.

EMSL has a history of being on the forefront of scientific discovery made possible by the wide-ranging expertise of its research staff and its extensive collection of scientific facilities and instrumentation. This issue of *The Molecular Bond* explores the science being made possible with EMSL's Quiet Wing. Also known as the Q-Wing, this facility is one the most advanced quiet laboratories in the world for high-resolution imaging capabilities. EMSL's Q-Wing supports various research areas of importance to DOE, including climate, biological, environmental and energy systems. This issue's cover story highlights several users who are utilizing the Q-Wing to research bacteria in complex soil aggregates, to understand the behavior of a unique multicopper oxidase and to explore remediation methods using porous clay.

I encourage you to reach out to EMSL's scientific staff or our user program and let us know how we can collaborate to advance your research.

—Harvey

Retired EMSL leader M. Tom Thomas (left) always takes a tour of the user facility while attending the M.T. Thomas Award for Outstanding Postdoctoral Achievement event named in his honor. Thomas and Arnab Dutta, this year's award recipient, visited some of the labs Dutta used during his research at EMSL on bio-inspired molecular catalysts. Read more about this year's award ceremony on page 5. (EMSL file photo)

NEWS & KUDOS

Hofmockel Named Lead Scientist

Kirsten Hofmockel

Kirsten Hofmockel has joined EMSL as lead scientist for Integrative Research. She will have a principal role in developing cross-cutting research studies spanning EMSL's science themes.

Hofmockel's research focus is environmental biology. Most recently she was a professor in the Department of Ecology, Evolution and Organismal Biology at Iowa State University since 2008. She earned the Iowa State University Award for Early Achievement in Research in 2014. She also received the National Academies Teaching Educational Fellow in the Life Sciences awarded by the National Academy of Sciences, Division of Earth and Life Studies, and the National Research Council in 2011.

Starting in 2010, Hofmockel was the lead or co-principal investigator on $6 million in externally funded projects. She has authored or co-authored more than 30 peer-reviewed journal publications, and she has delivered more than 30 invited presentations at major conferences and institutions since 2000.

Before becoming a professor at ISU, Hofmockel was a postdoctoral scholar at the University of Michigan Soil Microbiology Laboratory. She earned both a doctorate in ecology and a master's in environmental management from Nicholas School of the Environment at Duke University and held a number of research assistant positions at several institutions. Her bachelor's degree with honors is from Pennsylvania State University.

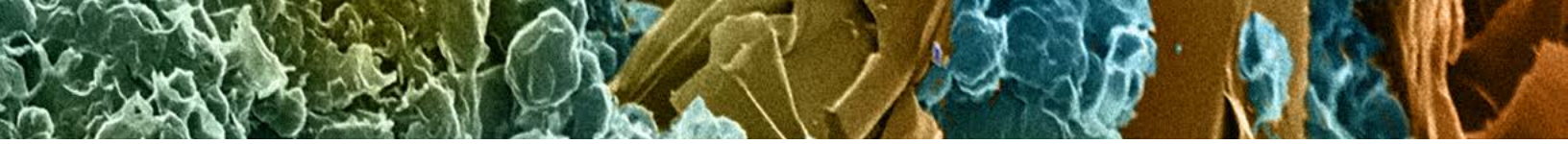
Annual Meeting Poster Competition Winners Announced

The winners of EMSL's annual meeting student poster competition are: first place-Venkateshkumar Prabhakaran, second place-Ashleigh Schwarz and third place-Ashish Bhattarai.

Venkateshkumar Prabhakaran, PNNL

Prabhakaran is with Pacific Northwest National Laboratory and received a cash award of $350. Schwarz is with EMSL and got a cash award of $250. Bhattarai is with Washington State University and received an award of $100.

The poster session was held Sept. 17 as part of EMSL Integration 2015: Energy Materials and Processes for Advanced Batteries and Catalysis. Posters were an opportunity for students and users to share their specific research with other meeting attendees. The student poster competition was open to full-time undergraduate and graduate students.



Orr a Co-PI of Center Studying Effects of Nanoparticles on Environment

Galya Orr

Galya Orr, a senior research scientist at EMSL, is a co-principal investigator at the Center for Sustainable Nanotechnology that studies nanoparticles in emerging technologies and their effects on the environment. Based at the University of Wisconsin-Madison, the multi-institutional research center recently received a five-year, nearly $20 million renewable grant from the National Science Foundation to expand existing operations.

"The purpose of the center is to explore how we can make sure these nanotechnologies come to fruition with little or no environmental impact," said Robert Hamers, director of the center and a professor of chemistry at the UW-Madison. "We're looking at nanoparticles in emerging technologies."

According to Orr, EMSL has been playing an important role in the success of the center. "EMSL expertise and resources have been acknowledged as strengths by reviewers of the center" said Orr, EMSL capability lead for Cell Isolation & Systems Analysis.

Orr's and EMSL's scientific contributions to the center will continue. For a molecular-level understanding of the cellular interactions and intracellular fate of nanomaterials in living cells, EMSL's quantitative, super-resolution and single-molecule fluorescence microscopy among other techniques will be utilized for the center's research.

As part of her involvement in the center, Orr will receive research funding for five years, renewable for additional five years. She will also have a full-time postdoctoral fellow funded by UW-Madison who will be working in EMSL on Orr's and the center's research projects.

In addition to EMSL and UW-Madison, scientists from Northwestern University, UW-Milwaukee, University of Minnesota and University of Illinois were involved in the center's first phase of research, which began in 2012 with a NSF grant. Joining the center for the next five-year phase are Tuskegee University, University of Maryland-Baltimore County, Johns Hopkins University, The University of Iowa, Augsburg College and Georgia Tech.

