the Molecular Bond

EMSL

SCIENTIFIC INNOVATION THROUGH INTEGRATION

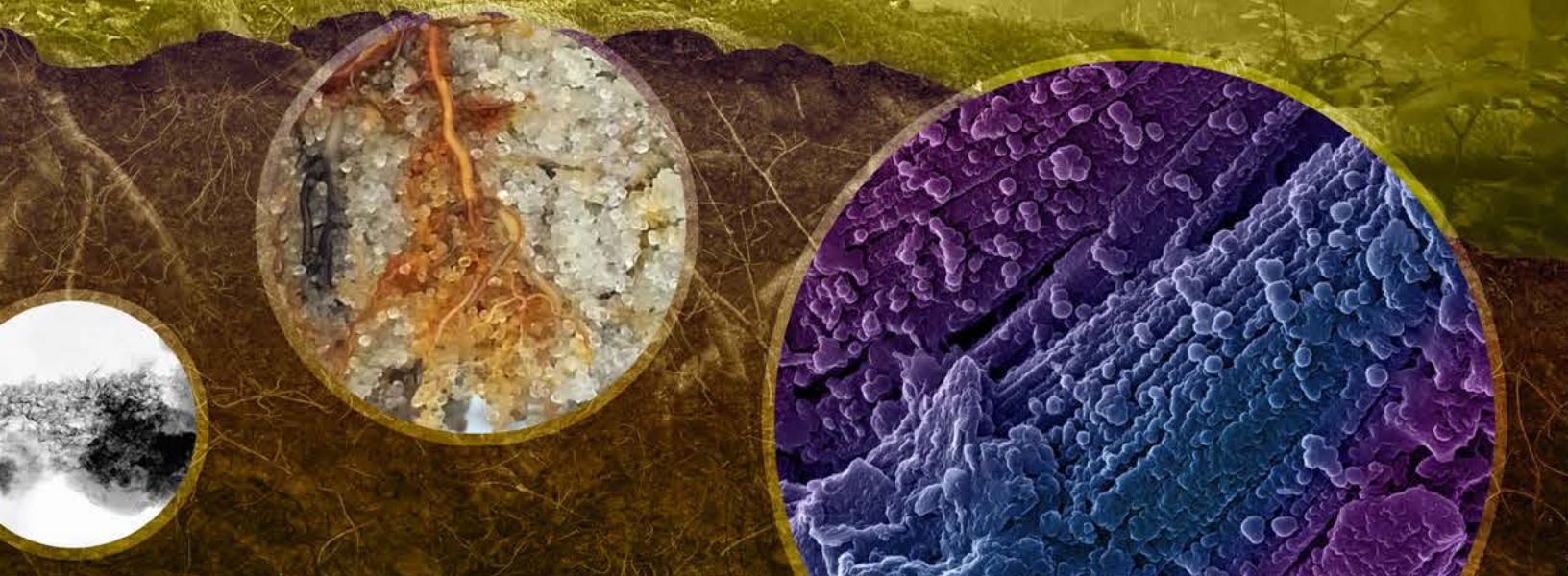
December 2014

EMSL's Radiochemistry Annex

It's Getting **Hot** in There

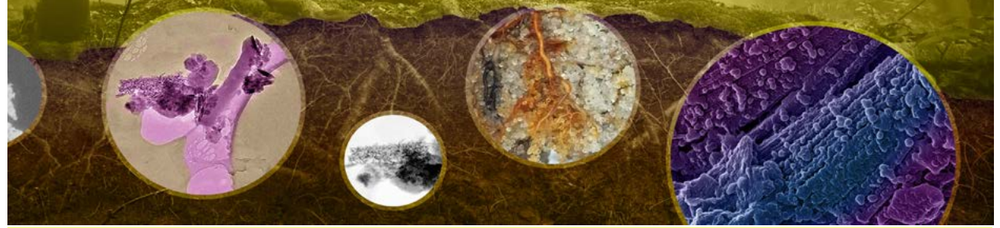
Also inside this issue:

T&SE Postdoc Position Closing
21 T Magnet Arrives
Improving CO_2 Sequestration
Enhanced Carbon-cycle Models



About the Cover

Researchers studying terrestrial and subsurface ecosystems are able to turn to the capabilities and scientific expertise at EMSL and its Radiochemistry Annex. The science images featured along the bottom are samples from within the rhizosphere of natural plants growing in a contaminated Savannah River Site wetland. The images were generated using EMSL resources, including X-ray computed tomography, scanning transmission electron microscopy and helium ion microscopy, (Images provided by Daniel Kaplan, Savannah River National Laboratory.)



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/emslweb

To request additional copies or to subscribe, contact: EMSL Communications at email: emslcom@pnnl.gov

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Libor Kovarik, EMSL scientist, was a member of the research team studying metal catalysts for steam methane reforming reactions highlighted in the "Improving Biofuel Production" science highlight on page 12. In this photograph, Kovarik is using the environmental transmission electron microscope housed in EMSL's Quiet Wing. EMSL's ETEM provides in situ capabilities that enable atomic-resolution imaging and spectroscopic studies of materials under dynamic operating conditions. (EMSL file photo)

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FROM THE DIRECTOR

Allison Campbell

I'm pleased to share with you this issue's cover story on the EMSL Radiochemistry Annex. It's a specialized facility we opened about a year ago and one we had envisioned from the early days of EMSL.

