the Molecular Bond

EMSL

SCIENTIFIC INNOVATION THROUGH INTEGRATION

April 2016

Double Teaming

Dual collaborations using EMSL and DOE JGI to speed and amplify research impact

Also inside this issue:

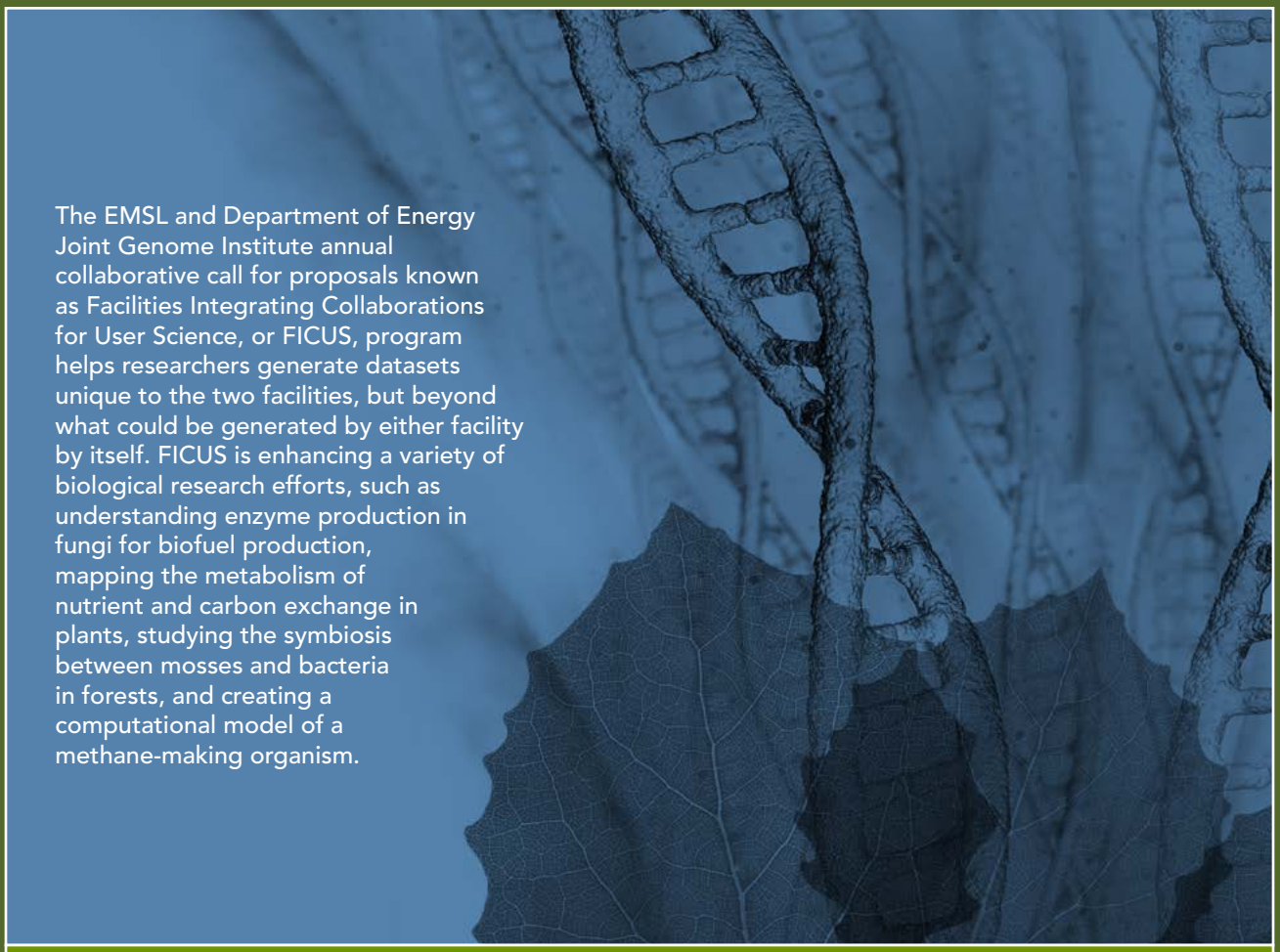
21T Mass Spectrometer Dedicated

Save the Date for EMSL Integration 2016

Check out a Special Issue of *Microscopy Today*

A new Method to Study Sea Spray Aerosols

Creating Hydrogen form Biomass



The EMSL and Department of Energy Joint Genome Institute annual collaborative call for proposals known as Facilities Integrating Collaborations for User Science, or FICUS, program helps researchers generate datasets unique to the two facilities, but beyond what could be generated by either facility by itself. FICUS is enhancing a variety of biological research efforts, such as understanding enzyme production in fungi for biofuel production, mapping the metabolism of nutrient and carbon exchange in plants, studying the symbiosis between mosses and bacteria in forests, and creating a computational model of a methane-making organism.

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

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

EMSL

Pacific Northwest NATIONAL LABORATORY

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U.S. DEPARTMENT OF ENERGY

EMSL held a scientific symposium before the 21T mass spectrometer dedication ceremony on April 14. The presenters included scientists Lili Paša-Tolić, EMSL; Sergey Nizkorodov, University of California at Irvine; Akos Vertes, The George Washington University; and Kelly Wrighton, The Ohio State University. (EMSL file photos)

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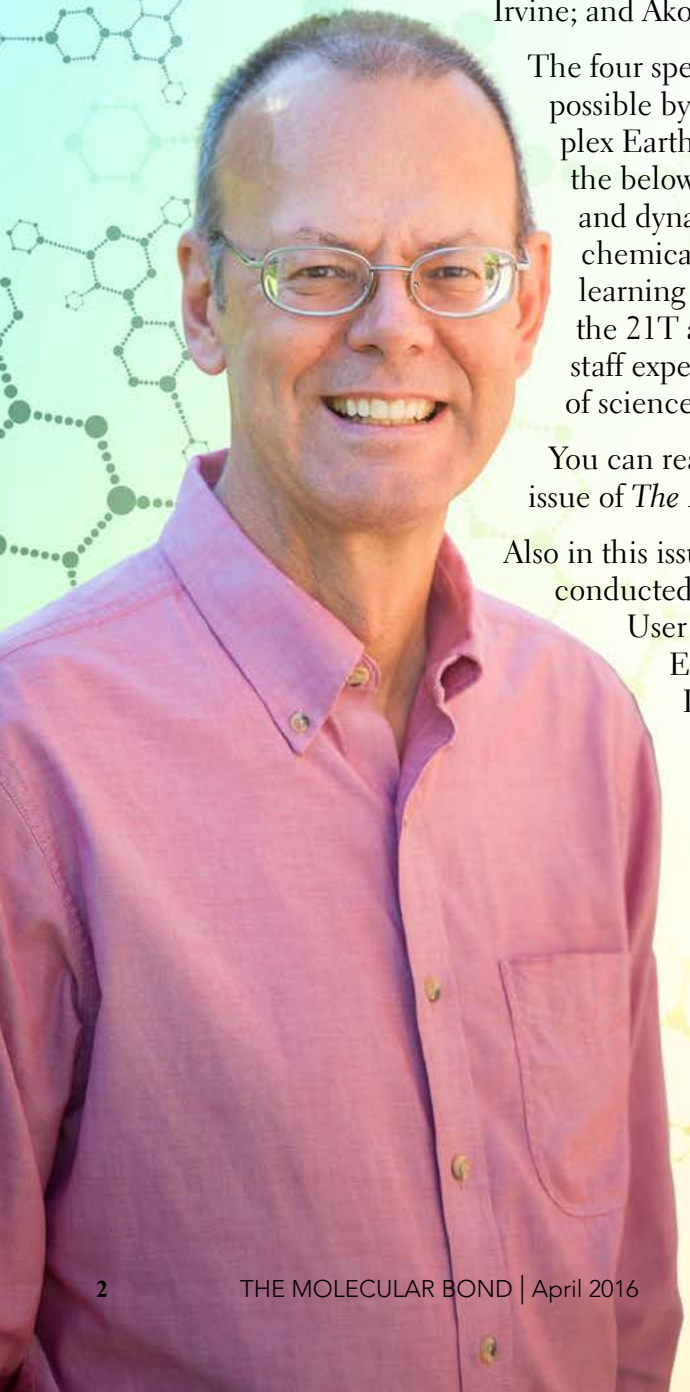
EMSL