Orr Named one of 100 Inspiring Women in STEM

INSIGHT Into Diversity magazine has selected Galya Orr, a senior research scientist at EMSL, as a recipient of 100 Inspiring Women in STEM Award. She was profiled in the magazine's September issue along with 99 other honorees.

Orr, EMSL capability lead for Cell Isolation & Systems Analysis, was nominated for the award with three colleagues: Rebecca Klaper, a professor at the University of Wisconsin-Milwaukee; Catherine Murphy, Markunas professor at the University of Illinois at Urbana-Champaign; and Christy Haynes, a professor at the University of Minnesota. The four women, together with three other co-principal investigators, founded the Center for Sustainable Nanotechnology, or CSN, funded by the National Science Foundation. The center is a multi-institutional partnership devoted to investigating the fundamental molecular mechanisms by which nanoparticles interact with biological systems.

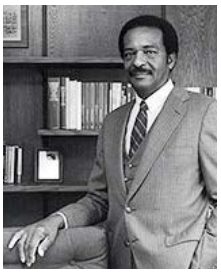
"The CSN is a research center that crosses institutional and disciplinary boundaries by providing an inspiring training environment for scientists at the undergraduate, graduate, and postgraduate levels," noted the award write-up in the September issue of *INSIGHT Into Diversity*. "With the goal of increasing diversity and female representation in STEM fields, these women have created a center that is composed of nearly 50 percent women – a high number in the field of chemistry."

Orr's many honors include the 2010 Outstanding Mentor Award from the Department of Energy's Office of Science and the 2010 Fitzner-Eberhardt Award Nominee for Outstanding Contributions to Science and Engineering Education.

Orr has been in her current role as capability lead since 2010. She has been a scientist at EMSL and Pacific Northwest National Laboratory since 2000. She earned a Ph.D. from University of Arizona and a bachelor's of arts from Technion - Israel Institute of Technology. Orr has authored or co-authored more than 43 peer-reviewed journal articles since 2000.

INSIGHT Into Diversity is the oldest and largest diversity magazine and website in higher education. The national award honors 100 women in professions whose work and achievements as researchers, teachers and mentors inspire a new generation of young women to consider careers in science, technology, engineering and math, or STEM. Read the September issue at http://bit.ly/1NomdBc

Wiley Postdoc Fellowship Position Now Open



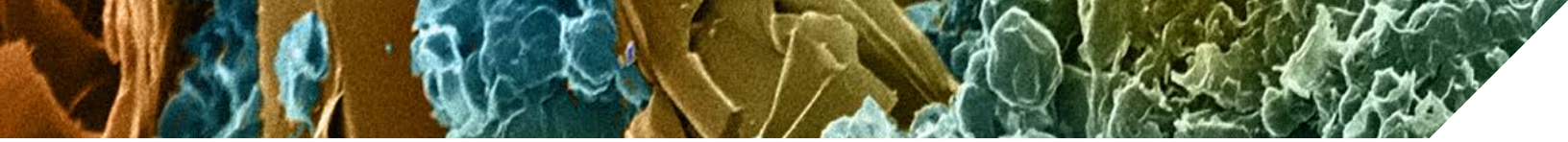
Dr. William R. Wiley

EMSL is currently accepting applications for its William Wiley Distinguished Postdoctoral Fellowship. The position closes Nov. 14.

Starting in 2010, EMSL established the fellowship to attract high-performing, newly graduated Ph.D. scientists who have the potential to become full-time scientific staff at EMSL.

Candidates must display superb ability in scientific research and must show promise of becoming outstanding leaders in their research areas. In addition to a current curriculum vitae and unofficial transcripts, all candidates must submit a statement of research interest aligning with one or more of EMSL's science themes. Candidate should upload one PDF file that includes these components. Applications lacking these components will be declared ineligible.

The recipient will serve a one-year term, with the possibility of the fellowship being renewed for a total of three years. The



position includes a high starting salary, and an additional allocation for research support and travel.

Applications must be submitted through PNNL's jobs website.

The fellowship is named after a former Pacific Northwest National Laboratory director and the visionary leader of EMSL, Dr. William R. Wiley. For more information on postdoctoral programs at EMSL and PNNL, visit the postdoc website: http://postdoc.pnnl.gov/

Bolton and Shilling Serving in Interim Capacities

Harvey Bolton and John Shilling have both agreed to function in interim leadership roles at EMSL until permanent replacements are named.

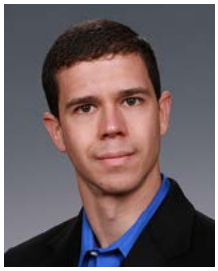
Harvey Bolton

Bolton

Bolton is interim EMSL director. He follows Allison Campbell who was EMSL director for more than a decade and is now acting associate laboratory director of the Earth and Biological Sciences Directorate at Pacific Northwest National Laboratory. Bolton was EMSL's associate director for Science and Technology for the past year and before that he was a division director of biological sciences at PNNL.

An environmental microbiologist, Bolton has more than 25 years of experience leading projects and teams focused on Department of Energy's Office of Biological and Environmental Research mission areas, including microbiology, geochemistry and hydrology together to address problems in contaminant behavior and elemental cycling in the environment. Bolton has held scientific leadership positions at PNNL of increasing responsibility for the past 25 years, from individual group manager to division director.

Bolton conducted research at PNNL for nearly 15 years before moving into leadership positions. He holds a Ph.D. and Master of Science in soil microbiology from Washington State University and a bachelor's degree from The University of Rhode Island.



John Shilling

Shilling

Shilling is interim lead for EMSL's Atmospheric Aerosol Systems Science Theme. He replaces Alex Guenther who left the lab.