Early on, EMSL leadership recognized we could apply our molecular-level expertise to studying radiological samples. It wasn't until we identified radiological space in a new facility next door at Pacific Northwest National Laboratory and received American Recovery and Reinvestment Act funds to purchase new instruments that we could realize this vision.

Today, the Radiochemistry Annex is a point of pride for EMSL. It represents our perseverance and belief in the value of molecular-level studies. I'm also proud of the science that our researchers and our users have already undertaken in the past year.

We expect to advance our understanding of elemental composition, chemical speciation of contaminants, microbial associations and chemical solubility of contaminants – all with the goal of informing remediation strategies.

EMSL's Radiochemistry Annex is one of the most modern radiochemistry laboratories in the world. I invite you to read about how we're advancing science and the mission of our Department of Energy sponsor, the Office of Biological and Environmental Research, through expertise and equipment in the Annex. If your research could benefit from collaborations with our scientific team and with access to the Annex, consider submitting a user proposal in our annual call, which opens next month.

—Allison

Researchers will soon have the highest clarity molecular characterization of complex systems with the arrival of the magnet for EMSL's new 21 Tesla Fourier Transform Ion Cyclotron Resonance Mass Spectrometer. A crew moved the 22-ton magnet in late November into its permanent location in one of EMSL's mass spec laboratories. EMSL anticipates the 21 T FT-ICR MS being ready for user community access in 2015. Read more about the science being made possible by this new instrument in the article "21 Tesla Mass Spectrometry Magnet Arrives at EMSL" on page 5.

NEWS & KUDOS

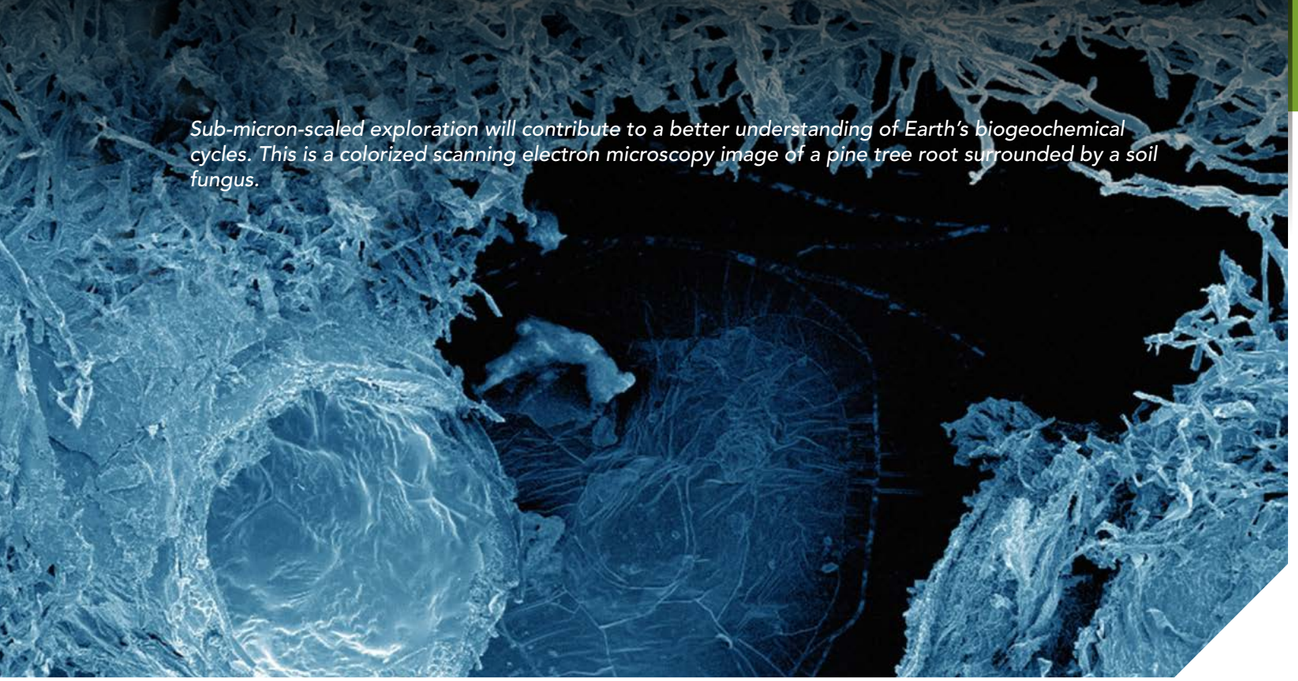
T&SE Postdoc Position Closes Dec. 28

EMSL is accepting applications for the 2015 Terrestrial and Subsurface Ecosystems Postdoctoral Appointment through Dec. 28, 2014.

The appointment is designed to attract high-performing, newly graduated junior Ph.D. scientists with research interests that include a mix of modeling/simulation and experimental approaches that lead to improving the representation of terrestrial ecosystem processes in the land components of Earth system models. The appointment is funded directly by the Department of Energy's Office of Biological and Environmental Research Terrestrial Ecosystem Science program.

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 EMSL's Terrestrial and Subsurface Ecosystem Science Theme.