FROM THE DIRECTOR

Harvey Bolton

We recently had a major event at EMSL – the dedication of our new 21 Tesla Ultra-high Resolution mass spectrometer, or 21T for short. Held on April 14, activities included a scientific symposium, dedication ceremony, tour of the 21T lab and a reception.

The event was a success, but for me, the highlight was the scientific symposium featuring scientists from EMSL and our user community. The distinguished presenters included Lili Paša-Tolić, EMSL; Kelly Wrighton, The Ohio State University; Sergey Nizkorodov, University of California at Irvine; and Akos Vertes, The George Washington University.



The four speakers presented some excellent examples of the science made possible by EMSL's 21T. Paša-Tolić is using the 21T to characterize complex Earth systems. Wrighton is studying the chemistry and dynamics of the belowground carbon cycle. Nizkorodov is examining the chemistry and dynamics of atmospheric aerosols. And, Vertes is decoding the chemical language of microbes and plants. I am looking forward to learning about more groundbreaking research by other users thanks to the 21T and the capabilities available at EMSL, as well as the EMSL staff expertise that allows these resources to advance the frontiers of science.

You can read more about the dedication ceremony and the 21T in this issue of *The Molecular Bond*.

Also in this issue is a feature article on some of the research projects being conducted through FICUS, or Facilities Integrating Collaborations for User Science. FICUS is a collaborative science program between EMSL and Department of Energy Joint Genome Institute, or DOE JGI, that combines EMSL's unique scientific resources and computational capabilities with cutting-edge genomics at DOE JGI. The article includes interviews with Steven Harris at University of Nebraska, Jonathan Cumming at West Virginia University, Philip Weyman with the J. Craig Venter Institute in San Diego, Zaida Luthey-Schulten at the University of Illinois at Urbana-Champaign and EMSL staff. This cover story helps illustrate the variety and depth of biological research that is possible by utilizing two DOE user facilities.

If your research could benefit from the 21T or participation in the FICUS program, please consider submitting a user proposal.

—*Harvey*

Following the tour of the mass spectrometry lab during EMSL's 21T dedication ceremony on April 14, several of the central players responsible for the development of the 21T mass spectrometer gathered for a photograph. Pictured are (from left to right) EMSL Program Manager Paul Bayer, DOE Office of Biological and Environmental Research; EMSL Scientist Lili Paša-Tolić, spectrometer task lead; Pacific Northwest National Laboratory Chief Science and Technology Officer David Koppenaal, project technical lead and magnet task lead; Associate Director Sharlene Weatherwax, DOE Office of Biological and Environmental Research; and EMSL Scientist Jared Shaw, project team member. (EMSL file photo)

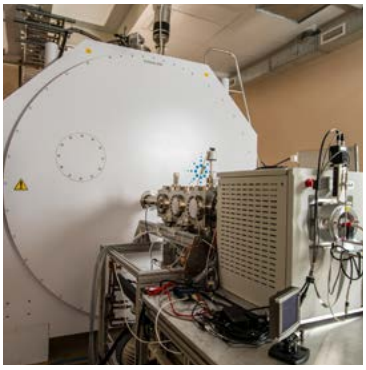
NEWS & KUDOS

Powerful Mass Spectrometer Opens New Vistas for Scientists

Scientists worldwide now have access to a powerful new resource at EMSL at the Pacific Northwest National Laboratory, or PNNL, to help them address pressing science challenges related to the environment, biology and energy.

The new 21 Tesla Ultra-high Resolution mass spectrometer, or the 21T for short, allows scientists to analyze and separate atoms and molecules according to their size and molecular structure with a clarity and precision well beyond conventional mass spectrometers.

Officials from EMSL, PNNL, DOE's Office of Science, DOE's Pacific Northwest Site Office, elected officials and scientists gathered on April 14 to celebrate the science that will be made possible by the 21T, which is available for use by scientists around the world. The topics scientists are already exploring with the instrument include:



The 21T – the 21 Tesla Fourier Transform Ion Cyclotron Resonance Mass Spectrometer – located at EMSL is available for use by scientist around the world.

- Understanding how fungi break down rugged plant materials more effectively than nearly anything humans can produce economically. The question is at the heart of efforts to create new fuels and products from biological materials that contain a tough natural material known as lignocellulose.
- How climate change affects carbon in soil and vice versa. The fate of the carbon beneath our feet — a huge reservoir of potential greenhouse gases — is intertwined with the future of our planet's climate.
- How particles of pollution interact with naturally occurring particles in our atmosphere, affecting how sunlight is deflected from Earth or absorbed by the atmosphere.

Read the rest of the PNNL news release: http://1.usa.gov/1Sgao1j.

DOE Bestows Achievement Award on 21T Project

The Department of Energy, or DOE, recently awarded its Achievement Award to the Office of Science's High Resolution and Mass Accuracy Capability Development Project. The project led to the development of EMSL's 21 Tesla Fourier-Transform Ion Cyclotron Resonance, or 21T FTICR, mass spectrometer.

"It was abundantly clear to all of us that this project was successful only through the team's hard work and dedication over the past six years," said Project Manager Scott Tingey, PNNL Earth

The Office of Science's High Resolution and Mass Accuracy Capability Development Project receives the DOE Achievement Award at a ceremony in Washington, D.C. Pictured are (from left to right): Paul Bayer, DOE Office of Biological and Environmental Research; Russ Warren, DOE Pacific Northwest Site Office; Deputy Secretary of Energy Elizabeth Sherwood-Randall; David Koppenaal, PNNL; and Scott Tingey, PNNL.

and Biological Sciences Directorate chief operating officer. "I would like to congratulate each one of you on this award and on the successful completion of this project."

