EMSL

THE MOLECULAR BOND

AUGUST 2014

IT TAKES TEAMWORK

Also inside this issue:

Bioengineering Better Biomass

DOE JGI/EMSL Collaborative Science Projects

Special Science Call Continues

Improving Pore-Scale Predictions

Translating Microbial Communication

About the Cover

Fungi may play both a direct and indirect role in carbon cycling. Colleen Hansel from Woods Hole Oceanographic Institution has teamed up with colleagues at the Smithsonian Institute, as well as scientists from EMSL and the DOE Joint Genome Institute, to study how fungi use indirect pathways to cycle and degrade 'recalcitrant carbon' – so called for its resistance to enzymatic breakdown. The fungi oxidize soluble manganese to form manganese oxide minerals that oxidize and degrade carbon. This is an image of the Mn(II)-oxidizing fungus *Stilbella aciculosa* – the fungal biomass is white and the brown color is manganese oxide mineral.

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

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Retired EMSL leader M. Tom Thomas (right) takes an annual tour of the user facility when he attends the M.T. Thomas Award for Outstanding Postdoctoral Achievement event named in his honor. Before this year's event, Thomas visited some of EMSL's mass spectrometry labs with PNNL Biological Sciences Deputy Division Director Joshua Adkins. Adkins nominated this year's recipient, Ernesto Nakayasu, who used these capabilities in his research on protein degradation.