Information on how to apply, selection criteria and the selection process is available at http://www.emsl.pnnl.gov/emslweb/news/tse-postdoc-position-open.



Sub-micron-scaled exploration will contribute to a better understanding of Earth's biogeochemical cycles. This is a colorized scanning electron microscopy image of a pine tree root surrounded by a soil fungus.

Baer Named AVS Trustee

Don Baer

The membership of AVS: Science and Technology of Materials, Interfaces, and Processing has elected Don Baer a trustee on the society's Scholarship and Award Committee.

The committee comprises six members known as trustees. Elected by the society's membership, the trustees are entrusted with the process and recipient selection of all society scholarships and awards.

"Recognition of outstanding scientific research and technological innovation is one of AVS' most important activities," said Baer, EMSL's Science Theme lead for Energy Materials and Processes. "It's a great honor to have been elected a trustee."

Baer has been an AVS Fellow since 2001 and earned the AVS Albert Nerken Award in 2009.

AVS, formerly American Vacuum Society, is an interdisciplinary, professional society that supports networking among academic, industrial, government and consulting professionals involved in a variety of disciplines related to materials, interfaces and processing.

Orr to Join Editorial Advisory Board

Galya Orr

Galya Orr has been asked to be a member of the editorial advisory board of *Chemical Research in Toxicology*, a peer-reviewed scientific journal published by the American Chemical Society.

Orr is a senior research scientist and the Cell Isolation and System Analysis capability lead at EMSL. She joins the board in January.

Chemical Research in Toxicology provides a venue for the presentation of research relevant to all aspects of the chemical basis of toxic responses. The journal is produced by ACS Publications, which is a division of the American Chemical Society.

21 Tesla Mass Spectrometry Magnet Arrives at EMSL

Scientists seeking to characterize complex environmental and biological materials are one step closer to using EMSL's new 21 Tesla Fourier Transform Ion Cyclotron Resonance Mass Spectrometer. The magnet, a critical piece of the system, was delivered to EMSL in late November.

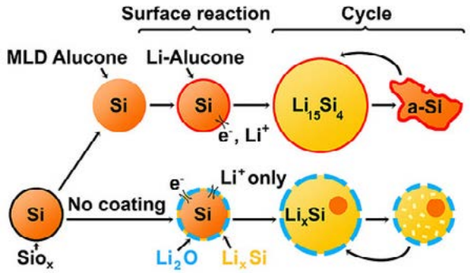
The 21 T FT-ICR MS will be one of only two in the world with this high of a magnetic field strength. The 21 Tesla field strength allows for higher resolution and higher mass accuracy measurements that ensure identification of molecular constituents in complex samples and materials. It will enable greater characterization of large intact proteins in microbial communities or natural organic matter in soils and aerosols.

Workers carefully move the magnet for EMSL's new 21 T FT-ICR MS system into the EMSL building.

Agilent Technologies' Magnet Science Facility outside of Oxford, England, manufactured the magnet for the 21 T FT-ICR MS system. The magnet is just one part of the overall instrument; EMSL is building the other customized spectrometer and data acquisition/instrument control parts of the system. The system is being developed to advance the science mission of the DOE Office of Biological and Environmental Research, and was funded as a Major Item of Equipment by BER. EMSL anticipates the capability being ready for user community access in 2015.

Lengthening the Life of Silicon Electrodes in Li Batteries

A new study could help researchers develop longer-lasting rechargeable lithium batteries. In a study published in the journal *ACS Nano*, researchers using EMSL expertise and instruments showed how an aluminum glycerol coating makes high-capacity silicon electrodes more durable, and could lead to a replacement for lower-capacity graphite electrodes.



Silicon nanoparticles coated in alucone (yellow spheres outlined in orange) expand and contract easily on charging and use. But left to their native silicon oxide covering (yellow spheres in blue), they break down fast on recharging.

"Understanding how the coating works gives us an indication of the direction we need to move in to overcome the problems with silicon electrodes," said Chongmin Wang, a senior research scientist at EMSL.