The project team designed and built the 21T FTICR mass spectrometer to characterize complex biological and environmental materials to advance the science mission of the Office of Science's Office of Biological and Environmental Research. The instrument's high 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.

Special Issue of *Microscopy Today* with EMSL Research now Available

The March 2016 special issue of *Microscopy Today* guest edited by Laboratory Fellow and EMSL Science Theme Lead Don Baer is available online. The special edition focuses on advances and applications of surface analysis methods and features articles co-written by EMSL scientists and users at University of Washington based on their EMSL research.

The special issue includes five articles, and Baer is a co-author on two of the EMSL-contributed research articles. The first, "Use of XPS to Quantify Thickness of Coatings on Nanoparticles" was co-written with David Castner and Yung-Cheng Wang, both with the University of Washington. Baer also co-authored "Multimodal and *In-Situ* Chemical Imaging of Critical Surfaces and Interfaces in Li Batteries" with EMSL scientists Arun Devaraj, Mark Engelhard, Chongmin Wang and Zihua Zhu.

Christopher Anderton, EMSL, and Lara Gamble, University of Washington, jointly wrote the third EMSL-contributed article "Secondary Ion Mass Spectrometry Imaging of Tissues, Cells and Microbial Systems."

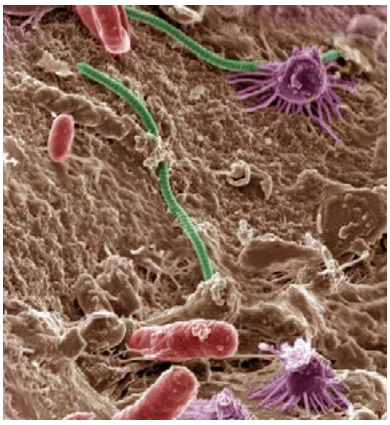
Microscopy Today is a trade magazine owned by the Microscopy Society of America.

Read the March 2016 special issue of Microscopy Today: http://bit.ly/1RP07H3.

EMSL Science Theme Lead Don Baer guest edited the March 2016 special issue of *Microscopy Today* that features EMSL research

Microbes Adaptability to Climate Change

Microbes in soil are central to Earth's carbon cycle by converting carbon and other elements in the soil into carbon dioxide and other gases that are released into the atmosphere. Scientists at Pacific Northwest National Laboratory, or PNNL, EMSL and Washington State University using EMSL capabilities determined microbial communities in soil may not be as adaptable to climate change as previously thought. The team's findings, published in *PLOS One*, are based on a 17-year study of transplanted soils on a mountain in eastern Washington state. The scientists analyzed the composition of the microbial communities, their enzyme activity and their rates of respiration and found less adaptability than expected, even after nearly two decades.



Microbes in the soil are central players converting carbon into greenhouse gases.

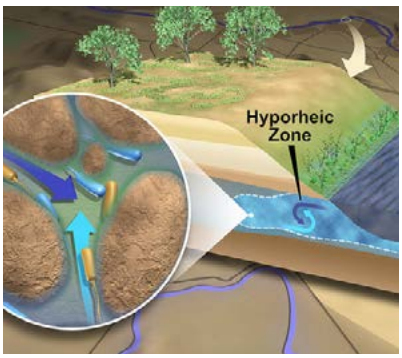
Reference: Bond-Lamberty B, H Bolton, S Fansler, A Heredia-Langner, C Liu, LA McCue, J Smith, and V Bailey. 2016. "Soil Respiration and Bacterial Structure and Function after 17 Years of a Reciprocal Soil Transplant Experiment." *PLOS One* 11(3): e0150599. DOI: 10.1371/journal.pone.0150599.

Read the PNNL news release: http://1.usa.gov/1UIYWif.

Read the PNNL Physical Sciences Division research highlight: http://1.usa.gov/1q75YjL.

Microbes Take Center Stage in Workings of 'the River's Liver'

A research team from Pacific Northwest National Laboratory, or PNNL, EMSL and The Ohio State University studied microbial activity near rivers in an area known as the hyporheic zone, which includes the sediment where river water mixes with groundwater. The team found rising river waters deliver carbon to microbes in the hyporheic zone, which causes an increase in microbial activity leading to a boost in emissions of carbon dioxide, methane and other greenhouse gases. The scientists counted microbial cells and characterized organic carbon using capabilities at EMSL. Their findings were published April 7 in *Nature Communications*.



Scientists call the area along a river where river water and groundwater mix the hyporheic zone. The circular inset illustrates some of the features of this zone, including tiny grains of sediment, water from both sources mixing, and the microbes that actively ply these waters and sediments.

Reference: Stegen JC, JK Fredrickson, MJ Wilkins, AE Konopka, WC Nelson, EV Arntzen, WB Chrisler, RK Chu, RE Danczak, SJ Fansler, DW Kennedy, CT Resch, and M Tfaily. 2016. "Groundwater-Surface Water Mixing Shifts Ecological Assembly Processes and Stimulates Organic Carbon Turnover." *Nature Communications*. DOI: 10.1038/NCOMMS11237.

Read the PNNL news release: http://1.usa.gov/1MsnCJh.

Wang Appointed a Principal Editor of *JMR*

Gary Messing, editor-in-chief of the *Journal of Materials Research*, or *JMR*, has invited EMSL Scientist Chongmin Wang to serve as a principal editor for the journal. Wang's appointment to the editorial board is immediate.

Chongmin Wang

JMR is the official journal of the Materials Research Society and is a premier materials science journal devoted to publishing new research that demonstrates significant impact or advance of scientific understanding of interest to the materials research community.

As a principal editor, Wang will choose scientifically qualified reviewers to review each submitted manuscript assigned to him. Wang can act as one of the reviewers if the article is in his area of expertise. Once a manuscript has been reviewed, Wang will recommend if it should be accepted, revised or rejected based on technical correctness and significance advancing the scientific understanding of the technical topic. Another role as principal editor is to help Messing identify opportunities for review papers and *JMR* special focus issues.

The Materials Research Society publishes *JMR* in partnership with Cambridge University Press.

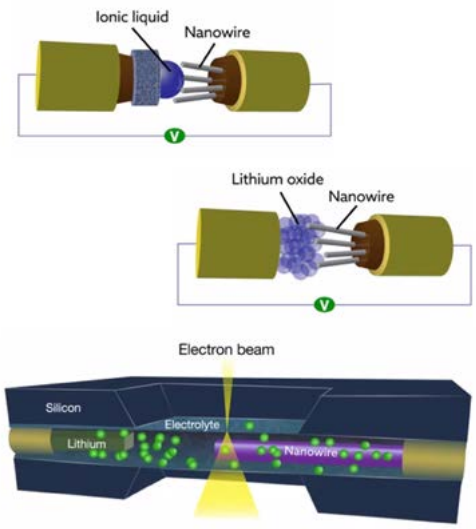
Wang's Paper of the Year Research Featured in Video

EMSL Scientist Chongmin Wang's review article about *in situ* transmission electron microscopy battery research that was named by the *Journal of Materials Research*, or *JMR*, as the 2015 *JMR* Paper of the Year has been turned into a video.

