theMolecularBond

EMSL

SCIENTIFIC INNOVATION THROUGH INTEGRATION

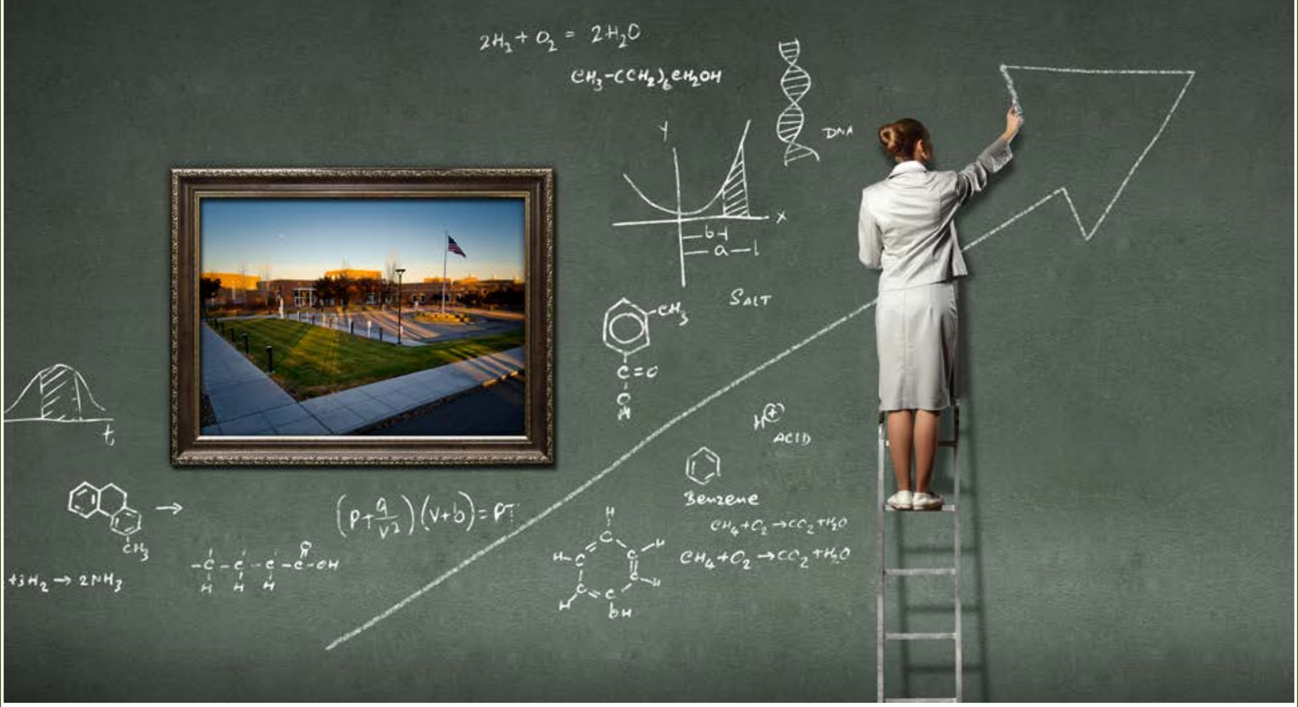
June 2016

EMSL user program facilitates transferable postdocs

Postdocs develop expertise in broad-reaching research and applicable techniques

Also inside this issue:

EMSL offers postdoctoral researchers, better known as postdocs, a unique opportunity to explore their personal research interests, collaborate with a community of users, assist an internationally recognized team of scientists, and enhance personal skills and expertise as they develop themselves for a career in the sciences. Four current EMSL postdocs tell their stories, discuss their research and share their experiences as members of a user facility's scientific staff.



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

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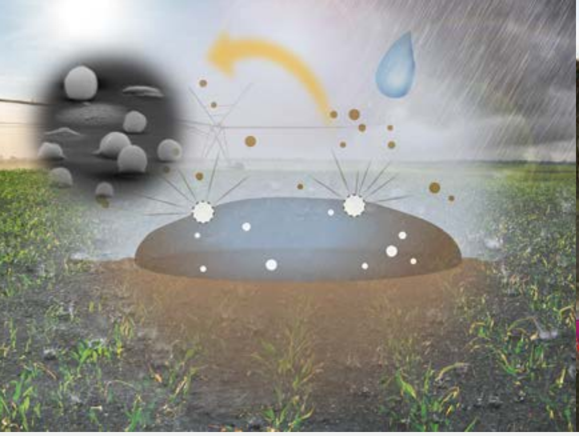
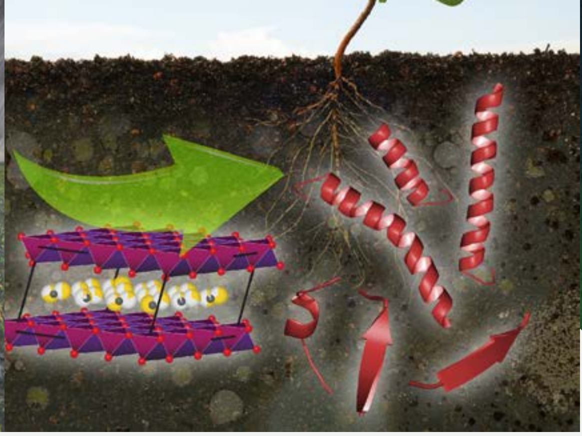
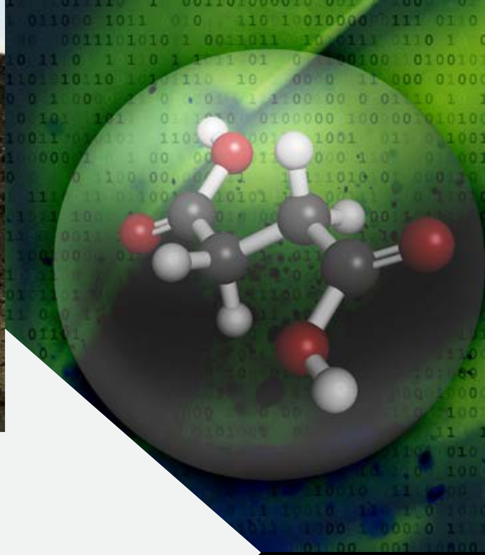
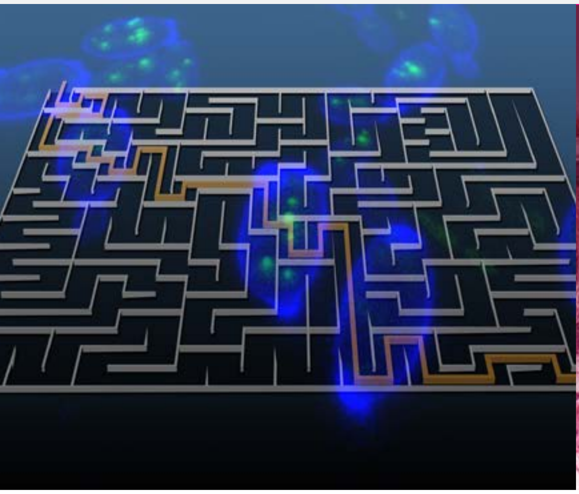
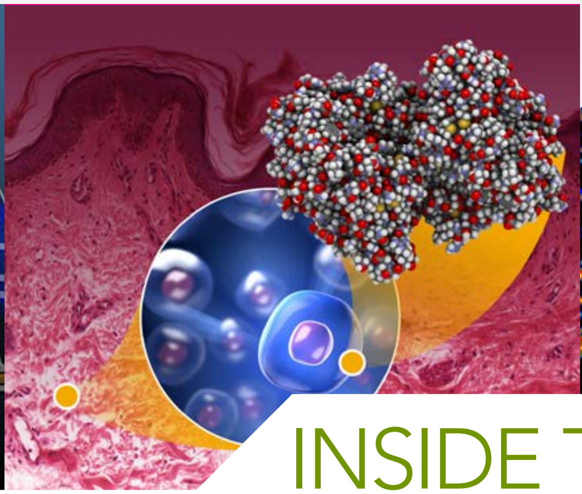
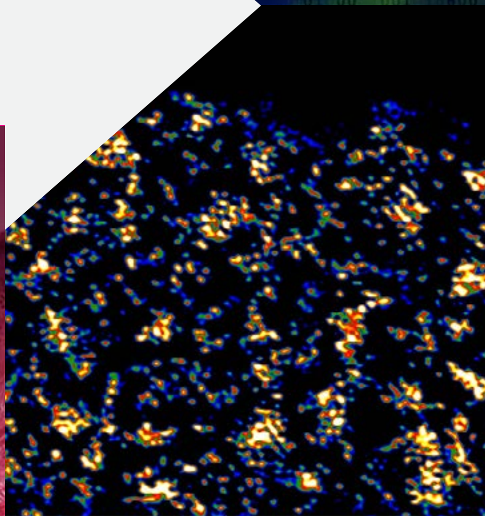