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FROM THE DIRECTOR

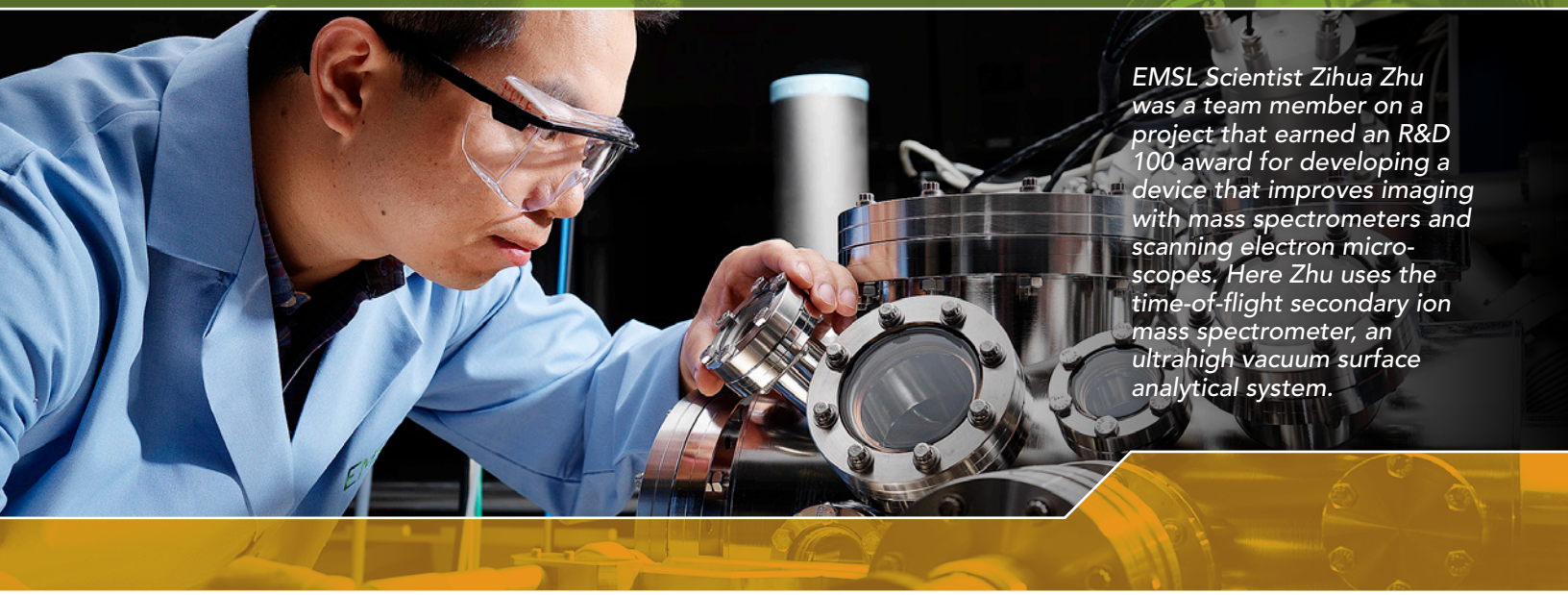
Allison Campbell

Collaboration has always been in EMSL's DNA, from when the user facility was just a dream of Bill Wiley's. Back then, science was stovepiped by discipline and with single-investigator studies. Molecular science was the horizontal translation we needed to bridge the gaps and build teams.

Today, we bring together teams from across disciplines and across facilities to drive greater innovation in energy, environment and biology. We've been doing it for 17 years and continue to create new ways of collaborating. In this month's issue of *The Molecular Bond*, you'll read about some of the mechanisms we've used to enhance collaboration and, as a result, scientific impact.

We encourage you to consider how you could engage with us – whether through scientific partner proposals, our annual calls, or special calls for first science on new capabilities and instruments. As Margaret Mead famously said, "Never doubt that a small group of thoughtful, committed people can change the world. Indeed, it is the only thing that ever has."

—Allison



EMSL Scientist Zihua Zhu was a team member on a project that earned an R&D 100 award for developing a device that improves imaging with mass spectrometers and scanning electron microscopes. Here Zhu uses the time-of-flight secondary ion mass spectrometer, an ultrahigh vacuum surface analytical system.

NEWS & KUDOS

DOE JGI/EMSL Announce 2015 Collaborative Science Projects

The Department of Energy Joint Genome Institute and EMSL have accepted 12 projects submitted during the 2104 call for Collaborative Science Initiative proposals.

The collaborative call represents a unique opportunity for researchers to combine the power of genomics and molecular characterization in one research project to help advance the missions of the DOE's Office of Biological and Environmental Research. The selected researchers will have access to the capabilities of both user facilities.

"These approved projects represent an excellent cross-section of research in biogeochemistry, carbon cycling and biofuel/bioproduct production," said Scott Baker, EMSL's Science Theme Lead for the Biosystem Dynamics and Design Science Theme. "It's very exciting to continue our collaboration with DOE JGI, and I look forward to the insights and impact these projects will produce."

Researchers submitted a total of 31 proposals during the call. The 12 approved projects will kick off in fiscal year 2015 and run for up to 18 months. These projects fall within the second collaborative call by EMSL and DOE JGI since the first in winter 2013.

BER, which is within DOE's Office of Science, stewards both EMSL and DOE JGI, and both user facilities play critical roles in supporting DOE's energy, environment and basic research missions.

Scheibe Named Lead Scientist for EMSL Computing

Tim Scheibe

EMSL has selected Tim Scheibe as lead scientist for Multiscale Modeling and High Performance Computing, a role recently created to emphasize its importance to EMSL's mission.

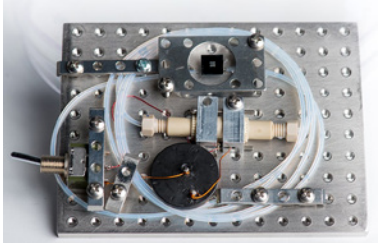
"Multiscale modeling cross cuts and underpins all of EMSL's Science Themes and is central to the DOE Office of Biological and Environmental Research's missions," says EMSL Director Allison Campbell.

As lead scientist, Scheibe will work across EMSL to develop and implement a science strategy for multiscale modeling and high performance computing, including attracting high-quality staff and an active user community. He will also provide client relationship management for EMSL's Molecular Sciences Computing Capability.

Scheibe's primary research focus is on characterization and modeling of multiscale heterogeneity and its impacts on reactive transport in groundwater systems. His research projects include both computational and field experimental elements.