Entitled "*In situ* TEM and spectroscopy studies of rechargeable batteries under dynamic operating conditions," the video was produced by Research Square for The Materials Research Society, or MRS, which publishes *JMR* in partnership with Cambridge University Press. Watch the video: http://bit.ly/1Ms5JKI.

The type of innovations summarized in the award winning paper and shown in the video contributed to Wang being named one of the three 2016 MRS Innovation in Materials Characterization Award winners. The video shows the stages of development that went into the creation of batteries that could be examined inside the microscope.

Reference: Wang CM. 2015. "*In situ* transmission electron microscopy and spectroscopy studies of rechargeable batteries under dynamic operating conditions: A retrospective and perspective view." *Journal of Materials Research* 30(3):326-339. DOI:10.1557/jmr.2014.281.



Images from the video "*In situ* TEM and spectroscopy studies of rechargeable batteries under dynamic operating conditions" based on EMSL Scientist Chongmin Wang's 2015 *Journal of Materials Research* Paper of the Year.

Plan to Attend EMSL Integration 2016

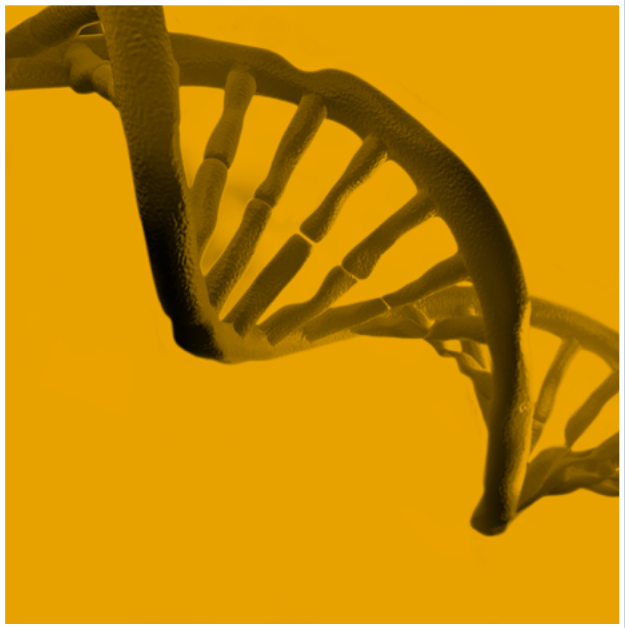
This year's user meeting – EMSL Integration 2016: Multiscale Ecosystems Analysis & Design – will be held Sept. 12-13 at EMSL in Richland, Wash. The 2016 science meeting takes a holistic view of the terrestrial carbon, nutrient and hydrologic coupled cycles including exchange and transformations between the atmosphere, plant, microbe and soil components at molecular to ecosystem scales. EMSL Science Theme Lead Nancy Hess and Plant Sciences Director Christer Jansson are jointly organizing the meeting.

Researchers from around the world and from academia, industry and government research labs are encouraged to attend. The meeting is open to EMSL users and non-users.

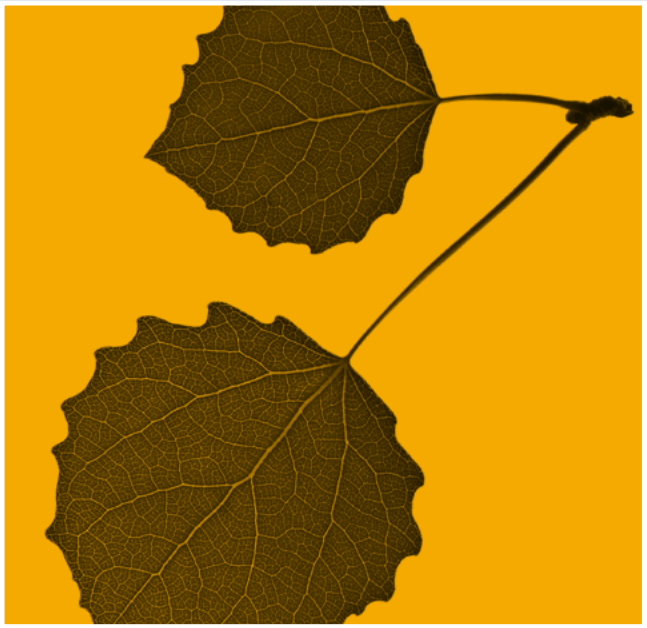
Mary Firestone, professor of soil microbiology in the Department of Environmental Studies, Policy and Management at the University of California at Berkeley, will open the meeting as the keynote science speaker.

The meeting will also feature internationally recognized plenary speakers.

Watch for more information!



Double Teaming



Dual collaborations using EMSL and DOE JGI to speed and amplify research impact

Borrowing a page from Aristotle, the philosopher who said "the whole is greater than the sum of its parts," an innovative program with EMSL and the Department of Energy Joint Genome Institute, or DOE JGI, in California, gives scientists a chance to combine the expertise and capabilities from both user facilities. With the opportunity to pursue one research project at two institutions, scientists can leverage disparate resources, shave years off their project times and amplify the impact of their work.

"Asking the scientific community to propose novel ways for user facilities to work together," is the way Scott Baker, the Biosystem Dynamics and Design EMSL Science Theme lead, describes the collaborative approach called Facilities Integrating Collaborations for User Science, or FICUS.

Created in 2013, originally under the name of the JGI-EMSL Collaborative Science Initiative, the program, which focuses on DOE missions in bioenergy and environment, combines EMSL's unique imaging and omics resources and computational capabilities with cutting-edge genomics at DOE JGI, enabling scientists to conduct fundamental science experiments in ways they couldn't with projects undertaken separately at either user facility. Before this, researchers had to apply to each facility on their own in accordance with separate review schedules and selection processes. That approach could add years to research efforts, noted Terry Law, EMSL's User Program Services manager. EMSL and DOE JGI are both DOE Office of Science User Facilities.

"We realized that if these two programs worked interactively with each other, then we could exponentially increase the possible results for our users," said Law.

Opening Doors

Access to both user facilities was invaluable for Steven Harris, a plant pathologist at the University of Nebraska, in his efforts to better understand enzyme production in a filamentous fungus called *Aspergillus nidulans*.

For years, these fungi have been workhorses in biofuel production, food processing and other industries, said Harris. "What's not well understood is the 'plumbing' of the fungal cells. We don't really know how they get the enzymes out," he added.