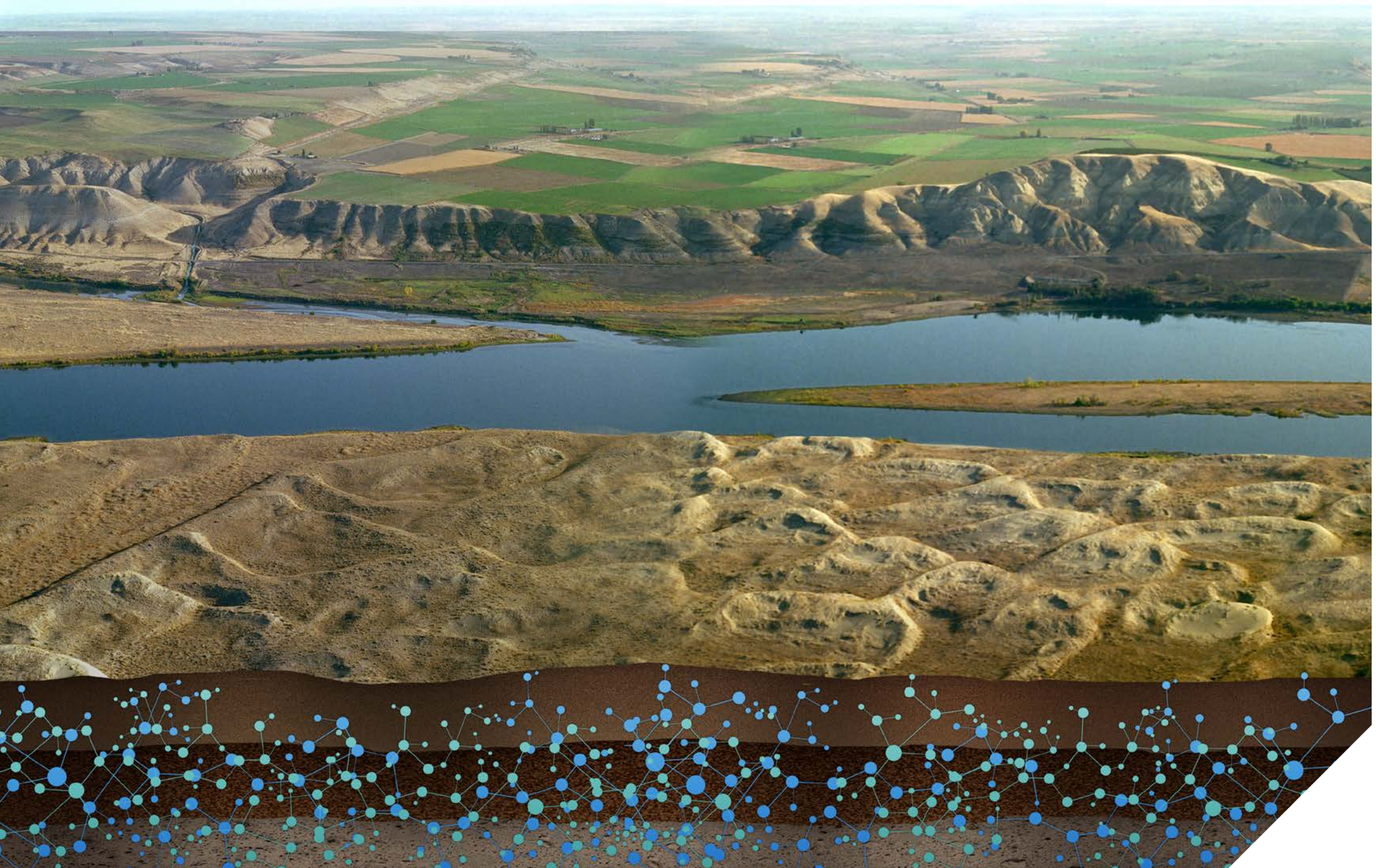
The researchers did not know how the rubber-like aluminum glycerol coating, called alucone, improved the performance of the silicon electrodes. To better understand how it worked, Wang and his research team used EMSL resources, including *in situ* transmission electron microscopy to watch the particles being charged and discharged.

Reference: He Y, D Piper, MengGu, J Travis, S George, S Lee, A Genc, L Pullan, J Liu, S Mao, J Zhang, C Ban and C Wang. October 27, 2014. "*In Situ* Transmission Electron Microscopy Probing of Native Oxide and Artificial Layers on Silicon Nanoparticles for Lithium Ion Batteries." *ACS Nano*. DOI: 10.1021/nn505523c.

EMSL's Radiochemistry Annex

It's Getting **Hot** in There

Understanding the chemical fate and transport of radionuclides



Scientist Daniel Kaplan has found it challenging to study radionuclides in contaminated wetlands due to the radioactive hazard and the biogeochemical complexity of the subsurface soils. Fortunately, he's able to safely pursue his research at EMSL's Radiochemistry Annex.

"Very few facilities in the U.S. have capability to do radiological work, the highly specialized equipment and scientific expertise of the Radiochemistry Annex," says Kaplan, a senior fellow scientist at Savannah River National Laboratory. He's one of several scientists who are working with EMSL through a Special Science Call for Proposals to do high-impact research at the Annex.

Located across the street from the main EMSL facility, the Annex opened in early 2014. It offers 6,000 square feet of lab space designed to safely study radionuclide samples in terrestrial and subsurface ecosystems. It houses advanced spectroscopic and imaging technologies as well as a full suite of instruments for sample preparation and analysis in a contiguous space. Like all EMSL capabilities, those in the Annex are available to the scientific community at typically no cost for openly published research.

Uranium Sequestration

Jeffrey Catalano, an associate professor at Washington University in St. Louis, was one of the prospective users approved to utilize the Annex's capabilities during the Special Science Call. Working with him are Daniel Giammar and Lindsay Troyer, both with Washington University in St Louis. They are studying the use of phosphate to remediate subsurface uranium contamination with funding by the Department of Energy's Office of Biological and Environmental Research.

"One of BER's mission goals is to develop a robust scientific understanding of physical, chemical and biological processes of contaminated subsurface systems for effective decision making on environmental remediation and stewardship," says Catalano.

At sites around the world, including some DOE facilities, uranium has been released into the subsurface. Uranium has become dissolved in the groundwater and can migrate toward waterways. These sites are challenging to treat because uranium is spread over a large area deep below the ground. One possible remediation approach is with an *in situ* treatment method. This entails injecting a chemical into the contaminated area that makes uranium less soluble so that it does not migrate in groundwater, thus reducing the potential health hazard posed by the radionuclide.