Zhu Part of Team to Receive R&D 100 Award

EMSL Scientist Zihua Zhu was a member of a team of researchers at Pacific Northwest National Laboratory working at EMSL that received an R&D 100 award from *R&D Magazine* for developing SALVI, short for System for Analysis at the Liquid Vacuum Interface. The device allows solid-liquid interface observation while imaging with mass spectrometers or scanning electron microscopes.



A team of scientists at PNNL working at EMSL received an R&D 100 award from *R&D Magazine* for developing SALVI, short for System for Analysis at the Liquid Vacuum Interface. The device allows solid-liquid interface observation while imaging with mass spectrometers or scanning electron microscopes.

The idea for SALVI emerged from the interfacial study of atmospheric aerosols and was first submitted as an EMSL user proposal in 2006. Members of the team began developing the SALVI device in 2008 and it has evolved in different configurations as an application for several proposals.

Funding for SALVI came from a number of sources, among them the Department of Energy's Office of Basic Energy Sciences condensed phase program, the PNNL Chemical Imaging Initiative, the PNNL Use at the Facility Funds and the EMSL user program, to name a few.

SALVI is being commercialized by Structure Probe, Inc. and its SPI Supplies Division, both of West Chester, Penn.

Guenther on Highly Cited Researchers 2014 List

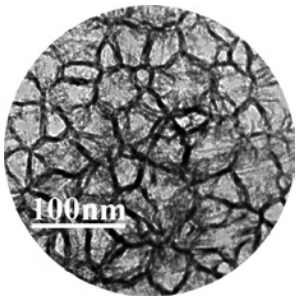
Alex Guenther

Highly Cited Researchers named Alex Guenther, an atmospheric scientist at EMSL, among the top cited researchers in average citations per paper in the category of geosciences. Guenther is the lead for EMSL's Atmospheric Aerosol Systems Science Theme and a PNNL Laboratory Fellow.

The ranking was found with InCites, a Thomson Reuters analytical tool that combed their database of indexed published papers from 2002-2012. Representing the top 1 percent in their field, only 250 researchers in each field were selected based on total citations to their papers published during this period.

Guenther is an international leader in atmospheric and terrestrial ecosystem research. He has published more than 250 peer-reviewed journal articles with 16,000 citations. Guenther was also identified as highly cited researcher by the 2014 ISI Essential Science Indicator.

Silicon Sponge Improves Li-ion Battery Performance



Researchers have developed a sponge-like silicon nano-material (shown here under a microscope) to replace the graphite electrode in lithium-ion batteries.

Researchers at EMSL, Pacific Northwest National Laboratory and the University of California, San Diego, developed and tested a sponge-like silicon material to replace the graphite traditionally used in one of the electrodes in a lithium-ion battery – silicon has more than 10 times the energy storage capacity of graphite. A paper describing the material's performance as a lithium-ion battery electrode was published July 8 in *Nature Communications*.

"Silicon has long been sought as a way to improve the performance of lithium-ion batteries, but silicon swells so much when it is charged that it can break apart, making a silicon electrode inoperable," said PNNL Fellow Ji-Guang "Jason" Zhang. "The porous, sponge-like material we've developed gives silicon the room it needs to expand without breaking."

EMSL Scientist Chongmin Wang tested the team's sponge-like silicon electrode through a series of charges and discharges using an *in-situ* transmission electron microscope to view the physical and chemical changes the battery undergoes during operation. The team observed that during charging, the new electrode mostly expanded into the empty spaces created by the material's porous structure, and the electrode did not break down.

Reference: Xiaolin L, M Gu, S Hu, R Kennard, P Yan, X Chen, C Wang, M Sailor, J Zhang and J Liu. July 8, 2014. "Mesoporous Silicon Sponge as an Anti-Pulverization Structure for High-Performance Lithium-Ion Battery Anodes," *Nature Communications*. DOI: 10.1038/ncomms5105.

Nakayasu Honored with 2013 M.T. Thomas Award

Ernesto Nakayasu

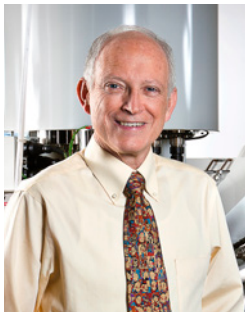
Ernesto Nakayasu received the 2013 M.T. Thomas Award for Outstanding Postdoctoral Achievement at a ceremony at EMSL on Aug. 19. He was a post-doctoral research associate at Pacific Northwest National Laboratory for more than three years studying protein degradation in biological systems.