With funding from the National Science Foundation, in his university lab Harris used "old-fashioned," plate-based assays to generate and screen hundreds of mutants for ramped up enzyme production. Then he went high-tech, sending 50 of those fungal overachievers to DOE JGI for genome sequencing to identify relevant mutations.

From that list of candidate genes, coupled with well-mapped genetics of *A. nidulans*, Harris selected an even smaller number of mutants for individual testing. "The idea is that it will provide insights into specific pathways – the plumbing – and potentially nail the regulatory points that could be manipulated for much more enzyme production," said Harris.

With EMSL's expertise, Harris is also looking at "secretome," the stuff that gets shipped out of the cell, from 25 of those sequenced mutants. "We can imagine that some of those fungi might just produce a lot more of everything, but the more interesting phenotypes are the mutants that make more of some things than of others," said Harris.

In addition, he hopes the helium ion microscope in EMSL's Quiet Wing can be used to look at cell surface features on fungi, to see if the effects of different subsets of mutants are reflected on their surface structure or the organization of cell walls. Ultimately, he wants to generate a data set big enough to hunt for patterns in mutations and enzyme production.

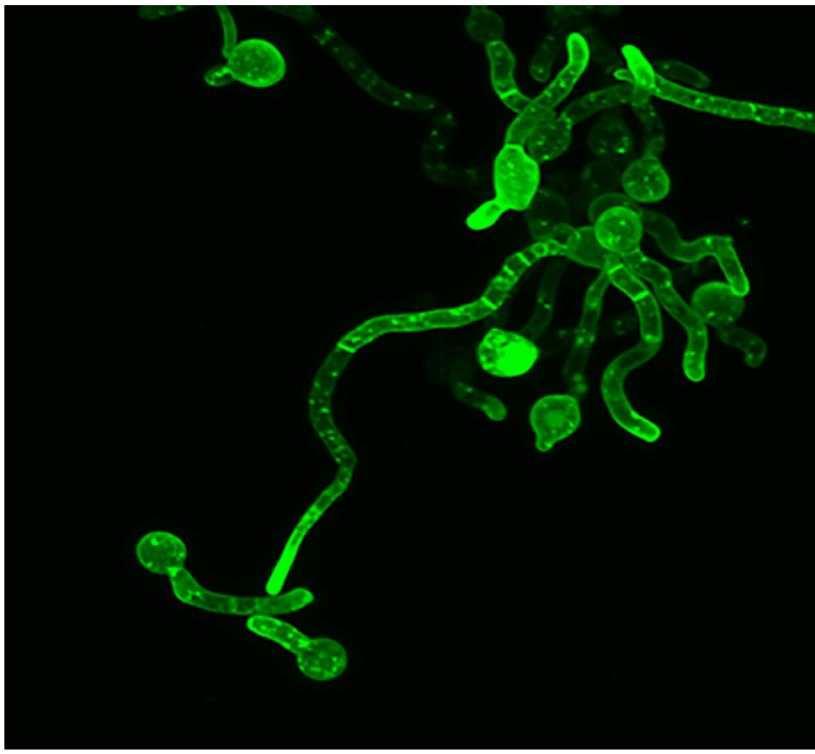
Yet, even from the limited set he has now, Harris found candidates for "regulators" that he plans to pursue further this summer. "I'm hoping we can open up new doors to make production of these enzymes more efficient. That would be beneficial in making biofuels more cost competitive in the future."

FICUS
Facilities Integrating Collaborations for User Science

JGI
JOINT GENOME INSTITUTE
DEPARTMENT OF ENERGY

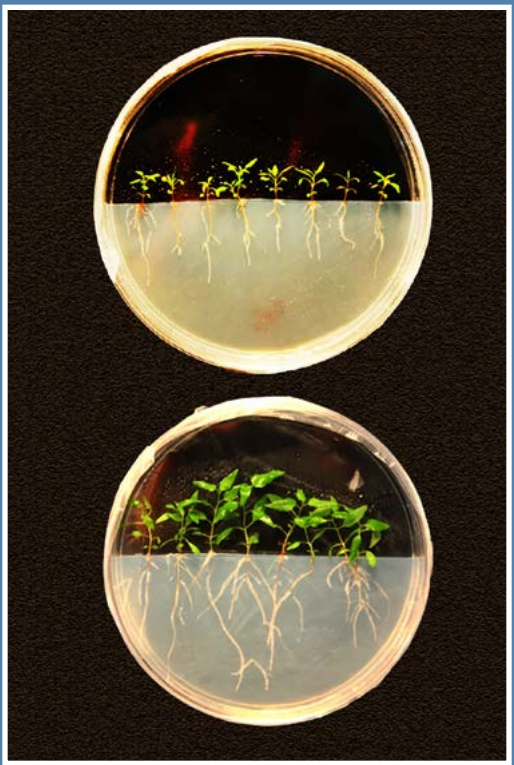
EMSL

This image shows the localization of a secreted enzyme (beta-glucosidase) in *A. nidulans* hyphae that have been grown on cellulose. The enzyme was fused to the green fluorescent protein (GFP) to facilitate localization. (Image provided by Steven Harris, University of Nebraska.)



These are aspen tree seedlings grown without or with L. bicolor and at low and high P_i in sand-vermiculite solution culture. (Image provide by Jonathan Cumming, West Virginia University.)

Shown are aspen trees growing with (bottom) and without (top) bacteria. (Image provide by Jonathan Cumming, West Virginia University.)



Better Together

Two projects exemplify what FICUS can do to help users explore complex interactions between plants and bacteria or fungi.

The pairing of EMSL's proteomics capabilities with DOE JGI's sequencing expertise was also just what Jonathan Cumming, a biologist at West Virginia University, needed to map the metabolism of nutrient and carbon exchange among trees and communities of soil ectomycorrhizal, or ECM, fungi and plant-growth promoting bacteria.

Millions of years ago, plants evolved to rely on soil fungi and bacteria to provide access to nutrients and protection from pathogens. In return, soil-based organisms get carbon from the plants. "Everyone brings a special covered dish to the potluck," said Cumming. By studying such complex interactions with a simplified system consisting of Pseudomonas bacteria, fungi and one tree, we can put together a story about how each of these microbes contributes and interacts with the genome of the host plant to make it a better, tougher plant in the environment, he said. "There's a lot of foundational knowledge about how this works, but the metabolic and genomic underpinnings aren't well known," said Cumming.

Such information could be used to improve soils that may, for example, be too saline or acidic to support plant growth. In particular, supplies of the second most important agricultural fertilizer – phosphorus – are expected to dwindle in the next 50 years, adding to global food and fuel insecurity.

With an experimental model using either aspen trees or black cottonwood trees, Cumming is analyzing how microbes change the physiology of the plant in response to limited phosphorus resources. His grid of greenhouse planters is divided into sections that include: trees alone, trees growing in soil with ECM fungi, trees with soil bacteria or all three together. Each grouping then gets all the needed nutrients, or is stressed by limited amounts of phosphorus. The data from DOE JGI will contribute to a template of the tree's gene expression and transcription under these changing conditions. At EMSL, with the help of scientists Young-Mo Kim and Stephen Callister, they'll determine which proteins are in action.