Every month EMSL develops science highlights based on research using EMSL expertise and capabilities and published in peer-reviewed journals. These are the science illustrations featured in this issue of *The Molecular Bond* on pages 11 and 12.

INSIDE THIS ISSUE

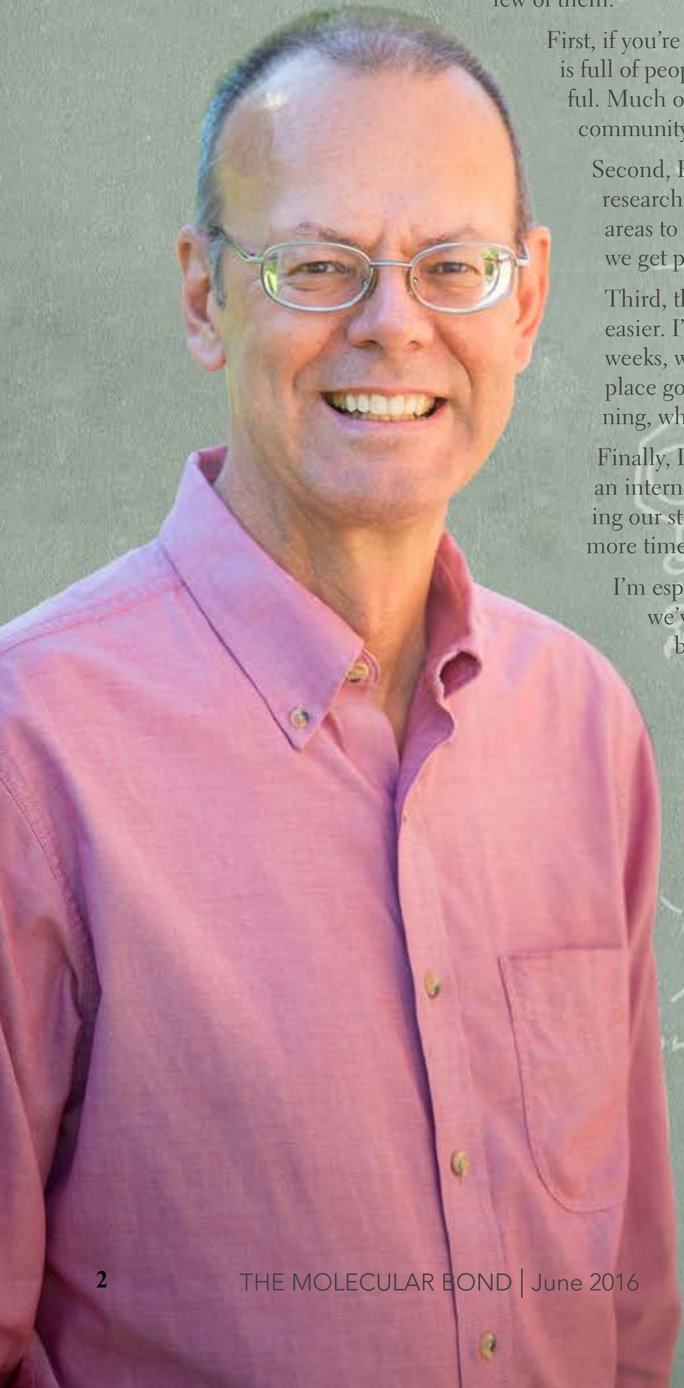
FROM THE DIRECTOR

Harvey Bolton

My 10-month tenure as the interim director of EMSL has been one of the most humbling, challenging, hectic, educational and immensely rewarding experiences I've had in my nearly 30 years with Pacific Northwest National Laboratory. It will soon come to an end as Liyuan Liang, from Oak Ridge National Laboratory, joins EMSL this summer as our new director.

I'm grateful to have served in this role, but I look forward to returning to my former position as EMSL's deputy director.

Leading an institution with the scope and prestige of EMSL teaches you all kinds of things. Here are just a few of them:



First, if you're not a 'people person' you're probably not going to end up at a user facility. EMSL is full of people who are dedicated to ensuring our users get the help they need to be successful. Much of the work of EMSL staff is focused on serving the needs of the scientific user community, often without public acknowledgement or accolade.

Second, EMSL's collaborative environment is special. I'm energized when I see our researchers in a spirited discussion in the hallways and coming together in collaboration areas to tackle scientific challenges. Science is important to people here. It's not just what we get paid to do, it's our passion.

Third, the work of former EMSL Director Allison Campbell made my interim role much easier. I'm thankful for the highly skilled and competent staff she put in place. In my first weeks, while I was grappling with a learning curve that was shockingly steep, you kept the place going, the programs functioning, the deadlines met. The engine of EMSL kept running, which gave me time to figure things out.

Finally, I've learned about myself: I like being a manager. My career objective is not to be an internationally known scientist. I find satisfaction and professional fulfillment from helping our staff build scientific programs and advance their careers. I look forward to having more time for this once Liyuan settles in.

I'm especially proud of several accomplishments this year, including the excellent people we've hired for key positions, the 21 Tesla ultra-high resolution mass spectrometer becoming available for users, the progress on the DTEM – dynamic transmission electron microscope program, and working with Don Baer to transition EMSL's current Energy Materials and Processes Science Theme to the Molecular Transformations Science Theme to encompass research of greater interest to our sponsor, the Department of Energy's Office of Biological and Environmental Research.

Liyuan brings expertise, prestige and relationships that will begin an exciting new chapter for EMSL. Her background, research and scientific focus will be a perfect fit here. My experience as an interim director has equipped me to help her as she becomes the new EMSL director and starts to make her mark on EMSL.

I want to thank everyone for entrusting me with this position, particularly the many EMSL staff who patiently answered questions I probably should have already known, and those who helped in numerous ways.

The future of EMSL is bright. I feel fortunate to be a contributor.