A research scientist, Shilling is an atmospheric chemist with expertise in measuring aerosol gas- and particle-phase chemical composition and gas/particle interactions. He is an expert in aerosol gas and particle measurements and in applying mass spectrometry to problems in atmospheric chemistry. Shilling led a project to design and build an aerosol measurement laboratory and environmental chamber in PNNL's Atmospheric Measurement Laboratory.

Shilling came to PNNL in 2008 as a staff scientist. He was a post-doctoral associate at Harvard University. He earned a Ph.D. in analytical/atmospheric chemistry from the University of Colorado.

Dutta Accepts 2014 M.T. Thomas Award

Arnab Dutta received EMSL's 2014 M.T. Thomas Award for Outstanding Postdoctoral Achievement on Sept. 30 following a presentation on his research at EMSL entitled "Developing synthetic H2 oxidation electrocatalysts with enzymatic features."

"Thank you for considering me worthy of this award," said Dutta while accepting the commemorative plaque from Tamas Varga, M.T. Thomas Award selection committee chair.

Dutta is the 19th M.T. Thomas Award honoree since 1996. The selection committee recognized him for his "scientific progress as a postdoc, the quality of his work, and his productivity as measured by the number and potential impact of his publications."

2014 M.T. Thomas Award recipient Arnab Dutta (center holding plaque) stands with (from left to right) Physical Science Division Director Bruce Garett; Associate Division Director for Catalysis Science Wendy Shaw, who nominated Dutta for the award; award namesake M. Tom Thomas; Norma Thomas; and EMSL Scientist Tamas Varga, selection committee chair.

Dutta has published seven scholarly papers, with one in process, based on his research using EMSL resources. He is the first author on four of these papers, including one in *PNAS*. The average impact factor of his seven papers is 11.6.

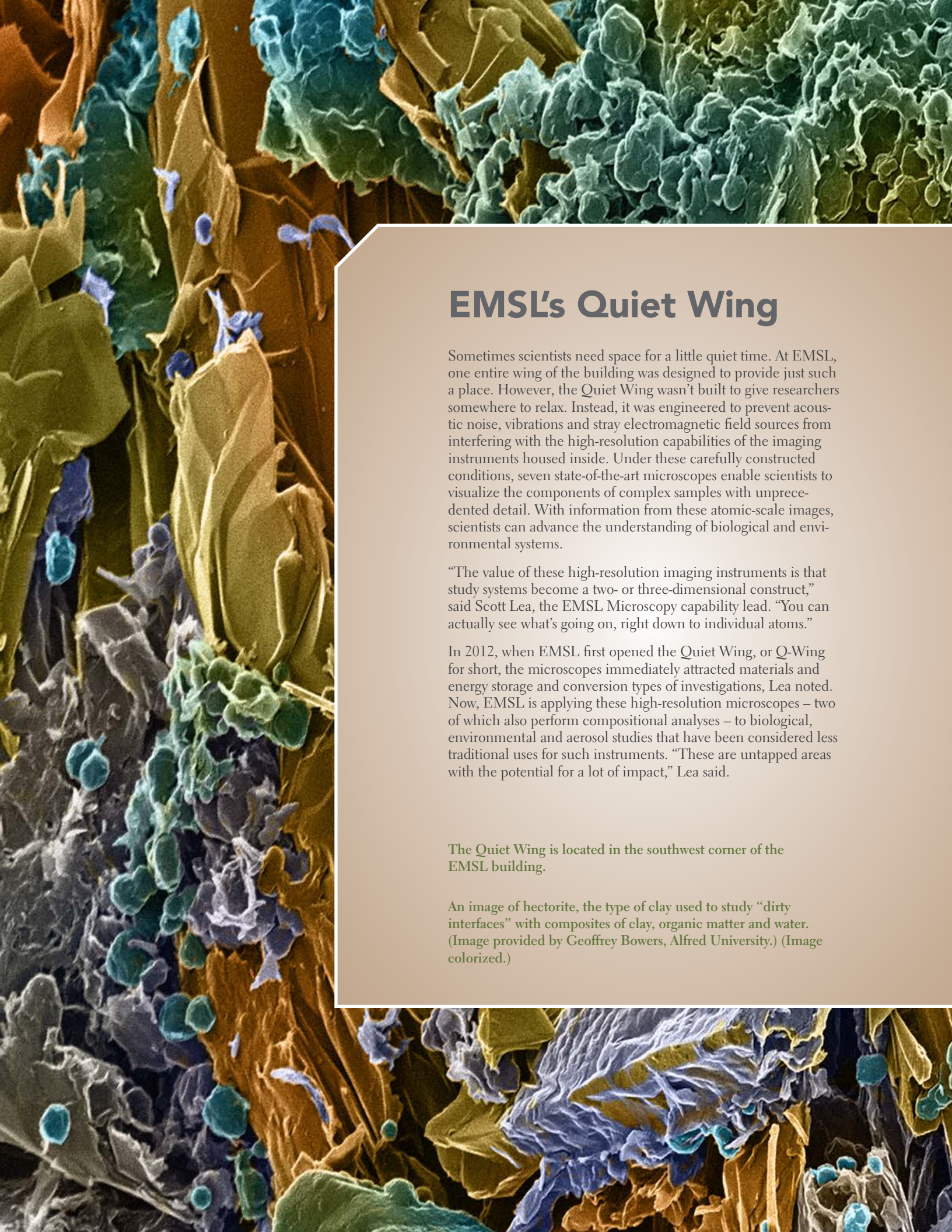
He is currently an assistant professor at Indian Institute of Technology Gandhinagar, India.