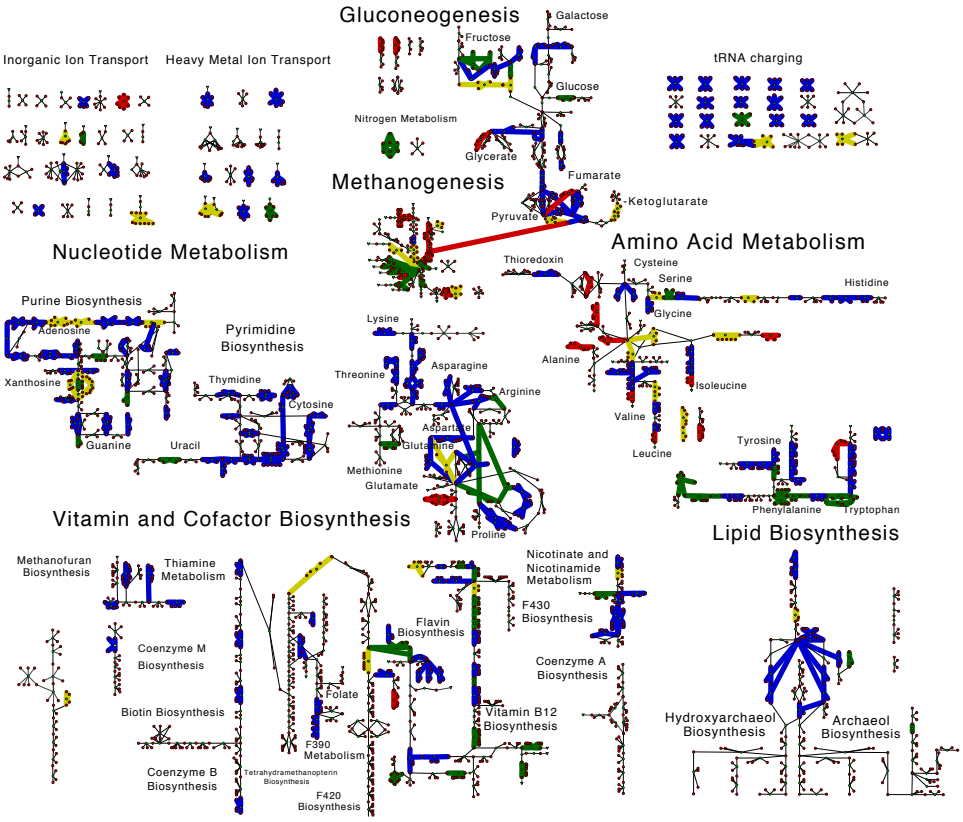
"The strength of the program is the breadth of information from both user facilities," said Cumming. "You can get the fully integrated information needed to understand, predict and show how the plant's machinery is functioning, and then how it responds to microbes and environmental stresses."

Ultimately, he hopes to take this information to another DOE Office of Science User Facility, the Advanced Photon Source at the Argonne National Laboratory in Illinois, to model the proteins determined by genes that are being transcribed and how that correlates with the metabolites found in the samples.

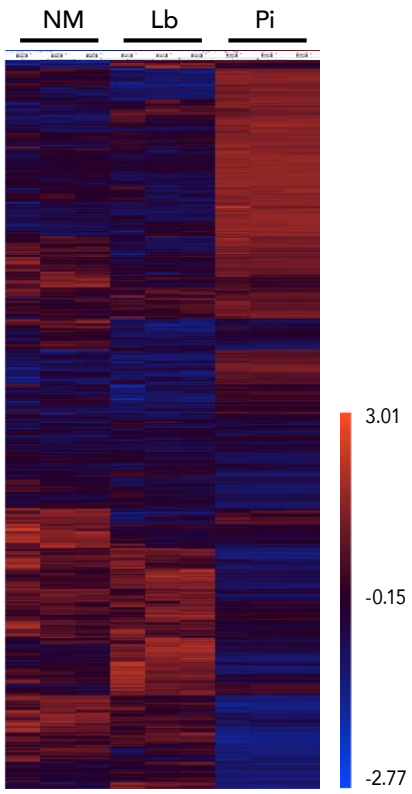
"These scientists have tons of experience doing things we don't typically do," said Cumming of the FICUS program. "I don't have the equipment or the skills to get down to that fine scale chemistry, but I have the imagination to think of what could be going on and these programs can help me get at those answers."

In a similar manner, Philip Weyman, a synthetic biologist at the J. Craig Venter Institute in San Diego, leveraged resources from the FICUS program to study the symbiosis between feather mosses and filamentous cyanobacteria in boreal forests.

The floor of these slow growing "snow forests," which comprises about 30 percent of the world's forest cover, are hotbeds of nitrogen fixation as a result of the relationship between mosses covered with filamentous cyanobacteria. Yet this critical, interrelated system was only recently discovered in the early 2000s, noted Weyman.



This is a mapping of all the known metabolic reactions in *M. acetivorans*. Colored lines indicate reactions that are regulated. More specifically, these reactions have proteins that are regulated by carbon growth substrate. These reactions are points in the metabolism where the organism can divert or constrain flux to change the way it is growing. Different colors compare different growth conditions. (Image provided by Zaida Luthey-Schulten Group, University of Illinois at Urbana-Champaign.)



Shown is a heatmap of ectomycorhizzal fungi, which form close associations – along with bacteria – with tree roots. The ECM trade access to nutrients for carbon from the plants. (Image provide by Jonathan Cumming, West Virginia University.)

Although there are well-described models of cyanobacteria interactions with plants, far less was known about their molecular activities with mosses, said Weyman. So, Weyman's colleagues at Stockholm University, Ulla Rasmussen and her student Denis Warshan, isolated bacteria and sent samples to DOE JGI for sequencing and transcriptome data. With that information, the team obtained proteomics from EMSL. But, he also wanted to get at the genetic relationship between bacteria and moss. "Often we look at photosynthesis or nitrogen reactions in these bacteria in ways that are divorced from the natural environment, but this was a chance to study them together," he said.

Weyman and his colleagues studied three different strains of cyanobacteria in a series of "treatments" – without moss, filtered to only allow chemical contact with moss and in full association with moss – and then got genome sequencing, transcriptomics and proteomics for both bacteria and moss.

"The synergy of capabilities at EMSL and DOE JGI enables us to make hypotheses about these interactions," said Weyman. With knockout models of bacteria, designed to completely lack a particular gene, he can then watch for what abolishes the ability to form these symbioses. "We'll get so many new ideas on how these interactions happen," he said.

Further down the line, with better understanding of the critical genes involved in creating these symbioses, field tests might make it possible to find which genes are getting upregulated for nitrogen fixation under different environmental conditions – such as warmer temperatures, he said.