—Harvey

Pacific Northwest National Laboratory scientist Bruce Arey is using EMSL's helium ion microscopy located in the Quiet Wing. Arey will be one of the instructors for the EMSL Integration 2016 capability tutorials and the helium ion microscope will be one of the instruments used in the training. Find out more about EMSL Integration 2016 on this page. (EMSL file photo)

NEWS & KUDOS

Registration Now Open for EMSL's Annual Science Meeting

Registration is now open for "EMSL Integration 2016: Multiscale Ecosystems Analysis & Design." The annual science meeting will be held Sept 12-13 at EMSL in Richland, Wash. Keynote speaker Mary Firestone, professor of soil microbiology in the Department of Environmental Studies, Policy and Management at the University of California at Berkeley, will kick off the meeting.

This year's meeting will focus on 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 Terrestrial and Subsurface Ecosystems 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.

The agenda includes:

- Sept. 12 – Science meeting with keynote and plenary presentations.
- Sept. 13 – All-day workshop featuring tutorials focusing on the rhizosphere science challenges and recent innovations.

The keynote address will be followed by additional plenary speakers including:

- David McNear, University of Kentucky
- Peter Thornton, Oak Ridge National Laboratory
- David Weston, Oak Ridge National Laboratory
- Rytas Vilgalys, Duke University
- Alex Guenther, University of California-Irvine

Tutorials will be offered on Sept. 13. These include:

- ^{57}Fe Mössbauer spectroscopy
- Using isotopic tracers to track C flow through microbial systems
- Quantitative confocal and super resolution fluorescence microscopy and cell isolation approaches to study plants and microbes
- Electron microscopy imaging and analysis, TEM or SEM/HIM
- Laser ablation mass spectrometry for spatially resolved chemical characterization of soils and roots
- Techniques in magnetic resonance
- Secondary ion mass spectrometry
- Molecular science computing

Cost is $65 for students and $135 for nonstudents. Registration information and access to the registration page is available on the Integration 2016 website, along with more information about accommodations, badging and contacts http://1.usa.gov/1WH44UW.

Liang Named Director of EMSL

World-class chemist Liyuan Liang has been selected as director of EMSL. She replaces Harvey Bolton, who has been serving as interim director. Liang will join EMSL and Pacific Northwest National Laboratory mid-summer from Oak Ridge National Laboratory.

"Dr. Liang brings outstanding experience providing strategic vision and planning to advance high-impact cross-disciplinary research," said Allison Campbell, associate director at PNNL and leader of the laboratory's Earth and Biological Systems Directorate. "Her experience leading projects and teams of scientists focused on research supporting the Department of Energy and other government sponsors is a perfect fit for EMSL and PNNL."

At Oak Ridge, Liang helped set research strategy, directed investments in strategic new research areas and led large teams of scientists tackling some of the nation's most important scientific problems. She oversaw the Office of Institutional Planning,

Liyuan Liang (Courtesy of Northeastern University)

managed the laboratory's ARPA-E programs, was a Distinguished Scientist in the Shull-Wollan Center at Oak Ridge's Spallation Neutron Source and served as a joint professor at the University of Tennessee.

At EMSL, Liang will be responsible for setting a scientific vision that attracts outstanding staff scientists and users of EMSL facilities and programs, promotes innovative research, and fosters the creation of robust scientific teams and communities.

In addition to her career at Oak Ridge, Liang has held faculty positions at the University of South Carolina and the University of Wales, Cardiff. A frequently invited speaker at scientific meetings, she is the author of more than 125 peer-reviewed articles and co-editor of the book *Neutron Applications in Earth, Energy and Environmental Sciences*. Liang was elected Fellow of the American Association for the Advancement of Science for research leading to 'the discovery of mercury methylation genes in anaerobic bacteria'. Liang received her Bachelor of Science in civil engineering from Northeastern University, and a Master of Science and Ph.D. in environmental chemistry from the California Institute of Technology.

Read the PNNL news release: http://1.usa.gov/1Ocj9LI

EMSL Scientists Named Laboratory Fellows

Ljiljana Paša-Tolić

Tim Scheibe

Pacific Northwest National Laboratory recently appointed EMSL scientists Ljiljana Paša-Tolić and Timothy Scheibe as Laboratory Fellows, one of PNNL's highest ranks for its scientific and engineering staff.

Paša-Tolić, lead scientist for mass spectrometry at EMSL, demonstrates leadership in mass spectrometry and proteomics, especially top-down proteomics. The impact of Paša-Tolić's work is evident in her international reputation and successful completion and establishment of EMSL's new 21 Tesla ultra-high resolution mass spectrometer.

Scheibe, lead scientist for multiscale modeling and high-performance computing at EMSL, is recognized for his leadership in establishing the connection between those two disciplines. He has an international reputation in understanding subsurface fluid flow and reactive transport modeling.

Laboratory Fellow is one of the highest honors bestowed by PNNL and is only given to those scientists and engineers who have demonstrated exceptional quality research and development in science and engineering as validated by their peers and external reviews.

Hofmockel Receives DOE's Early Career Research Program Funding

Kirsten Hofmockel

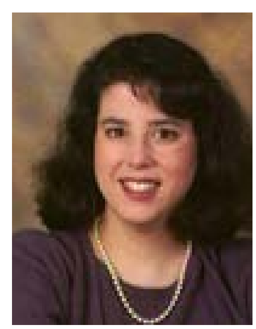
Kirsten Hofmockel, lead scientist for integrative research at EMSL, was one of 49 scientists selected by the Department of Energy's Office of Science to receive significant funding for research as part of DOE's Early Career Research Program. The effort, now in its seventh year, is designed to bolster the nation's scientific workforce by providing support to exceptional researchers during the crucial early career years, when many scientists do their most formative work.

Hofmockel's research project is "Molecular Interactions of the Plant-Soil-Microbe Continuum of Bioenergy Ecosystems," and was selected by DOE's Office of Biological and Environmental Research. She will study the science around bioenergy crops, such as switchgrass and corn that are grown as a potential source of energy. She will do experiments both in her laboratory and in experimental plots at the Great Lakes Bioenergy Research Center looking at microbial activity in the soil in which bioenergy crops are grown.

Her project will look at how crop selection and soil properties influence soil micro-organisms, which play a huge role in the fate of carbon in soil. She will study what those microbes are doing to transform carbon and other compounds in the soil, the potential of soil to hold vast amounts of carbon, what happens to the microbes once they die, and the effects of growing bioenergy crops on soil and its microbes.

DOE's Office of Science selected 49 scientists from across the nation to receive awards. The recipients were selected from a large pool of university- and national laboratory-based applicants. Selection was based on peer review by outside scientific experts.

Lipton Named Mass Spectrometry Capability Lead



Mary Lipton

Effective May 1, Mary Lipton became the lead for EMSL's mass spectrometry capability. She replaces Robby Robinson, who is now supporting the Earth and Biological Sciences Directorate at Pacific Northwest National Laboratory.

A senior staff scientist, Lipton also serves as an adjunct professor at Washington State University-Tri-Cities at both Pullman and Richland, Wash. She is nationally recognized for her research in microbial proteomics, specifically for developing and applying new mass spectrometry-based technologies for the characterization of environmental and pathogenic microbes, microbial communities and plants.