The award was named in honor of retired EMSL leader M. Tom Thomas, and acknowledges outstanding accomplishments by postdoctoral fellows who conduct their research at EMSL. The award includes a commemorative plaque and a cash prize.

EMSL on YouTube – iDirector

Former EMSL Director Allison Campbell talks with EMSL Scientist Bingbing Wang about his career path to EMSL and his atmospheric science research into ice nucleation of atmospheric particles. The video is part of Campbell's monthly iDirector interview series available on EMSL's YouTube channel at http://bit.ly/1vy5t02.

The Silent Treatment



EMSL's Quiet Wing

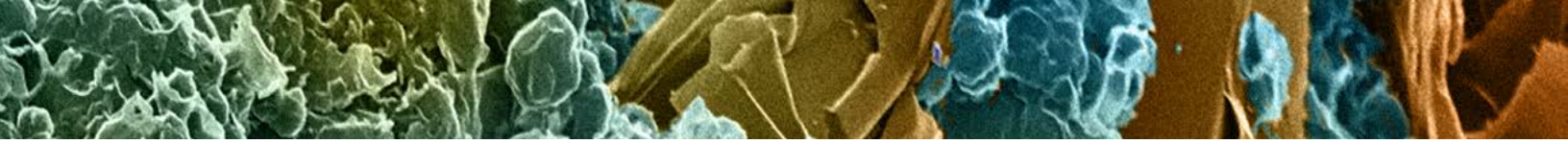
Sometimes scientists need space for a little quiet time. At EMSL, one entire wing of the building was designed to provide just such a place. However, the Quiet Wing wasn't built to give researchers somewhere to relax. Instead, it was engineered to prevent acoustic noise, vibrations and stray electromagnetic field sources from interfering with the high-resolution capabilities of the imaging instruments housed inside. Under these carefully constructed conditions, seven state-of-the-art microscopes enable scientists to visualize the components of complex samples with unprecedented detail. With information from these atomic-scale images, scientists can advance the understanding of biological and environmental systems.

"The value of these high-resolution imaging instruments is that study systems become a two- or three-dimensional construct," said Scott Lea, the EMSL Microscopy capability lead. "You can actually see what's going on, right down to individual atoms."

In 2012, when EMSL first opened the Quiet Wing, or Q-Wing for short, the microscopes immediately attracted materials and energy storage and conversion types of investigations, Lea noted. Now, EMSL is applying these high-resolution microscopes – two of which also perform compositional analyses – to biological, environmental and aerosol studies that have been considered less traditional uses for such instruments. "These are untapped areas with the potential for a lot of impact," Lea said.

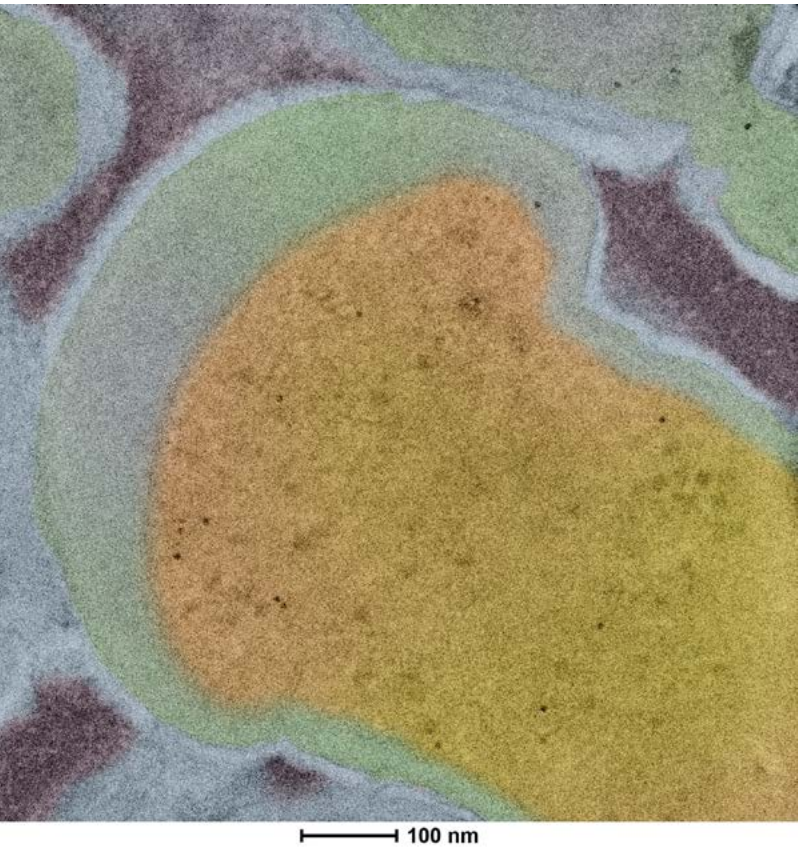
The Quiet Wing is located in the southwest corner of the EMSL building.

An image of hectorite, the type of clay used to study "dirty interfaces" with composites of clay, organic matter and water. (Image provided by Geoffrey Bowers, Alfred University.) (Image colorized.)



Quiet Work

Early evidence of that impact came during the Q-Wing's ramp-up phase. An initial test case for the high-resolution transmission electron microscopes, or TEMs, turned up high-quality images which identified nanoparticulate uraninite being formed by bacteria. The samples came from a decade-old study on uranium remediation led by Ken Kemner, head of the Molecular Environmental Science Group at the Argonne National Laboratory, and EMSL's Alice Dohnalkova. Although their previous work inferred the presence of isolated ions of reduced uranium from X-ray absorption spectroscopy, at the time there was no technique that could directly image those ions.[1] "It was a verification of an idea we put forth almost a decade ago," said Kemner.