Other researchers tested an *in situ* treatment method by injecting dissolved phosphate into the subsurface at the Hanford Site in southeastern Washington. The intent was for the phosphate to react with uranium to create uranium-phosphate solids, insoluble phases that would not migrate.

(continued on page 8)

Jeffrey Catalano

"It turns out the subsurface system is a bit more complicated than previously thought," says Catalano. "The initial tests didn't work as expected."

According to Catalano, the chemical reactions caused by adding phosphates to a subsurface system aren't well understood enough to be able to predict what will happen when this remediation method is used. His team's experimental investigation at the Annex is trying to understand when uranium-phosphate solids form, their composition and solubility, what other solids form and what other reactions occur.

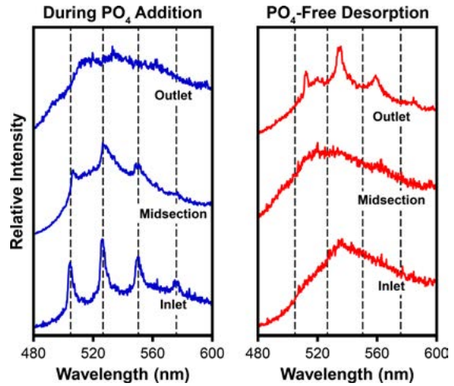
Catalano and his team have been working on this phosphate remediation project for three years, but they have only been utilizing EMSL's capabilities through the Special Science Call since September. As part of the proposal, they are using EMSL's fluorescence, cryogenic spectrometer to determine the chemical forms of uranium in the samples formed under different conditions. With the radiological X-ray photoelectron spectrometer, better known as XPS, they can study nucleation behavior on mineral surfaces to determine how much uranium and phosphate are on the mineral surfaces. They're also investigating field-site sediments, in particular the calcium-phosphate solids, under high resolution microscopy with the Annex's radiological focused ion beam scanning electron microscope, or FIB/SEM, and radiological transmission electron microscope, or TEM.

At this point in the study, most of the EMSL data is from the fluorescence, cryogenic spectrometer. They are finding uranium-phosphate solids only precipitate under a limited set of conditions. In most cases, uranium instead adsorbs to other solids, likely newly formed calcium phosphates, and can actually be easily remobilized when phosphate addition ends.

"Until we had the EMSL data, we didn't know the chemical reactions weren't forming dedicated uranium-phosphate solids," says Catalano. "And that's not what we expected."

Catalano anticipates receiving XPS data in mid-December, and the microscopy work will be done in the spring.

"We're just starting to get data from EMSL, but from what I've seen so far, the information from the Radiochemistry Annex will help us make better predictions of how effective remediation methods are over the longer term," says Catalano.



For their research on the use of phosphate to remediate subsurface uranium, Jeffrey Catalano's team analyzes cryogenic laser fluorescence spectra of uranium in sediments reacted with uranium-bearing groundwater in flow-through column experiments. During addition of phosphate (left) uranium-phosphate solids form, as indicated by the dashed vertical lines, but these materials are most concentrated near the point of phosphate addition; none forms near the outlet of the column. After shutting off phosphate addition and continuing to flow uranium-bearing groundwater through the column (right), the uranium-phosphate solids dissolve completely, releasing uranium to groundwater and leaving behind some residual adsorbed uranium.

Hematite-technetium Interface

Nathalie Wall, an assistant professor of chemistry at Washington State University, is another scientist whose proposal to use the Annex was approved through the Special Science Call. She is supervising Larissa Gribat, a WSU graduate student, to study the chemistry of the hematite-technetium interface and its effect on technetium mobility. The Department of Defense is funding this study.

Technetium, or Tc, is a radioactive fission product often present in nuclear waste. It tends to be more mobile in the environment than other fission products.

"There is a lack of knowledge of the fundamental chemistry of Tc that would explain its mobility in complex systems, such as the environment," says Wall.

Tc in the environment has two oxidation states, Tc(VII) and Tc(IV). Generally, Tc(VII) is soluble and highly mobile in the environment, especially in water; and Tc(IV) is insoluble and quite immobile. It was thought the best way to remediate Tc(VII) was to add a reducing agent, microbes or a mineral to form Tc(IV) and immobilize it. Unfortunately, this remediation process only works in the laboratory, not in an environmental system. Tc(IV)

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can form soluble, mobile compounds with molecules in nuclear waste or the environment.

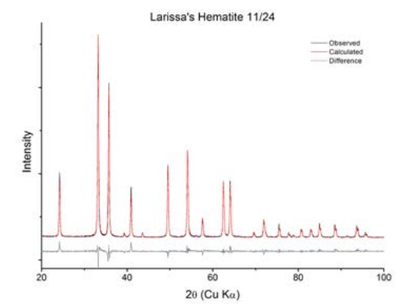
"The idea Tc in one state is very soluble compared to the other one isn't completely correct," says Wall. "Tc(IV) is less soluble than Tc(VII), but in an environmental system it's not insoluble; it's still slightly soluble. The problem is we don't know exactly how much, because there's a lack of thermo-dynamic data."