Lipton came to PNNL in 1993 as a postdoctoral fellow and became a staff scientist at the lab in 1998. She holds a Bachelor of Science in chemistry from Juniata College in Huntingdon, Penn., and a Ph.D. in biochemistry from the University of South Carolina,

NEWS & KUDOS

Columbia. Since 2001, Lipton has served as principal investigator for more than 10 projects with funding ranging from $150K to $1.5M. She has been the lead author or co-author on more than 120 peer-reviewed journal articles.

Paša-Tolić Named Interim EMSL Chief Scientist

Laboratory Fellow and EMSL scientist Ljiljana Paša-Tolić has accepted the role of interim chief scientist for the EMSL user program. She will replace David Stahl, who will become EMSL's chief scientist for microbiology.

As interim chief scientist for the user program, Paša-Tolić will lead efforts to build user communities in EMSL's Science Theme research areas and reach out to raise awareness of EMSL to the Department of Energy's Office of Biological and Environmental Research principal investigator community.

Paša-Tolić is currently the lead scientist for mass spectrometry at EMSL, a position she will retain with her new responsibilities. PNNL recently named her a Laboratory Fellow, one of its highest honors. Paša-Tolić holds a Ph.D., Master of Science and Bachelor of Science from the University of Zagreb in Croatia.

David Stahl

As chief scientist for microbiology, Stahl will have a greater focus on conducting science using EMSL capabilities. He will also help attract new users to EMSL, and support EMSL's and the Pacific Northwest National Laboratory's biological sciences and outreach strategies.

Stahl has an international reputation in studying the application of molecular microbial ecology to environmental engineering. In addition to his scientific duties at EMSL, Stahl is an environmental microbiologist at the University of Washington in Seattle. He will continue to hold a dual appointment and maintain his teaching and research position at the university. He received his bachelor's degree in microbiology from the University of Washington and his master's and Ph.D. in microbiology from the University of Illinois.

Bruce Named EMSL Communications Lead

Denice Bruce has been selected communications lead for EMSL starting May 2. She is responsible for leading communications activities critical to EMSL's unique capabilities and the innovative science and discovery achieved there.

Prior to EMSL, Bruce was at University of Kansas School of Medicine-Wichita where she was the director of public affairs. She brings considerable communication and public relations experience to her position at EMSL. She has worked as a nationwide communication consultant and trainer to the financial industry, has taught communication strategy and research in academia, and directed external communications for large engineering projects for a regional Midwest firm. Bruce holds a Master of Arts in communication from Wichita State University.

Paša-Tolić Part of a National Microbiome Initiative

Ljiljana Paša-Tolić, lead scientist for mass spectrometry at EMSL and Laboratory Fellow, is a core member of a team of scientists advising the White House on issues related to research on the microbiome, a community of microbes in a given environment.

On May 13, Paša-Tolić attended a White House briefing as the president's advisers announced more than $121 million in new funding from federal agencies for the National Microbiome Initiative. The federal dollars are in addition to more than $400 million from foundations, organizations, companies, universities and other laboratories.

Read the Pacific Northwest National Laboratory news release: http://1.usa.gov/1UiP2i6.

Read related article: http://1.usa.gov/1UxG5Ej.

Unexpected Discovery Leads to a Better Battery

Scientists at Pacific Northwest National Laboratory, EMSL and the University of Washington collaborated to study rechargeable zinc-manganese batteries as a low-cost, safe alternative to lithium-ion batteries; however, zinc-manganese batteries usually stop working after a few charges.

The research team built a zinc-manganese oxide battery and tested it using EMSL and PNNL capabilities. The team discovered manganese from the battery's positive electrode begins to sluff off, making the battery's active material inaccessible for energy storage. But after some manganese dissolves into the electrolyte, the battery gradually stabilizes and the storage capacity levels out, though at a much lower level.

An improved aqueous zinc-manganese oxide battery offers a cost-effective, environmentally friendly alternative for storing renewable energy and supporting the power grid.

The researchers have found a way to prevent the sluffing problem. The improved zinc-manganese oxide battery could become a cost-effective, environmentally friendly alternative for storing renewable energy and supporting the power grid. The findings were published in the journal *Nature Energy*.

Reference: Pan H, Y Shao, P Yan, Y Cheng, KS Han, Z Nie, C Wang, J Yang, X Li, P Bhattacharya, KT Mueller, and J Liu, 2016. "Highly reversible aqueous zinc/manganese oxide energy storage from conversion reactions," *Nature Energy*. DOI: 10.1038/nenergy.2016.39.

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

EMSL USER PROGRAM FACILITATES TRANSFERABLE POSTDOCS


Erin Bredeweg

Postdocs develop expertise in broad-reaching research and applicable techniques

Science's 2014 'The Transferable Postdoc' article argued that postdoctoral researchers need broad beyond-the-bench skills to stay competitive; and *Nature's* 2015 'The Future of the Postdoc' story illustrated some harsh realities of an academically driven career. EMSL, the Environmental Molecular Sciences Laboratory, a DOE scientific user facility at Pacific Northwest National Laboratory, or PNNL, offers postdocs a unique advantage in addressing these and similar challenges early in their scientific careers.

EMSL provides postdocs with the opportunity to hone skills and explore new research tools and options. By the time they leave EMSL, postdocs have experience working on a variety of projects, helping to develop new tools, learning management skills for shared instruments and contributing to user-defined projects.

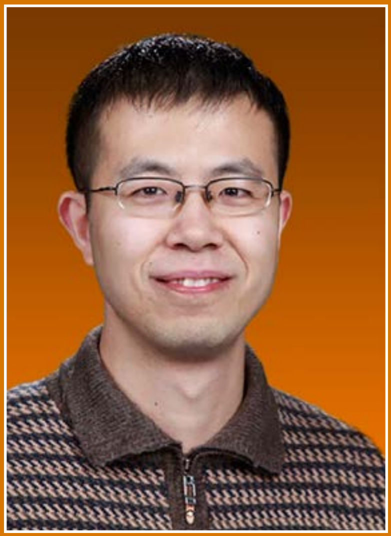
"Here researchers have freedom. We get people with a fresh love of science," says Nancy Washton, EMSL nuclear magnetic resonance, or NMR, and electron paramagnetic resonance capability lead.

"We get the cream of the crop of postdocs," says Mark Bowden, EMSL spectroscopy and diffraction capability lead. They excel at the broad research topics that comprise EMSL's mission-driven programs.

Postdocs at EMSL have diverse interests supported by the facility's structure and state-of-the-art instrumentation. Four postdocs share their experiences.

Mark Borkum

Manjula Nandasiri



Peng Lin

"I HAVE THE OPPORTUNITY TO FIGURE OUT HOW TO DO SOMETHING THAT NOBODY'S DONE BEFORE"

A Computer Scientist in a Chemist's World

Mark Borkum describes the road to becoming a postdoc at EMSL as "a long story."

While working on his Ph.D. at the University of Southampton, Borkum investigated applications of semantic web technologies to support chemistry research, focused on chemical health and safety. When a travel grant sent him to work with Karl Mueller at PNNL and the Pennsylvania State University, Mueller and collaborator Washton began courting him to join EMSL. Now, Borkum builds cyber infrastructure to assist Washton's NMR group in their studies of bacterial metabolism.

Microorganisms digest organic matter in the soil, producing trace gases like carbon dioxide, methane and nitrogen compounds that can affect energy transfer through the atmosphere. But climate models lack constraints on the kinetics and materials bacteria break down. "If you have pine needles or maple leaves, do microorganisms use a different pathway to break each down?" asks Washton.