"The whole process is very user friendly from a biologist's point of view," said Weyman. "I provide samples and get a whole host of refined sets of data in return."

Model Organisms

Generating massive amounts of data is the goal of Zaida Luthey-Schulten, a biophysical chemist at the University of Illinois at Urbana-Champaign. She wants a molecular-level dossier – genomics, transcriptomics, proteomics, ribosome counts and everything else she can find – to create a computational model of a methane-making organism in the Archaea domain.

Perhaps best known for their emissions from cows, methanogens are single-celled, anaerobic microbes that are an important source of energy and can also perform the last step in converting biomass into methane in the carbon cycle. Even though Carl Woese, a prominent evolutionary

biologist at the University of Illinois, was the first to identify the Archaeal methanogens and use them to establish his phylogenetic tree of life, little is known about them. The methanogens and other organisms in the third domain of life have not been characterized as well as their relatives on bacterial and eukaryal branches. However, Luthey-Schulten and her students plan to change that situation, and they turned to the combined expertise of EMSL and DOE JGI to help make that happen.

With funds from the DOE and a NASA astrobiology grant (because research suggests these organisms could thrive on Mars) her team proposed a two-step plan: first, RNA sequencing data from DOE JGI would help them make predictions about how the organism grows in varied conditions; then, from EMSL, detailed information about the number of ribosomes in these methanogens could help begin building a computational model.

These ribosomes are at the core of protein synthesis, explained Luthey-Schulten. In many bacteria they account for a large percentage of the macromolecules, so if you want to start understanding how gene expression is connected to protein synthesis and metabolism, you need to know how many ribosomes there are.

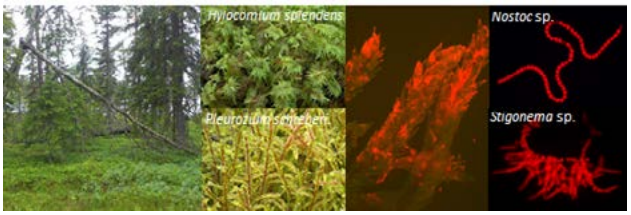
Luthey-Schulten's research group is also extending and refining a metabolic network using RNA sequencing information from DOE JGI. In addition, they plan to use EMSL's imaging expertise to track proteins bearing fluorescent labels during methanogenesis, the primary metabolic pathway that produces methane.

Another ongoing collaboration between Luthey-Schulten's lab and EMSL involves proteomics, growing cells under different conditions to get the relative abundance of proteins to then tie those results to RNA sequencing data and create constraints for intracellular metabolic fluxes, noted Joseph Peterson, a member of Luthey-Schulten's team. These kinds of data are like getting the satellite version of a street map for the metabolome; it can tell you the flow of traffic, whether there are stop lights, parked cars or other potential bottlenecks – and what determines what goes there in terms of metabolic fluxes, said Luthey-Schulten.

"All of this contributes to making a good model for understanding an Archaea," said Luthey-Schulten. "These organisms play an important role in making methane and in the carbon economy on Earth ... and maybe even Mars."

So far, 28 research projects have benefitted from paired resources available through the FICUS program. A fourth call for joint EMSL-DOE JGI research proposals just closed. In the future, other national user facilities may be included, too. Already there are projects shared between EMSL and the Atmospheric Radiation Measurement Climate Research Facility so we've started considering how to broaden our scope, noted Law. "We're always thinking of ways that could expedite scientific discovery," she said. ■

Elizabeth Devitt is a science journalist and freelance writer.



Philip Weyman, J. Craig Venter Institute, is studying the symbiosis between feather mosses and filamentous cyanobacteria in boreal forests. The far left image is a boreal forest. The next images are (top) *Hylocomium splendens*, commonly known as feather moss and (bottom) *Pleurozium schreberi*, red-stemmed feather moss. The middle image is feather moss colonized by cyanobacteria. The red color is auto-fluorescence, due to photosynthetic pigment. The last images are (top) *Nostoc*, a genus of cyanobacteria and (bottom) *Stigonema*, a filamentous blue-green algae. (Images provided by Ulla Rasmussen and Denis Warshan, University of Stockholm.)

EMSL, the Environmental Molecular Sciences Laboratory, a DOE Office of Science User Facility located at Pacific Northwest National Laboratory in Richland, Wash. EMSL offers an open, collaborative environment for scientific discovery to researchers around the world and its integrated computational and experimental resources enable researchers to realize important scientific insights and create new technologies.

DOE JGI, the Department of Energy Joint Genome Institute, a DOE Office of Science User Facility located in Walnut Cree, CA, is the only federally funded high-throughput genome sequencing and analysis facility dedicated to genomes of non-medical microbes, microbial communities, plants, fungi and other targets relevant to DOE missions in energy, climate and environment.

SCIENCE HIGHLIGHTS

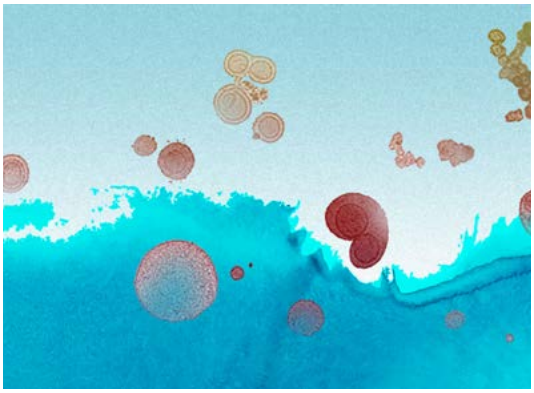
Freezing Sea Spray Aerosols to Study their Natural State

New method preserves sea spray aerosols for studying their natural structure

Scientists can now trap sea spray aerosols in their natural state and accurately characterize their particle structure using a new microscopy approach.

This approach will enable scientists to more easily investigate the influence of sea spray aerosols on climate and the environment.

Funding: This work was supported by the DOE Office of Science (Office of Biological and Environmental Research), including support of EMSL, a DOE Office of Science User Facility; the National Science Foundation; and National Institutes of Health.



Publication: Patterson JP, Collins DB, Michaud JM, Axson JL, Sultana CM, Moser T, Dommer AC, Conner J, Grassian VH, Stokes MD, Deane GB, Evans JE, Burkart MD, Prather KA, and Gianneschi NC. 2016. "Sea Spray Aerosol Structure and Composition Using Cryogenic Transmission Electron Microscopy." *ACS Central Science* 2:40-47. DOE:10.1021/acscentsci.5b00344.

Participating Organizations: University of California, San Diego; EMSL; and the University of Iowa.