Ken Kemner is able to track the distribution of bacteria within complex soil aggregates. This image of a thin section of *Bacillus subtilis* was exposed to conjugated CdSe quantum dots and clearly demonstrates conjugated quantum dots are taken up by the bacteria. This information will be critical for determining the mechanism bacterial cells use to take up these quantum dots. (Image provided by Ken Kemner, Molecular Environmental Science Group at the Argonne National Laboratory.) (Image colorized.)

More recently, Kemner and fellow Argonne collaborator Sarah O'Brien used the Q-Wing's scanning transmission electron microscope, or STEM, to develop approaches to track the distribution of bacteria within complex soil aggregates. The ability to pinpoint the location of bacteria and monitor their activity will improve understanding of soil contaminant transport and fate, the bacterial drivers of carbon dioxide or methane released into the atmosphere, and the effects of microorganisms on plant roots.

However, bacteria ensconced in soil laden with minerals and other opacities can easily dodge detection with traditional X-ray methods. To capture images of bacteria, Kemner is tagging them with fluorescing quantum dots. These dots are nanoparticle-sized pellets of cadmium selenide that are conjugated with amino acids for bacterial uptake.

"With the transmission electron microscope, the Q-Wing is playing a key role in verifying that the quantum dots get into the bacteria via an active uptake mechanism," Kemner said. Once they nail down that mechanism, Kemner and his colleagues hope to popularize the use of these all-around nano-tracking devices.

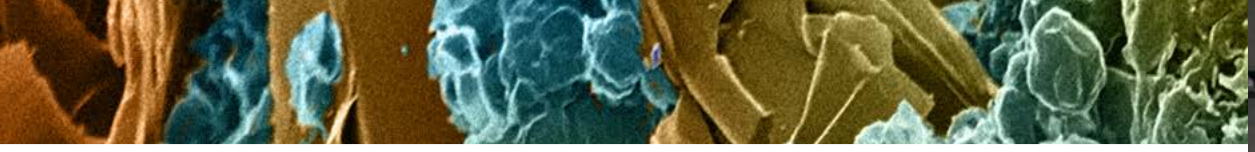
Support for this work was provided by the Department of Energy's Office of Biological and Environmental Research, or DOE BER, specifically, funding was provided by two programs: the Argonne Subsurface Biogeochemical Research Program Scientific Focus Area, which is funded by the DOE BER Subsurface Biogeochemical Research Program; and the Argonne Small Worlds project which is funded by the DOE BER Mesoscale to Molecules Program.

Obtaining atomic-level detail with Q-Wing instruments is also critical to Bradley Tebo, the associate director for the Institute of Environmental Health at Oregon Health and Science University in Portland. With funding from the National Science Foundation's Chemistry of Life Processes program, Tebo wants to understand the behavior of a unique multicopper oxidase, or MCO, that oxidizes manganese from a soluble Mn^{+2} state to an insoluble Mn^{+4}.

Unlike other well-characterized enzymes of its ilk, which catalyze single electron transfers, this unusual MCO also requires two accessory proteins to carry out this oxidizing activity in *E. coli*. Understanding this mechanism may shed light on how manganese conversions occur in the environment, where the availability of the mineral is important for photosynthesis and other key processes, explained Tebo.

"The outstanding scanning transmission electron microscopy capabilities in the Quiet Wing allow us to image single atoms of manganese, and the accessory proteins in the MCO complex," said Tebo.

As atoms of manganese link with oxygen, this mineral development can be followed on the STEM. With a time series of images taken during the reaction, Tebo hopes to determine whether the minerals immediately form a well-developed structure, or create an amorphous shape that later organizes into orderly sheets. He can also examine the accessory proteins to see



how they fold and where the protein subunits are bound to the MCO. Ultimately, he wants to discover whether the protein complex itself serves as a template for mineral formation, or whether some other control exists.

Once the mineralization process is understood, it might be modified to perform tasks such as targeted metal sequestration or – with a slightly altered redox potential – perhaps create a renewable catalyst that can directly deoxidize water to form hydrogen.

Such fine structural detail is equally important to see what happens to the sponge-like properties of clay after it's coated with natural organic material and exposed to water. Interactions at these dirty surfaces play key roles in remediation methods using porous clay to soak up environmental contaminants or in shale-based sequestration techniques that use clay pores in the shale rock as carbon storage chambers, explained Geoffrey Bowers, an associate professor of chemistry at Alfred University in New York.

After many years of exploring the properties of hectorite (a clay with minimal iron content) with EMSL's experts in nuclear magnetic resonance, or NMR, and X-ray diffraction, Bowers made "a concerted shift" to study the interfaces between clay and natural organic matter, or NOM. This research is supported by funds from the DOE's Office of Basic Energy Sciences, Geosciences program.

"We have reasonable ideas about how pristine clay affects the transport of ions in the near surface soils and we know organic matter is good at picking up heavy metals like iron and arsenic," said Bowers. "But it's important to know what happens when you put them together because in surface soil you're almost never going to find clay that's not in intimate contact with NOM."

With his longtime collaborator, R. James Kirkpatrick, dean of the College of Natural Science at Michigan State University, Bowers turned to the Q-Wing's helium ion microscope, or HIM, to get a more holistic view of this complex system. The HIM is similar in concept to a scanning electron microscope, but has higher spatial resolution, greater depth of field and increased sensitivity to small changes at the clay surface. With this instrument the researchers could study natural organic matter-clay composites at scales ranging from tens of nanometers up to one micron in size.

There's a long list of questions Bowers wants to answer with the HIM. For example: Do the samples have large amounts of organic matter preventing water or ions from accessing the clay fraction? Do the clays interact with NOM? What does the pore network look like before and after NOM is introduced? Are there chunks of hydrophobic organic matter that won't let water in, or do super-porous organic matter flocculent particles soak up more water than we expect?