Environmental changes affect how cells metabolize. Understanding the metabolites, or substances formed during metabolism, can help explain how bacteria adapt to new environmental conditions. NMR spectroscopy and mass spectrometry experiments provide data about the chemical and positional composition of these substances. But once this information has been gathered, identifying unknown components can be challenging. That's where Borkum comes in.

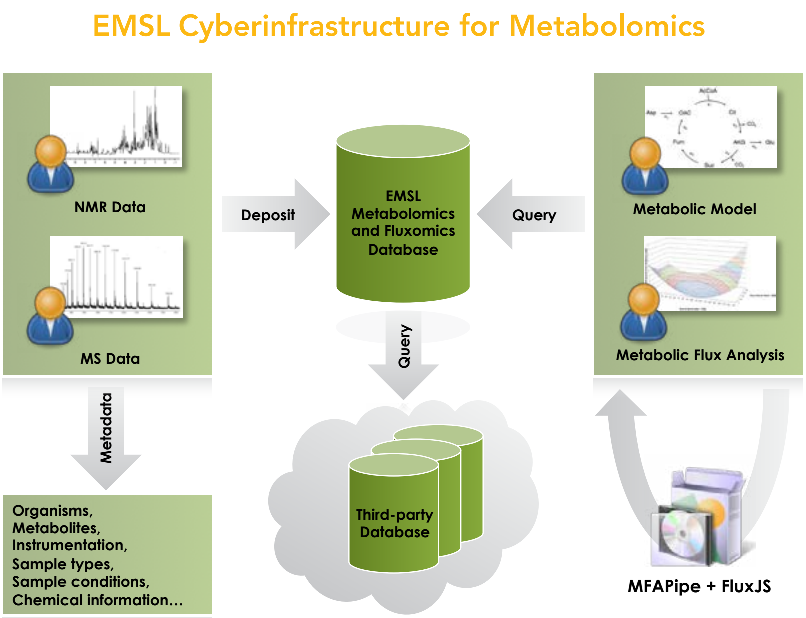
While databases exist for NMR or mass spectrometry data for some 500 metabolites, the vast majority of metabolites are unknown. Borkum is developing a novel database that is data-agnostic, providing a structure that can house not only NMR and mass spectrometry data, but any spectroscopic data. Like a refined Amazon search, it can search all existing data when provided with user input of the desired ranges for each parameter. The ability to cross-reference available data will make it easier to narrow down the possible identities of unknown compounds.

"Entire Ph.D. dissertations have been written about the integration of mass spectrometry and NMR spectroscopy data. Our system just does it," says Borkum.

Borkum also applies his background in computer science-based mathematics to fluxomics, the study of the flow of fluids and molecules within cells. From a network of biochemical reactions, each with known inputs and products, metabolic flux analysis algorithms infer the most important reactions. This means researchers can determine experiments to perform to understand the behavior of a given biological system. Currently available software handles data from mass spectrometry experiments only. Borkum and his colleagues also want to input data from NMR spectroscopy experiments, and need a general-purpose system to accommodate both types of data simultaneously.

"I have the opportunity to figure out how to do something that nobody's done before," says Borkum.

Thawing permafrost is an example why this matters. As the tundra warms, bacteria will become increasingly more active, eating away at organic matter that has been stable for centuries. How fast they do so and how their metabolic pathways change as a function of environment is a complicated and poorly understood process. Yet these processes are increasingly thought to play an important role in atmospheric emissions from the land surface, and that will impact long-term climate processes.



Mark Borkrum's Research – An illustration showing EMSL's cyberinfrastructure for metabolomics. (Image provided by Mark Borkum, EMSL.)

New Directions in Fungal Genetics

Erin Bredeweg's doctoral studies at Oregon State University focused on *Neurospora crassa* genetics. But she wanted to continue studying other fungal species and their applications in biofuel production. She had met Scott Baker, EMSL Science Theme lead for Biosystem Dynamics and Design, at a conference, and had spoken with a former labmate who was already at EMSL. Based on these discussions, she applied for a postdoc position in Baker's group that let her explore new directions in fungal genetics as well as imaging techniques.

She examines how the fungus *Yarrowia lipolytica* accumulates lipids in specific cellular compartments, or organelles, and how these accumulations vary between carbon-rich and nitrogen-poor environments. Scientists want to know what pathway causes cells to transition to lipid accumulation, so they can engineer organisms that rapidly make fats for biofuel production.

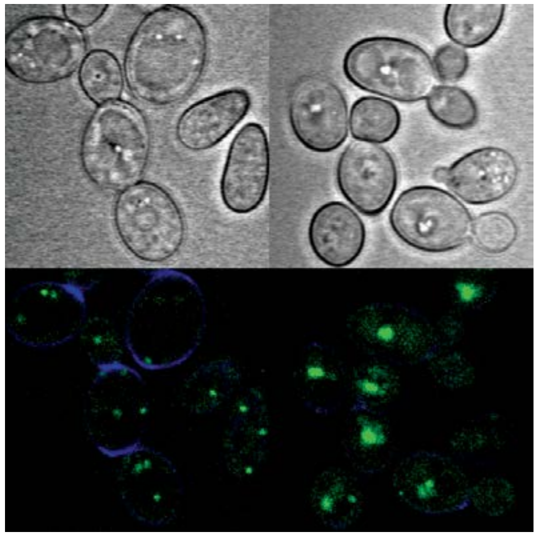
"A lipid body is like a fat droplet inside the cell, whose size depends on how long it remains in nitrogen-limited, nutrient-replete conditions," says Bredeweg.

To investigate *Yarrowia's* cell biology and metabolism, Bredeweg and colleagues developed the "*Yarrowia* Cell Atlas." This library of genetic strains expresses a specially engineered green fluorescent protein, also known as GFP, which emits a specific wavelength of light when hit by a laser. It becomes easy to follow the pathways of protein expression and to view organelle morphology in live cells, and therefore, where lipid accumulation occurs. Tagging enzymes suspected to play a role in fatty acid production further helps identify their location. With this background, Baker's group has developed a toolkit for live-cell organelle identification in *Yarrowia*, to better understand the cell during biofuel production.

"These cells have been studied, but they had to be altered to be visualized. With GFP tags, you can watch how cellular components interact in real time," says Bredeweg. They also observe how cells respond to the presence or absence of a particular nutrient.

Bredeweg enjoys access to a suite of EMSL microscopes. Modifications to these instruments make it possible to image cells and define imaging environments within small spaces. Her confocal laser-scanning microscope boasts a powerful, tunable laser and high-speed cameras for monitoring cell wall and lipid body growth.

With these tools, Bredeweg wants to ask specific scientific questions, such as how lipid accumulation works under conditions used in industry. "We've developed tools in a research lab setting, but aim for a more applied direction," she adds.



Erin Bredeweg's Research – These are *Yarrowia lipolytica* lipid droplets in nitrogen replete (left) and nitrogen-limited (right) media. The top images are transmission photomultiplier tube. The bottom images are lipid droplets labeled with a green fluorescent protein tag on protein erg6, which localizes to the lipid droplet. Blue is calcofluor white, a cell wall-specific stain. (Images provided by EMSL's Erin Bredeweg and Scott Baker.)

Upping the Charge of Batteries

Manjula Nandasiri first came to EMSL as an intern during his graduate studies at Western Michigan University, working on metal oxide thin films for applications in fuel cells and catalysis. Upon graduating, he returned as a postdoc to work with Bowden's spectroscopy and diffraction group on surface analysis for energy storage materials.