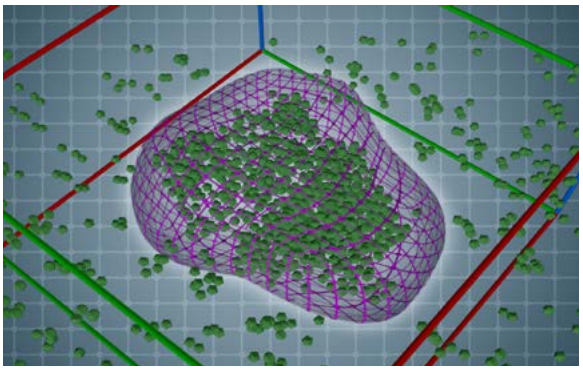
Directly Revealing Atomic-scale Phosphorus

New approach enables atomic-scale analysis in soft biological materials

Researchers examined the chemical identity and 3-D position of atoms in soft biological materials with a new approach using atom probe tomography, or APT.

An extension of the new specimen preparation technique can further enhance the APT study of organic and inorganic materials and nanoparticles relevant to energy and the environment.

Funding: This work was supported by the DOE Office of Science (Office of Biological and Environmental Research), including support of EMSL, a DOE Office of Science User Facility; and the Chemical Imaging Initiative conducted under the Laboratory-Directed Research and Development Program at PNNL.

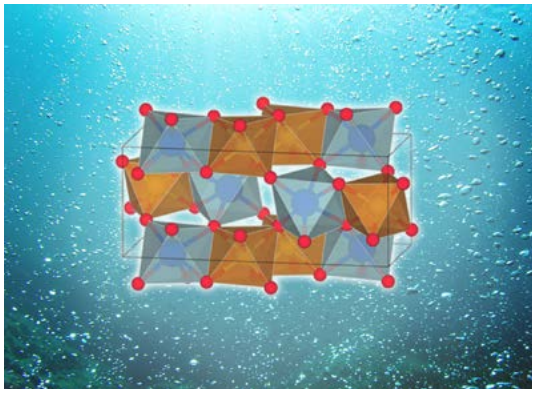


Publication: Perea DE, Liu J, Bartrand J, Dicken Q, Thevuthasan ST, Browning ND, and Evans JE. 2016. "Atom probe tomographic mapping directly reveals the atomic distribution of phosphorus in resin embedded ferritin." *Scientific Reports*. DOI: 10.1038/srep22321.

Metal Monouranates Found to be Highly Stable

A less common form of uranium may hold key to remediation efforts

A recent study examined in unprecedented detail the structural and thermodynamic properties of uranium containing compounds called metal monouranates. Metal monouranates are of considerable interest due to their relevance to nuclear technology.



The new findings on this understudied form of uranium help complete the picture of uranium solid-state chemistry and could improve models of and strategies for minimizing the environmental impact of uranium contamination.

Funding: This work was supported by DOE's Office of Science (Office of Biological and Environmental Research), including support of EMSL, a DOE Office of Science User Facility. Major funding was provided by the DOE Energy Frontier Research Center, Materials Science of Actinides, Office of Basic Energy Sciences. This work was also supported by the National Science Foundation, DOE GeoSciences and the Laboratory-Directed Research and Development Program at Los Alamos National Laboratory.

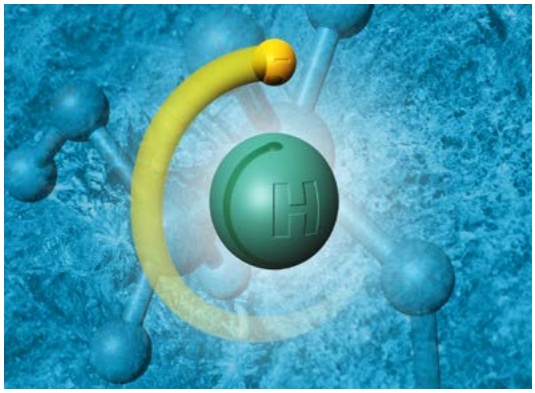
Publication: Guo X, E Tiferet, L Qi, JM Soloman, A Lanzirotti, M Newville, MH Engelhard, RK Kukkadapu, D Wu, ES Ilton, M Asta, SR Sutton, H Xu, and A Navrotsky. 2016. "U(v) in metal urinates: a combined experimental and theoretical study of $MgUO_4$, $CrUO_4$ and $FeUO_4$." *Dalton Transactions* 45,4622-4632. DOI: 10.1039/c6dt00066e.

Participating Organizations: University of California, Davis; EMSL; PNNL; Los Alamos National Laboratory; Argonne National Laboratory; Lawrence Berkeley National Laboratory; Nuclear Energy Center of the Negev, Israel; University of California, Berkeley; University of Michigan; and University of Chicago.

From Biomass to Hydrogen

Cobalt catalyst ideal for producing hydrogen through steam reforming biomass-derived ethylene glycol

Hydrogen production through steam reforming biomass-derived compounds is an economically feasible and environmentally benign way to efficiently use renewable energy resources. A recent study combined experimental and theoretical approaches to compare the hydrogen yield achieved by several different metal catalysts used for steam reforming ethylene glycol.



The findings show a cobalt catalyst had a much higher hydrogen yield than rhodium or nickel catalysts, making it a promising catalyst for steam reforming ethylene glycol for hydrogen production. Ethylene glycol is a component found in aqueous phases that are produced from the direct liquefaction of plant-derived cellulose or cellulosic oxygenates. The study could lead to the development of more efficient strategies to produce hydrogen from bio-derived aqueous phases as an environmentally friendly strategy to power diverse energy needs.

Funding: This work was supported by DOE's Office of Science (Office of Biological and Environmental Research), including support of EMSL, a DOE Office of Science User Facility; the DOE Office of Energy and Renewable Energy, Bioenergy Technologies Office; PNNL; and the National Energy Research Scientific Computing Center, a DOE Office of Science User Facility.

Publication: Mei D, VL Dagle, R Zing, KO Albrecht, and RA Dagle. 2015. "Steam Reforming of Ethylene Glycol over $MgAl_2O_4$ Supported Rh, Ni, and Co Catalysts." (2015). *ACS Catalysis*: 315-325. DOI: 10.1021/acscatal.5b01666.

Participating Organization: PNNL.

"The good thing about science is that it's true whether or not you believe in it."

-Neil deGrasse Tyson

About this Art

This material, fashioned from carbon nanotubes (grainy objects) and zinc oxide nanowires (fuzzy objects), could sharpen the potential of electrodes and help forge progress on much-needed energy storage technologies. The promising material was studied at EMSL. In the study, EMSL and University of Texas at El Paso scientists joined forces to improve electrode materials. Electrodes are important components of supercapacitors, or devices prized for their ability to deliver quick bursts of energy and to store electricity. The research was funded by Pacific Northwest National Laboratory's, or PNNL's, Laboratory-Directed Research and Development program; results ultimately could benefit transportation, electronic products and grid management.

Team Members

Shuttha Shutthanandan and Manjula Nandasiri, both with EMSL; Vijayakumar Murugesan, PNNL; and Karim Hasanul and Mohammad Shuvo of UTEP. The image was captured with a helium ion microscope in EMSL's Quiet Wing and colorized by Shutthanandan.