Nathalie Wall

Wall and Gribat designed their Annex research to gather the needed data using a combination of radiochemistry, electrochemistry and inorganic chemistry. Previous research has shown iron, or Fe, effects on the oxidation state of Tc. Iron exists naturally in the environment as Fe(II) or Fe(III). They want to see if $Fe(III)O_2$, or hematite, will re-oxidize Tc(IV) to Tc(VII) in an oxygen-free environment. Conversely, they want to put Tc(VII) in contact with an Fe(II) mineral and see if it reduces it to Tc(IV). They are using the Annex's XPS with attached environmental chamber to determine the oxidations state of the Tc samples.

"To understand the mobility of Tc, we need to understand the switch between the two Tc oxidation states – it's never been looked at in a systematic way," says Wall. "The reason we're doing this study is to see how an iron mineral affects the redox of Tc, because the redox of Tc influences and drives the mobility of Tc in the environment."

For Wall, a bonus of doing research at the Annex is its proximity to WSU's main campus in Pullman, Wash. She can cost-effectively send her students to Richland to gain



For their study of the hematite-technetium interface and its effect on technetium mobility, Nathalie Wall and Larissa Gribat use the radiological X-ray photoelectron spectrometer to generate a spectrum of hematite.

The rhizosphere, or root zone, is the focus of Daniel Kaplan and Peter Jaffe's wetland research. The rhizosphere is the region of soil that is chemically, hydraulically and microbially influenced by the presence of a root. (Image provided by Daniel Kaplan.)

the experience of working at a national scientific user facility with respected scientists. Gribat has made several trips to EMSL to oversee the project since it started two months ago. Wall says it has been an outstanding experience for Gribat.

Wall and Gribat's study aligns with BER's missions. Their findings will be helpful when remediating subsurface systems contaminated with Tc, including the Hanford Site and other DOE facilities. In addition, by knowing more about Tc chemistry, nuclear waste repositories can be designed to ensure Tc does not escape the boundary of the repository.

"This research will lead to a better understanding of Tc chemistry for better remediation and better containment of future nuclear waste. We'll have less environmental remediation to do in the future if we can fix the problem now," says Wall. "And by better understanding how Tc chemistry works in the environment, we can find a way to stop it. That will be a huge savings by not having to go back and remediate contaminated sites."

Uranium Redox Cycling

Kaplan is the principal investigator and Peter Jaffe, Princeton University, is his colleague on the wetland study in the Annex. Their BER-funded research explores the influence of iron and carbon on uranium redox cycling in wetlands with a focus on the plant root zone, or rhizosphere.

Kaplan and Jaffe are studying uranium contaminated wetlands on DOE's Savannah River Site. Over time, uranium radionuclides travel through the vadose zone – the area between the surface and the aquifer – and move through the aquifer and collect in a wetland or riparian zone until migrating into a waterway. In support of BER's missions,

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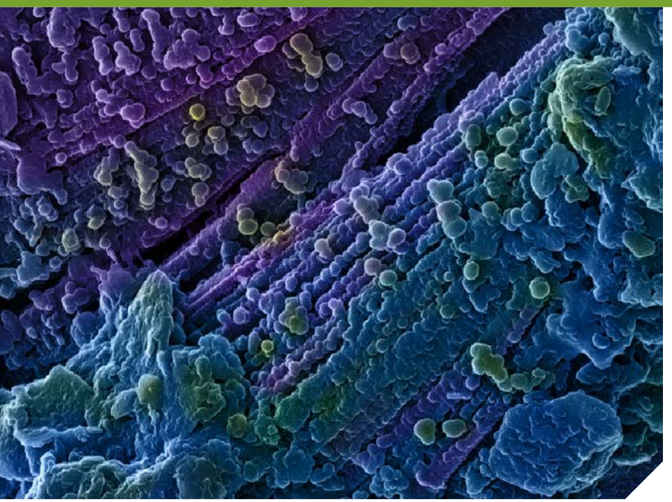


Daniel Kaplan and Peter Jaffe's earlier research on uranium contaminated wetlands used EMSL's helium ion microscopy in the Quiet Wing to image biogenic nano-iron oxides oriented along a root recovered from a wetland plant from the Savannah River Site. (Image taken by Bruce Arey, EMSL technologist.)

this research will help show how legacy radioactive waste is impacting the environment and will be used to help estimate any potential risk.

Wetlands consist of the rhizosphere and bulk soil, the area not penetrated by roots. A lot of geochemical reactions take place in wetlands due to the organic matter and microbial colonies. Their research at EMSL has discovered a difference in the iron chemistry between the rhizosphere and bulk soil. The rhizosphere has more iron nanoparticles and a greater percentage of organic matter, and the properties of the organic matter in the rhizosphere are also different than those in bulk soil.

"The rhizosphere accounts for a very small percentage of the total volume of these wetlands, but it seem to be accounting for a disproportionately large percent of uranium in that system," says Kaplan. "We're interested in finding the factors in the soils that have the greatest impact on chemistry – that's why we're focusing on the rhizosphere. Because of its scale – just millimeters – I've called on EMSL to help us to characterize the rhizosphere and do it with radioactive soils."