"It's challenging, because you have to work on other EMSL users' projects as well as on your own research. But I like that, because I've had the chance to collaborate with so many scientists," says Nandasiri.

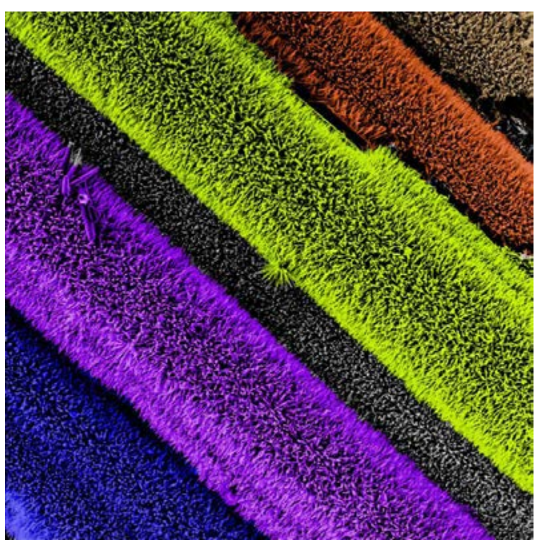
One research interest is developing next-generation lithium-sulfur battery materials. Rechargeable Li-S batteries of the future will have higher energy density and specific capacity than today's lithium-ion batteries. But scientists need to understand how surface layers develop on the electrodes and what causes them to fail. Nandasiri helps this effort by developing *in situ* chemical imaging tools to characterize electrodes.

A significant problem with Li-S batteries is that lithium polysulfides accumulate and 'clog' the electrodes. To combat this, scientists are developing electrolyte additives that form protective layers on the electrodes. "Electrolyte materials can control surface layer formation on electrodes under different conditions," notes Bowden, Nandasiri's mentor.

One way to study battery properties is to charge and discharge the battery, and then observe changes in the materials externally. However, Nadasiri cycles battery samples inside an X-ray photoelectron spectroscopy, or XPS, chamber so he can obtain chemical-specific information during their operational process.

XPS measures the elemental composition of the surface layer by irradiating the material with X-rays, while measuring the kinetic energy and number of electrons that escape from the material. XPS can also provide the oxidation state of the elements. EMSL's imaging XPS capability can also provide elemental and chemical mapping on the materials' surfaces.

In situ studies have shown a gradual increase of lithium polysulfides accumulating on the anode after one or two cycles. Initial results also show electrolyte decomposition, which leads to additional products forming on electrode surfaces during cycling. Chemical state maps show how these reaction products are

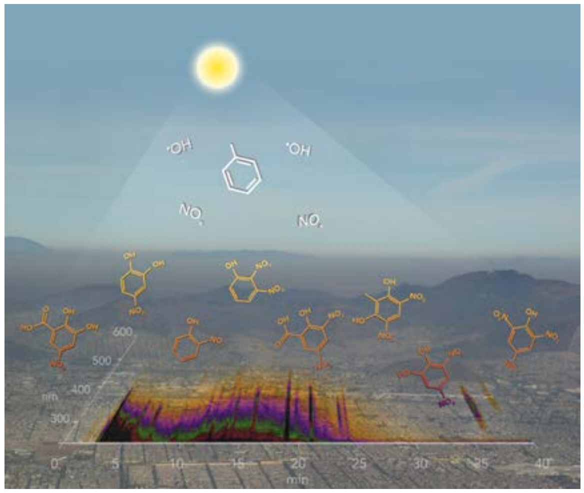


Manjula Nandasiri's Research – Helium ion microscopy image of supercapacitor electrode made from carbon nanotubes (grainy objects) and zinc oxide nanowires (fuzzy objects). This material was used to develop X-ray photoelectron spectroscopy characterization methods. (Image provided by Shuttha Shutthanandan, Manjula Nandasiri, EMSL; Vijayakumar Murugesan, PNNL; and Karim Hasanul and Mohammad Shuvo, University of Texas at El Paso.)

distributed on the electrode. These studies emphasize the potential of *in situ* XPS for understanding Li-S battery properties as new materials are developed.

Because XPS is a vacuum technique, it can only be used with vacuum-friendly electrolytes. “Other electrolyte systems require you to modify the technique. That’s the next step,” Nandasiri adds.

Studying Molecular-scale Processes to Understand Climate Processes



Peng Lin’s Research – Characterization of brown carbon chromophores in light-absorbing secondary organic aerosol generated from photo-oxidation of an organic aerosol, toluene, in the presence of NOx. Chemical composition and light-absorption properties of the product depend strongly on initial NOx concentration. (Cover image for Lin *et al. Phys. Chem. Chem. Phys.*, **Vol 17, Sept 2015.)**

Peng Lin came to EMSL from the Hong Kong University of Science and Technology to continue his graduate research on the physiochemical properties of atmospheric aerosols and their environmental impact.

“EMSL’s research theme fits my interest very well, so I decided to apply there. Alexander Laskin’s group is the most innovative team studying organic aerosols at the molecular level using ultra high-resolution mass spectrometry,” he says.

The brown haze of pollution hanging over many cities serves as a sobering reminder of what our energy consumption choices could look like in the future. Brown carbon, a light-absorbing organic aerosol, contributes substantially to this haze and can be an important contributor to climate forcing. But quantitative predictions of its contribution to climate forcing is challenging because of its compositional complexity. Aerosol properties depend on their molecular structures, and Lin develops methods to characterize brown carbon chemistry.

Brown carbon optical properties change over time as a result of oxidation and other reactions in the atmosphere. Obtaining molecular-level information about the rates of processes leading to these properties, meaning the chemical evolution of chromophore molecules responsible for color, is critical for including aerosol aging in climate models.

Recently, Lin and colleagues focused on brown carbon produced through reactions of organic aerosols with ammonium salts, both of which are abundant in the atmosphere. They identified the major chromophores responsible for light absorption, suggesting that under specific atmospheric conditions, nitrogen-containing compounds dictate brown carbon’s optical properties.

“Being a postdoc at a DOE user facility gives me access to state-of-the-art instrumentation, so I can spend more time developing methods for atmospheric research applications,” says Lin. “We need to develop analytical methods to make instrumentation suit our research goals.”

That means developing a range of spectroscopy techniques to establish predictive understanding of light absorption properties and their relationship to individual chromophore structure. Lin’s continued efforts will provide more detailed molecular-level understanding of brown carbon chemistry to improve parameterizations of aerosol absorption in global-scale climate models.

A Great Way to Start a Career

Postdocs at EMSL enjoy many unique opportunities to combine theoretical skills with practical problems, enhancing the potential for rich and varied careers. Not surprisingly, they, along with their mentors, advocate expanding user facilities’ role to further support new scientists in the greater community.

EMSL’s structure differs from traditional academic organizations. “The way experiments are pursued is not necessarily driven by a single person or advisor,” notes Bredeweg. Rather, it’s driven by larger program goals established by committees of scientists from around the world. And while Lin is happy with life at EMSL, he would like to see still more opportunities for new scientists to conduct research in a flexible, multi-disciplinary environment.

Adaptability is critical for career scientists. The EMSL user program offers investigators flexibility and an array of experiences that benefit both new and senior scientists, and most important, the scientific community. ■

Rachel Berkowitz is a freelance writer.