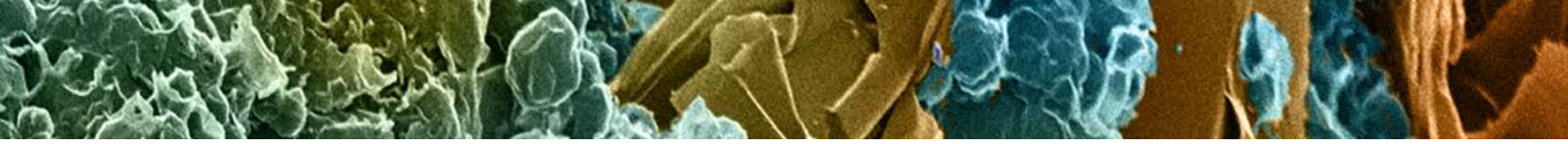
"Those are questions we can't answer with molecular-scale techniques we typically use such as molecular dynamics modeling or NMR," said Bowers. "But we need the answers to properly interpret our models and NMR results. That's where the Q-Wing comes into play."

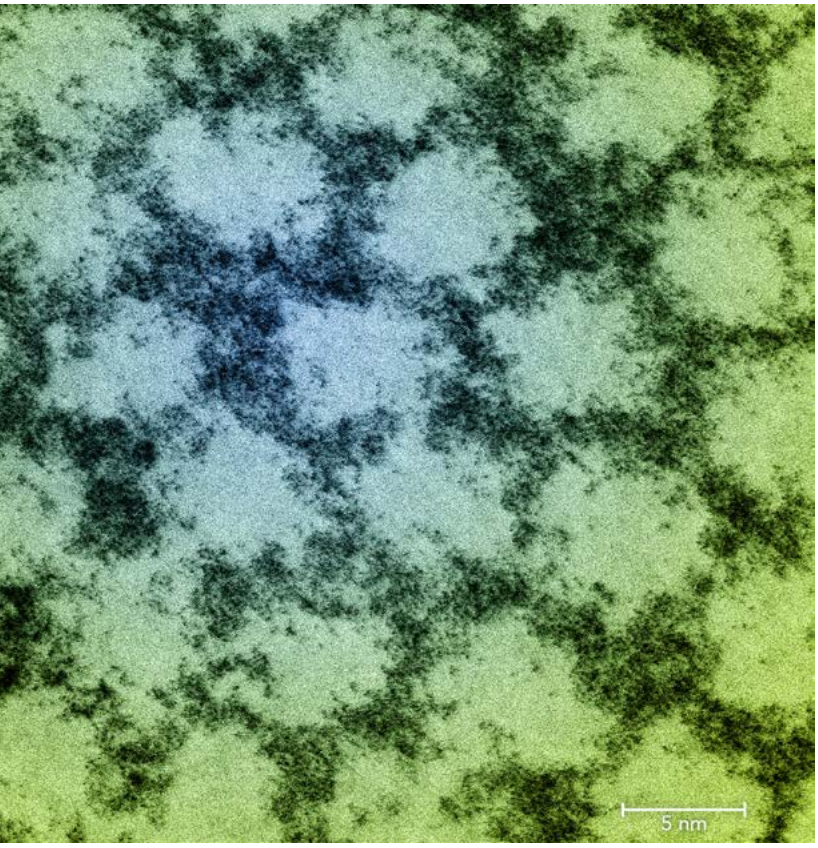
So far, Bowers has seen subtle surface changes that couldn't be captured with electron microscopy alone. For example, the basal surfaces of clay appear flat under the HIM lens. However, the composite material surfaces show "little hills and hummocks" that suggest there's a coating on the clay, said Bowers. Going forward, he'll study how altering the chemical conditions of clay-NOM composite suspensions influence that structure.

Another surprise from the Q-Wing studies was that some composite samples, under certain conditions, form "taffy-like strands" of NOM between the clay particles. These strands look like a "string of pearls," said Bowers, with the size of each pearl in the string correlating with other research results which suggest small 10-20 nm globules may be the state of NOM in solution. With further study, the types of structures formed in clay-NOM composites could be manipulated to improve targeted ion absorption.

Bowers and his colleagues are also exploring subsurface samples with Q-Wing microscopes. "We want to know what might happen if supercritical carbon dioxide is pumped into shale to sequester it," he said. "Will the ions in clay help form more stable mineralized carbon phases?"

Advancing the scientific understanding of various phenomena, including interfacial behavior, biological transformations and geochemical processes, the helium ion microscope is located in EMSL's Quiet Wing.





The circular shapes are individual particles of Mnx, a bacterial multicopper oxidase (MCO) protein complex that converts soluble, dissolved manganese into manganese minerals. The protein is studied in the laboratory of Bradley Tebo, and this image was captured on a scanning transmission electron microscope in the Quiet Wing by EMSL scientists Alice Dohnalkova and Libor Kovarik. (Image provided by Bradley Tebo, Oregon Health and Science University.)(Image colorized.)

There's no endpoint to his questions about these materials and how they affect transport, with or without supercritical CO_2 around, said Bowers. "I think we've opened the lid on a treasure chest, and the question is how far we are going to reach in there and pull out gold for the scientific community as a whole."

Breaking the Silence

Spreading the word about these Q-Wing capabilities is done primarily through meetings, said Scott Lea. "Either we're presenting our own work, or talking with investigators to understand what they're trying to do and see how we might be able to help them," he said.

Soon, scientists using the Q-Wing will have even better options available to study their research samples.