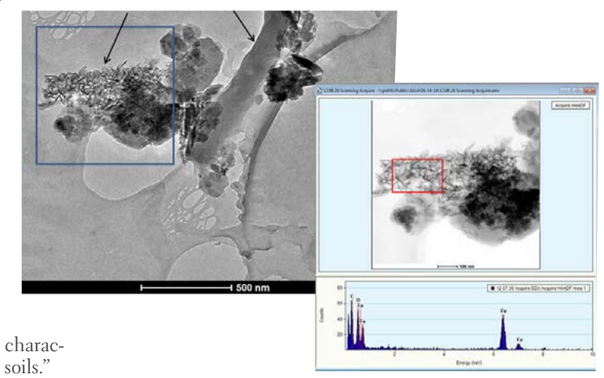
This Annex study will utilize a number of EMSL's spectrometry and microscopy capabilities, including the XPS, TEM, scanning probe microscope and electron microprobe. Kaplan and Jaffe chose to do their research at the Annex because of its unique instrumentation, ability to handle radioactive samples, and knowledgeable scientists who are experts at helping to interpret data and putting it into the appropriate context for their study.

Kaplan and Jaffe's Special Science Call research is a follow-up to a previous project using EMSL resources but not at the Annex. They used data from the earlier study to develop the Special Science Call proposal. While Kaplan and Jaffe's research at the Annex has only been underway for a few months, their research using EMSL resources is generating valuable information.

Daniel Kaplan

"Our work at EMSL has shown the chemical and biological differences between the rhizosphere and bulk soil – these findings are groundbreaking," says Kaplan. "None of these differences has been demonstrated before with uranium-contaminated sediments. We could have never done it without EMSL instrumentation and staff support."

EMSL is a national scientific user facility funded by the Department of Energy's Office of Biological and Environmental Research and located at Pacific Northwest National Laboratory in Richland, Wash. ■

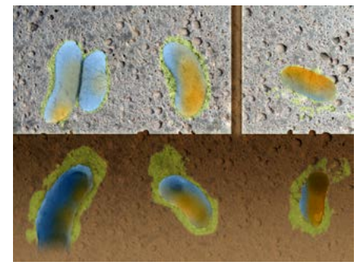


Daniel Kaplan and Peter Jaffe's research on uranium contaminated wetlands used EMSL's high angle annular dark field (HAADF) scanning transmission electron microscopy (STEM). It shows a rhizosphere sample showing a bacterium and nearly nano-geothite. (Image taken by Alice Dohnalkova, EMSL senior research scientist.)

SCIENCE HIGHLIGHTS

Geologic CO_2 Sequestration Inhibits Microbial Growth

Implications for microbial ecology and engineering processes



Carbon dioxide, or CO_2, sequestration in deep subsurface environments has received significant attention and investment as a way to reduce greenhouse gas emissions to the atmosphere. However, relatively little is known about the effect of CO_2 on the microbial community in the deep biosphere—the largest biosphere on earth. A recent study used a novel combination of techniques to reveal how CO_2 injection could affect physiology and stress responses of sulfate-reducing bacteria, which catalyze a key biogeochemical process in the deep subsurface.

Findings suggest CO_2 injected in subsurface systems likely acts as a driving force for shifts in microbial community structure, which in turn could influence the efficiency of the CO_2 sequestration process. Ultimately, research could lead to new strategies for improving the success of CO_2 sequestration and help reduce climate change.

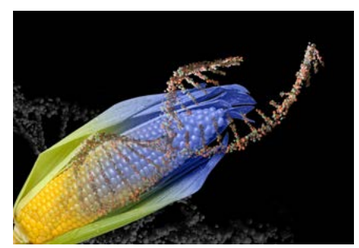
Funding: Portions of this research were supported by a Laboratory Directed Research and Development grant at Pacific Northwest National Laboratory. Extracellular polymeric substances characterization studies were funded by a DOE Office of Science Early Career Research Program Award. Remaining portions of this work were performed under a Science Theme Proposal using EMSL and sponsored by DOE's Office of Biological and Environmental Research.

Publication: Wilkins MJ, DW Hoyt, MJ Marshall, PA Alderson, AE Plymale, LM Markillie, AE Tucker, ED. Walter, BE Linggi, AC Dohnalkova and RC Taylor. 2014. "CO_2 exposure at pressure impacts metabolism and stress responses in the model sulfate-reducing bacterium *Desulfovibrio vulgaris strain Hildenborough*." *Frontiers in Microbiology*. DOI: 10.3389/fmicb.2014.00507

Participating Organizations: The Ohio State University at Columbus, PNNL and EMSL.

Enzymes with Agriculture and Biofuel Applications

Two plant enzymes maintain genetic stability



All eukaryotes have three essential DNA-dependent RNA polymerase enzymes. These enzymes control gene activity by constructing chains of RNA molecules using DNA genes as templates in a process called transcription. Beyond these three RNA polymerases, known as Pols I, II and III, plants are unique. They have two additional 12-subunit enzymes called Pols IV and V, which maintain genetic stability by silencing transposable elements, viruses and specific genes. A new study shows functionally distinct subtypes Pols IV and V exist in corn, revealing new RNA polymerases with novel functions in all plants.