Abiotic Pathway Makes Organic Nitrogen Compounds Available to Microbes and Plants

Manganese oxides found in some minerals interact with proteins to release organic nitrogen compounds into soils

The ability of plants and microorganisms to take up organic nitrogen in the form of amino acids and peptides has received increasing attention over the last two decades, yet mechanisms for the formation of such compounds in soil environments remain poorly understood. A new study reveals that manganese oxides found in some minerals fragment proteins to produce soluble peptides that could be released into the soil and directly taken up by microbes and plants.

The study reveals how mineral-mediated, abiotic processes can produce small peptides that could contribute to the availability of organic nitrogen to plants and microorganisms. Understanding the mechanism by which nitrogen is made bioavailable is key to understanding nutrient cycling within terrestrial ecosystems.

Funding: This work was supported by the Department of Energy's Office of Science, Office of Biological and Environmental Research, including support of EMSL, a DOE Office of Science user facility at Pacific Northwest National Laboratory; the William Wiley Distinguished Postdoctoral Fellowship at EMSL; and a research fellowship from the Institut fuer Bodenlandschaftsforschung, Leibniz Zentrum für Agrarlandschaftsforschung.

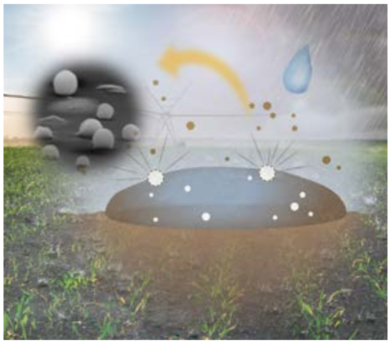
Publication: Reardon PN, SS Chacon, ED Walter, ME Bowden, NM Washton, and M Kleber. 2016. "Abiotic protein fragmentation by manganese oxide: Implications for a mechanism to supply soil biota with oligopeptides." *Environmental Science & Technology* 50 (7), 3486–3493. DOI: 10.1021/acs.est.5b04622.

Participating Organizations: Oregon State University, EMSL and the Leibniz Zentrum für Agrarlandschaftsforschung.

Rain Ejects Soil Organic Particles Into the Atmosphere

Precipitation events in agricultural areas and grasslands might be important contributors to cloud formation

Airborne organic particles play a critical role in Earth's climate, public health, air quality, and hydrological and carbon cycles, but sources of solid organic particles in the atmosphere are poorly understood. A new study shows rain events are an unrecognized contributor to airborne soil organic particles.



The findings suggest airborne soil organic particles could have important impacts on cloud formation and the absorption of solar radiation. Therefore, the study could be used to improve the accuracy of atmospheric models and to deepen our understanding of atmosphere-land interactions and how airborne organic particles influence Earth's climate.

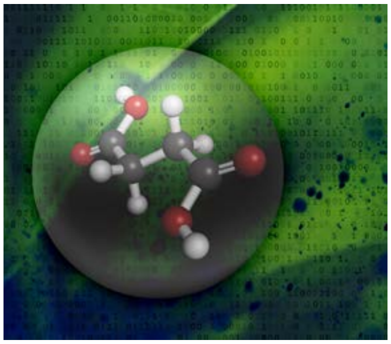
Funding: This work was supported by the Department of Energy Office of Science, Office of Biological and Environmental Research, including the Atmospheric System Research program; EMSL, a DOE Office of Science user facility at Pacific Northwest National Laboratory; Atmospheric Radiation Measurement, a DOE Office of Science user facility; the Chemical Imaging Initiative of the Laboratory-Directed Research and Development program at PNNL; the Advanced Light Source at Lawrence Berkeley National Laboratory, a DOE Office of Science user facility at Lawrence Berkeley National Laboratory; and the Office of Basic Energy Sciences Condensed Phase and Interfacial Molecular Sciences program.

Publication: Wang B, TH Harder, ST Kelly, DS Piens, S China, L Kovarik, M Keiluweit, BW Arey, MK Gilles and A Laskin. 2016. "Airborne soil organic particles generated by precipitation." *Nature Geoscience*. DOI: 10.1038/ngeo2705.

Participating Organizations: EMSL; Lawrence Berkeley National Laboratory; the University of California, Berkeley; and the University of Massachusetts, Amherst.

3-D NMR Method Enhances Analyses of Metabolic Networks in Cells

Data acquisition time dramatically reduced and metabolite identification amplified



More rapid and improved estimates of metabolic fluxes in cells are possible thanks to a new technique that combines ^{13}C-Metabolic Flux Analysis with non-uniform sampling nuclear magnetic resonance spectroscopy data.

Key insights into metabolic networks provided by the new technique could be used for synthetic biology-based efforts to modify living systems for production of metabolites or other products of interest, such as biofuels or fine chemicals.

Funding: This work was supported by the Department of Energy's Office of Science, Office of Biological and Environmental Research, including support of EMSL, an Office of Science user facility;

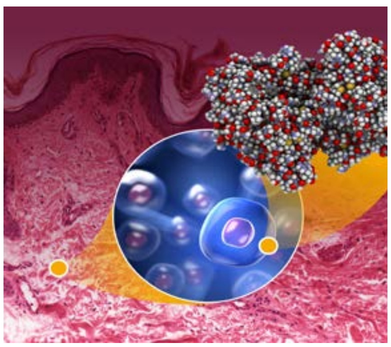
William Wiley Distinguished Postdoctoral Fellowship from EMSL; and an EMSL intramural research project entitled "Development of an Integrated EMSL Mass Spectrometry and Nuclear Magnetic Resonance Metabolic Flux Analysis Capability in Support of Systems Biology: Test Application for Biofuels Production."

Publication: Reardon PN, CL Marean-Reardon, MA Bukovec, BE Coggins, and NG Isern. 2016. "3-D TOCSY-HSQC NMR for metabolic flux analysis using non-uniform sampling." *Analytical Chemistry* 88, 2825–2831. DOI: 10.1021/acs.analchem.5b04535.

Participating Organizations: EMSL, Washington State University, Duke University Medical Center and Miami University.

Improving Lipid Yields for Biofuel Production

New insights into lipid metabolism in yeast could benefit biofuel production



Using a comprehensive system-wide approach, researchers identify regulators of metabolic pathways that drive lipid accumulation in a genetically tractable yeast species.

A better understanding of the metabolic pathways that regulate lipid accumulation in yeast could be harnessed to improve lipid yields and enhance the efficiency of biofuel production.

Funding: This work was supported by the Department of Energy's Office of Science, Office of Biological and Environmental Research, including support of EMSL, an Office of Science user facility; BER Genomic Science program; William Wiley Distinguished Postdoctoral Fellowship; and BER-funded Pan-omics program at Pacific Northwest National Laboratroy.

Publication: Pomraning KR, Y-M Kim, CD Nicora, RK Chu, EL Bredeweg, SO Purvine, D Hu, TO Metz and SE Baker. 2016. "Multi-omics analysis reveals regulators of the response to nitrogen limitation in *Yarrowia lipolytica*." *BMC Genomics* 17:138. DOI: 10.1186/s12864-016-2471-2.

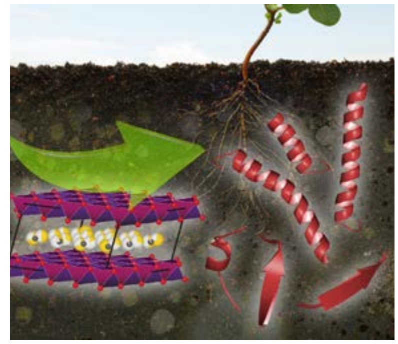
Participating Organizations: EMSL and PNNL.