Efforts by Nigel Browning, Pacific Northwest National Laboratory, and James Evans in EMSL are underway to develop a second-generation dynamic TEM that allows faster time resolution (in the nanosecond realm) as well as high spatial resolution. "We're trying to go three to six orders of magnitude faster," said Lea. "If we can do that, then we'll be able to see things like protein conformational dynamics such as helix or domain motions, aerosol growth and nucleation. There's no way to get this information now using electron-based approaches."

EMSL experts are also planning to add high-sensitivity, direct electron detector devices, or DEDs for short, on some of the Q-Wing instruments. Replacing the charge-coupled devices currently on the TEMs with these new devices will give microscopists high-resolution images with a smaller dose of electrons. The DEDs will be particularly advantageous for aerosol or biological samples that are more sensitive to beam damage caused by exposure to large doses of electrons. The liquid helium cryogenic transmission electron microscope is the first instrument slated for getting the new device, Lea said.

Another technique championed by the Chemical Imaging Initiative at PNNL that would give researchers more imaging information with fewer electrons is a mathematical method called compression sensing. This method provides similar information, but with less electron dose, by reducing the noise in the images.

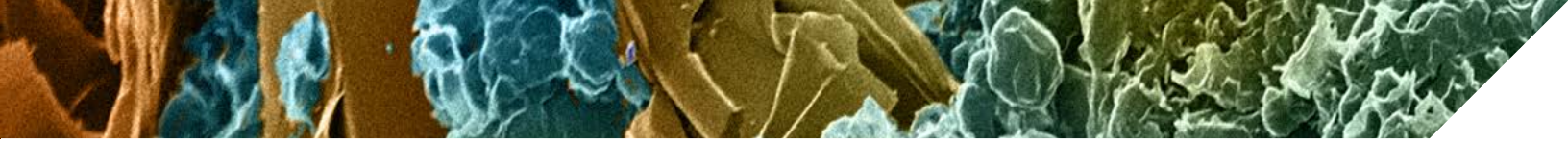
"These combined efforts should give us the ultimate in low-dose imaging, which is very important going forward for biochemical, environmental and aerosol research," said Lea. Still, he's eager to fill one empty instrument berth in the Q-Wing with the next advanced instrumentation. ■

Elizabeth Devitt is a science journalist and freelance writer.

EMSL, the Environmental Molecular Sciences Laboratory, is a national scientific user facility sponsored by the Department of Energy's Office of Science. Located at Pacific Northwest National Laboratory in Richland, Wash., EMSL offers an open, collaborative environment for scientific discovery to researchers around the world. Its integrated computational and experimental resources enable researchers to realize important scientific insights and create new technologies.

Reference:

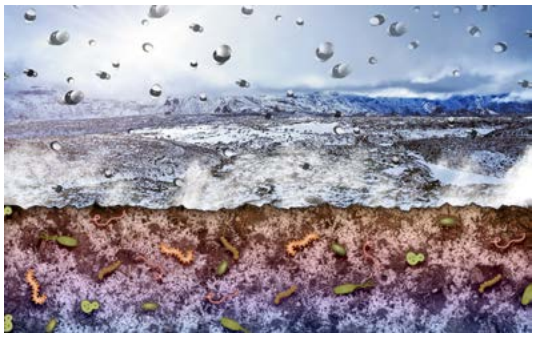
1. Dohnalkova A, Marshall M, Kemner K, Kennedy D, Genc A and Fredrickson J. 2014. "Bacterially-Produced Uraninite – Ultrastructural Characterization by High Resolution Imaging and Analyses." Goldschmidt conference in Sacramento, Calif.



SCIENCE HIGHLIGHTS

Arctic Changes

Thawing permafrost may not worsen climate change



Permafrost soils near the North Pole contain roughly twice the amount of carbon compared to that stored in the atmosphere today; but for now, most of this soil organic carbon is perennially frozen. However, Arctic warming is thawing permafrost soils and mobilizing previously frozen dissolved organic matter, or DOM, from deeper soil layers to nearby surface waters. The subsequent degradation of DOM by bacteria may cause a substantial increase in CO_2 release to the atmosphere, triggering a positive feedback loop that could amplify climate change. To better understand this risk, a recent study characterized the chemical composition of DOM drained from different depths in permafrost soils and related these compositional differences to its susceptibility to biological degradation.

The findings revealed deeper permafrost soil layers contain molecules that are more readily degraded by bacteria compared to shallow layers. However, higher degradation rates in the deep permafrost layer may not translate into a rapid increase in CO_2 release into the atmosphere. These findings could lead to more accurate global climate models and more effective strategies to mitigate climate change.

Funding: This research was supported by the National Science Foundation.

Publication: Ward CP and RM Cory. 2015. "Chemical composition of dissolved organic matter draining permafrost soils." *Geochimica et Cosmochimica Acta*. doi:10.1016/j.gca.2015.07.001

Participating Organizations: University of Michigan at Ann Arbor and EMSL.

Scarcity Drives Efficiency

Platinum can be an efficient fuel cell catalyst

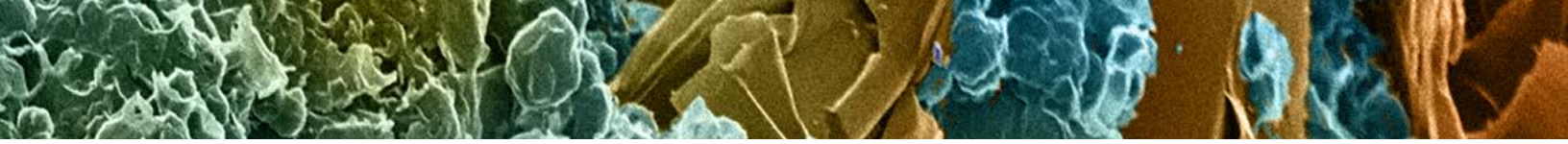
Platinum is an excellent catalyst for reactions in fuel cells, but its scarcity and cost have driven scientists to look for more efficient ways to use the precious metal. In a recent study, researchers developed a new class of catalysts by putting essentially all of the platinum atoms on the surface and minimizing the use of atoms in the core, thereby increasing efficient utilization of platinum for fuel cells.