By characterizing new subtypes of RNA polymerases, this study reveals novel insights into enzymes important for genome stability and gene regulation related to plant development. An understanding of how genome regulation influences biomass production and yield is important for optimized biofuel production and sustainable agriculture to meet the needs of growing populations and combat hunger around the world.

Funding: Portions of this research were supported by a National Institutes of Health grant, National Institutes of Health National Center for research resources, EMSL, Howard Hughes Medical Institutes, and Gordon and Betty Moore Foundation.

Publication: Haag J, B Brower-Toland, E Krieger, L Sidorenko, C Nicora, A Norbeck, A Irsigler, H LaRue, J Brzeski, K McGinnis, S Ivashuta, L Pasa-Tolic, V Chandler and C Pikaard. 2014. "Functional Diversification of Maize RNA Polymerase IV and V Subtypes via Alternative Catalytic Subunits." *Cell Reports* 9:378-390. DOI:10.1016/j.celrep.2014.08.067.

Participating Organizations: Indiana University, Bloomington; Monsanto Company, The University of Arizona, Tucson; PNNL; Florida State University, Tallahassee; National Institutes of Health and EMSL.

Carbon-cycle Models for Better Long-term Predictions

Reduced variation among models should improve precision

Projecting variations in the carbon cycle is important for predicting long-term climate changes. However, climate models used to predict climate change still have a large degree of uncertainty in simulating the terrestrial carbon cycle. To address this problem, two recent studies elucidated how uncertainties in representing surface and subsurface hydrology may influence simulations of the carbon cycle, and analyzed how current carbon-cycle models translate climate extreme events into responses in carbon fluxes.

Both studies revealed a high degree of uncertainty in carbon-cycle modeling, highlighting the need to determine the underlying sources of variation and improving the modeling of hydrologic processes in particular. Ultimately, the findings could enable models to more precisely project changes in the carbon cycle and predict long-term climate changes.

Funding: DOE Office of Science, Biological and Environmental Research through the Earth System Modeling program, and National Aeronautics and Space Administration through the Terrestrial Ecology Program.

Publication: Lei H, M Huang, L Leung, D Yang, X Shi, J Mao, D Hayes, C Schwalm, Y Wei and S. Liu. 2014. "Sensitivity of global terrestrial gross primary production to hydrologic states simulated by the Community Land Model using two runoff parameterizations." *Journal of Advances in Modeling Earth Systems*, 06. DOI: 10.1002/2013MS000252.

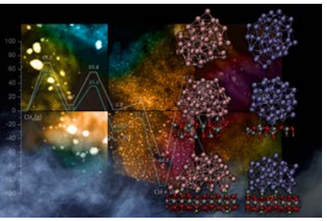
Funding: NASA ROSES Grant and European Community's Seventh Framework Program.

Publication: Zscheischler J, et al. 2014. "Impact of large-scale climate extremes on biospheric carbon fluxes: An intercomparison based on MsTMIP data." *Global Biogeochemical Cycles*, 28, 585–600. DOI: 10.1002/2014GB004826.

Participating Organizations: PNNL; Tsinghua University, Beijing; Oak Ridge National Laboratory; Northern Arizona University, Flagstaff; Max Planck Institute for Biogeochemistry; EMSL; Carnegie Institution for Science; Max Planck Institute for Intelligent Systems; Laboratoire des Sciences du Climat et de l'Environnement; University of Illinois at Urbana-Champaign; National Institute for Environmental Studies, Tsukuba; Auburn University, Alabama; Laboratoire de Glaciologie et Géophysique de l'Environnement, CNRS and Université Grenoble Alpes; Montana State University, Bozeman; NASA; and University of Maryland, College Park.

Improving Biofuel Production

Optimizing catalysts for steam reforming



Steam reforming is a method for converting biomass-derived light hydrocarbons and aromatics into a mixture of carbon monoxide and hydrogen that can be further converted to transportation fuels as well as valuable chemicals. This study combines experimental and theoretical approaches to shed light on the metal catalysts that maximize activity and stability for steam methane reforming, or SMR, reactions.

By providing an enhanced understanding of the performance of rhodium- and iridium-based SMR catalysts, this study will pave the way for optimally screening potential catalysts that will be most active and stable for steam reforming hydrocarbons. Ultimately, findings will lead to selection and development of high-performing SMR catalysts.

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Participating Organizations: PNNL and EMSL.

About this Art

Researchers at Pacific Northwest National Laboratory and EMSL are trying to create a low-cost, higher energy and power density storage technology to more effectively capture and release energy and manage the nation's energy problem. The scientists are designing new types of energy storage devices called supercapacitors using novel porous carbon composite electrodes and ionic liquid electrolytes. The supercapacitors can deliver a sudden burst of power in a short time. This technology has been already used on hybrid vehicles, electric trains, airplanes, computers and smart phones. The researchers imaged the sponge-like feature of the porous carbon composite electrode using the helium ion microscope in EMSL's Quiet Wing. This research was funded by PNNL Laboratory Directed Research and Development, and EMSL user support, sponsored by the Department of Energy's Office of Biological and Environmental Research.

The project team included Vijayakumar Murugesan and Gowri Manickam, both with PNNL, and Manjula Nandasiri and Shuttha Shutthanandan, both with EMSL. (Image colorized.)