How Organic Acids Form Atmospheric Particles

Studying how atmospheric aerosol particles form could improve climate models

Organic acids are an important component of atmospheric aerosols found in abundance in a variety of urban, rural and marine environments. A recent study combined experimental and theoretical techniques to shed light on their role in initial stages of aerosol particle formation.

Newly formed atmospheric aerosol particles can influence the formation and properties of clouds, potentially having a major impact on global climate. New insights into mechanisms controlling this process can be harnessed to develop more accurate climate models.



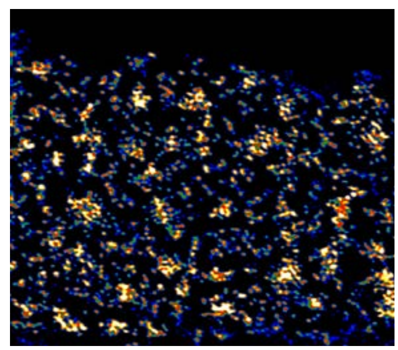
Funding: This work was supported by the Department of Energy's Office of Science, Office of Biological and Environmental Research, including support of EMSL, a DOE Office of Science user facility, the EMSL Intramural Aerosol Science Theme Funding; and Office of Basic Energy Sciences.

Publication: Hou G-L, M. Valiev, and X-B Wang. 2016. "Deprotonated dicarboxylic acid homodimers: Hydrogen bonds and atmospheric implications." J*ournal of Physical Chemistry* A 120(15), 2342-2349. DOI: 10.1021/acs.jpca.6b01166.

Participating Organizations: EMSL and PNNL.

Research Settles Debate on How Methane Forms

Understanding how methane forms could improve catalysts for fuel production



Methanogenic archaea produce more than 90 percent of Earth's atmospheric methane, totaling more than 1 billion tons of methane per year globally. A new study settles a longstanding debate on how this important fuel and powerful greenhouse gas is generated.

By identifying the key intermediate involved in methane formation, this study could lead to the development of better catalysts for fuel production as well as strategies to inhibit microbial production of a potent greenhouse gas.

Funding: Computation at EMSL was supported by the Department of Energy's Office of Science, Office of Biological and Environmental Research. All other work was supported by Office of Science, Office of Basic Energy Sciences and Advanced Research Project Agency – Energy.

Publication: Wongnate T, D Sliwa, B Ginovska, D Smith, MW Wolf, N Lehnert, S Raugei, and SW Ragsdale. 2016. "The radical mechanism of biological methane synthesis by methylcoenzyme M reductase." *Science* 352 (6288): 953-958. DOI: 10.1126/science.aaf0616.

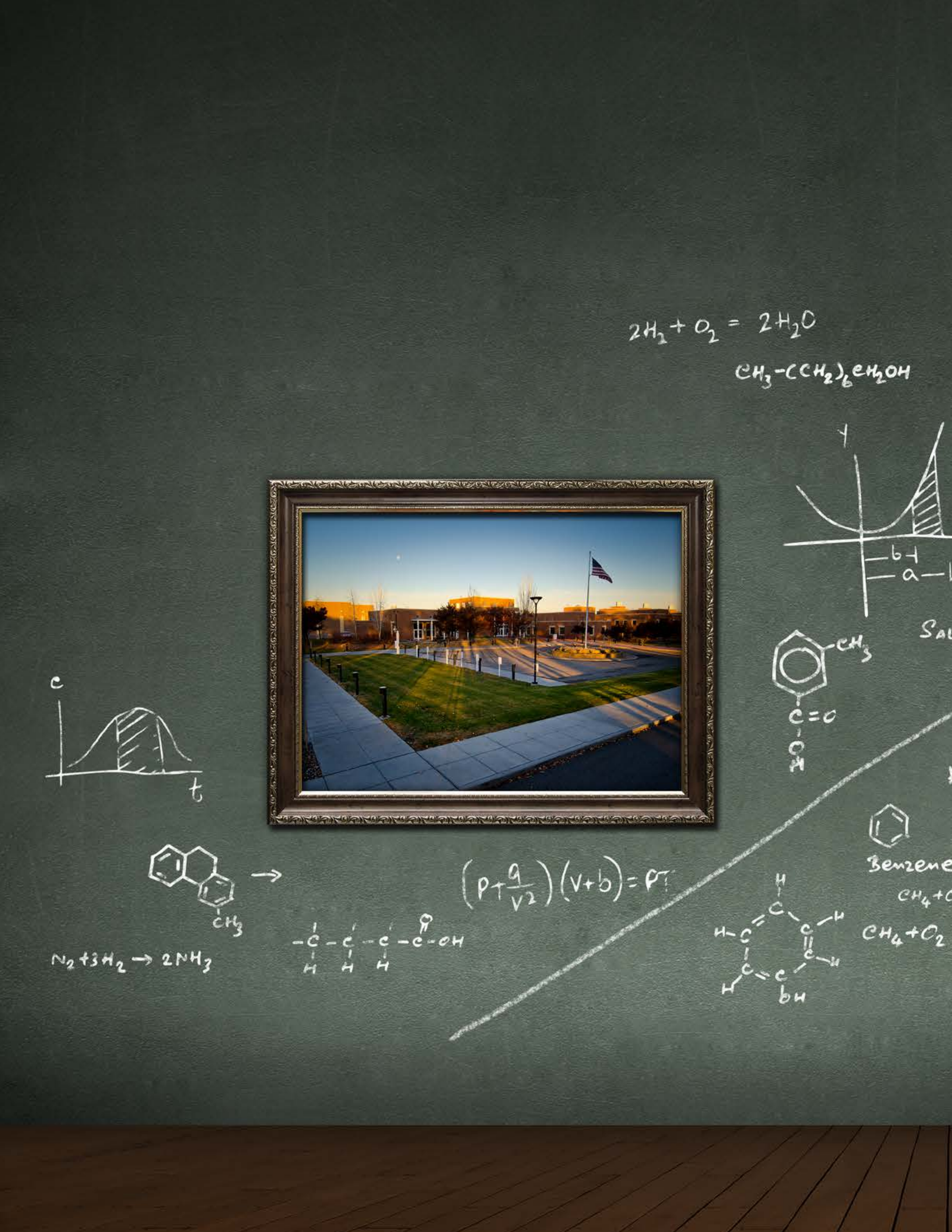
Participating Organizations: University of Michigan at Ann Arbor and PNNL.

About This Art

The study of these zinc oxide plates and how the plates nucleate and grow as secondary structures on zinc oxide surfaces contributes toward America's goal of a clean, abundant and secure energy future. Researchers are enhancing fundamental understanding of nucleation sites and growth characteristics. This is a vital step in making zinc oxide a more effective material for use in the development of high-energy storage systems, such as lithium-air and zinc-air batteries. The research is being conducted in facilities at Pacific Northwest National Laboratory and EMSL. The image was captured with a Helios 600 dual-beam focused ion beam/scanning electron microscope at EMSL. Funding was provided by the Department of Energy's Office of Basic Energy Sciences.

Team Members

Bruce Arey, Jun Liu, Yongsoon Shin and James De Yoreo, all from PNNL (Image colorized)


2H2 + O2 = 2H2O
CH3-(CH2)6CH2OH
N2 +3H2 → 2NH3
Benzene
CH4 +O2