The novel nanocage catalyst will help promote the sustainable use of platinum and other precious metals for energy and other industrial applications. The reduced costs associated with the novel nanostructures will encourage commercialization of this technology for the development of zero-emission energy sources.

Funding: This research was supported by the Department of Energy's Office of Basic Energy Sciences.

Publication: Zhang L, L Roling, X Wang, M Vara, M Chi, J Liu, S Choi, J Park, J Herron, Z Xie, M Mavrikakis and Y Xia. 2015. "Platinum-based nanocages with subnanometer-thick walls and well-defined, controllable facets." *Science Magazine*. DOI: 10.1126/science.aab080.

Participating Organizations: Georgia Institute of Technology, Emory University, Xiamen University, University of Wisconsin–Madison, Oak Ridge National Laboratory, Arizona State University, EMSL, Argonne National Laboratory and National Energy Research Scientific Computing Center.



Better Science

Molecular understanding sheds light on soil processes

Natural organic matter, or NOM, is a mixture of organic molecules derived primarily from the natural decay of plant matter. Understanding how NOM interacts with mineral surfaces is critical for a range of applications such as CO_2 sequestration, wastewater treatment and prevention of industrial fouling (the accumulation of unwanted material on solid surfaces). A recent study shed light on the molecular-scale roles calcium and other cations play in determining the structure and behavior of large NOM aggregates commonly found in nature.

These broad-reaching fundamental discoveries will improve predictive models used for understanding nutrient and carbon cycling at the earth's surface, CO_2 sequestration and the transport of environmental contaminants. This information could be used to improve strategies for remediating contaminated soil and groundwater.

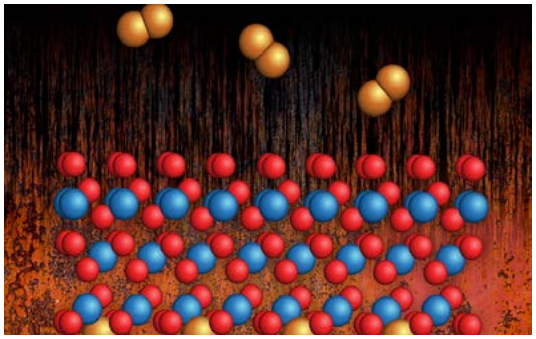
Funding: This research was supported by the Department of Energy's Office of Basic Energy Sciences.

Publication: Bowers GM, HE Argersinger, V Reddy, TA Johnson, BW Arey, ME Bowden and RJ Kirkpatrick. 2015. "Integrated Molecular and Microscopic Scale Insight Into Morphology and Ion Dynamics in Ca2+-Mediated NOM Floccs." *The Journal of Physical Chemistry C*. doi:10.1021/acs.jpcc.5b05509.

Participating Organizations: Alfred University, Michigan State University and EMSL.

New Models Closer to Nature

Better understanding could improve remediation



Uranium dioxide contains the less soluble and immobile form of uranium in nature, so it is the desired end product of bioremediation strategies for contaminated soil and groundwater. But when exposed to oxygen, UO_2 incorporates additional O atoms and the uranium oxidizes, transforming into the more soluble, mobile form of uranium that can be released into the environment. This study combined experimental and theoretical approaches to examine, at the atomic scale, the earliest stages of UO_2 oxidation under ambient conditions relevant to oxidation mechanisms in nature.

The findings show UO_2 oxidation spreads from the surface to deeper atomic layers in a complex pattern that does not follow classical diffusion. By shedding light on initial stages of oxidation in UO_2, the findings could improve predictions of how this essential material will corrode in a wide range of settings, including ore bodies, nuclear reactors, waste repositories and environmental cleanup sites.

Funding and Programs: This research was supported by the Department of Energy's Office of Basic Energy Sciences GeoSciences; National Science Foundation-Earth Sciences; Geosciences Research Program at PNNL through the DOE-BES and Subsurface Biogeochemical Research through the SLAC SFA Program.

Publication: Stubbs JE, AM Chaka, ES Ilton, CA Biwer, MH Engelhard, JR Bargar and PJ Eng. 2015. "UO_2 Oxidative Corrosion by Nonclassical Diffusion." *Physical Review Letters* 114:246103. doi:10.1103/PhysRevLett.114.246103.

Participating Organizations: University of Chicago, PNNL, EMSL, Advanced Photon Source and Berkeley Nanogeoscience Center.

About this Art

Scientists at Pacific Northwest National Laboratory and EMSL are trying to understand structure-property relationships in plasmonic nanoparticles and their assemblies. Shown is a silver nanoparticle assembly supported on a single sheet of graphene. Differences in phase contrast are highlighted. Electric fields can be localized and enhanced at the nanojunctions formed between the nanoparticles which comprise the 2-D assembly imaged. The research was funded by the Department of Energy's Office of Basic Energy Sciences and PNNL's Chemical Imaging Initiative. The 53x53 nm2 image was captured with a transmission electron microscope housed in EMSL's Quiet Wing.

Team Members

Project team members include: Patrick El-Khoury, Wayne Hess and Nigel Browning, all with PNNL; James Evans with EMSL; and Patricia Abellan, formerly at PNNL and now at SuperSTEM Laboratory, Daresbury.