The award was in recognition of his work with the potential for real societal impact, including development of methods to analyze proteins and determine enzymes using highly innovative mass spectrometry tools, development of an approach to integrate multiple omics methods to study proteins, and a breakthrough discovery of the mechanism of action of the first drug that can efficiently kill Methicillin-resistant *Staphylococcus aureus*, the "superbug."

During his time at PNNL, he authored or co-authored nine publications that used EMSL resources. He has a total of 50 publications in high-impact journals including *Nature, Journal of Clinical Investigations, Molecular Systems Biology* and *PNAS*.

Nakayasu is currently a research associate at Bindley Bioscience Center at Purdue University.

Baer Selected to Join Washington Academy of Sciences



Don Baer

Don Baer has been elected for membership into the Washington State Academy of Sciences. He is a PNNL Laboratory Fellow and Science Theme lead for EMSL's Energy Materials and Processes Science Theme.

The academy recognized Baer for advancements in understanding how physical and chemical processes at the surface of a material or nanoparticle influence the behavior of the material or its environment, enabling removal of contamination from water, for example. In addition to research, he also helped develop the design and operation of the EMSL user facility.

Baer joins with 17 other scientists and engineers from across Washington being recognized for outstanding scientific achievement and leadership. They will be honored at the academy's annual meeting in Seattle in September.

Special Science Call for Proposals Closes Soon

EMSL's Special Science Call for Proposals closes Sept. 15 for high-impact research that advances the DOE's Office of Biological and Environmental Research scientific missions by taking advantage of EMSL's recently established or developing technical resources.

Proposals should support EMSL's Science Themes, which are focused on leading-edge scientific research in atmospheric aerosols, feedstocks for bioproducts and biofuels, global carbon cycling, biogeochemistry and energy materials.

This call focuses on research topics enabled by these unique scientific resources at EMSL:

- Radiochemistry Annex
- Quiet Wing Microscopy and NanoSIMS Capabilities
- High Resolution and Mass Accuracy Mass Spectrometry Capability

External review and award decisions will be made upon receipt of the proposals to expedite access. Questions about this call should be directed to the User Support Office, 509-371-6003 or **emsl@pnnl.gov**.

Watch EMSL's iDirector on YouTube

EMSL Director Allison Campbell interviews Scientist Alex Laskin for iDirector.

EMSL Director Allison Campbell interviews EMSL Scientist Alex Laskin about his aerosol research, including his studies of brown carbon with the NanoDESI system. Campbell talked with Laskin as part of her monthly iDirector interview series available on EMSL's YouTube channel at **www.youtube.com/user/EMSLatPNNL**

2014 Wiley Distinguished Postdoctoral Fellows Named

For only the second time, two recipients have been named in the same year to be William R. Wiley Distinguished Postdoctoral Fellows. The 2014 honorees are Lyle Gordon and Abigail Ferrieri.

Lyle Gordon

Gordon earned his doctorate at Northwestern University, Evanston, Ill. His thesis was entitled "Buried organic-inorganic interfaces in biological minerals," and his research focused on characterizing the structure and chemistry of biological minerals to study the complex mechanisms that lead to their formation. As a graduate student, he pioneered the application of atom probe tomography to study the chemistry of buried organic-inorganic interfaces in biological minerals. This work was published in *Nature* in 2011. Beyond biological minerals, Gordon has studied a wide range of materials and biological systems, including Portland cement, nanoparticles, proteins and viruses, iron oxide, and calcium phosphates. Gordon is working in EMSL's microscopy group.

Abigail Ferrieri

Ferrieri earned her Ph.D. at the University of Missouri-Columbia. Her doctoral work examined dynamic induced responses of *Arabidopsis thaliana* to attack by insect herbivores to understand how plants coordinate these responses at the whole-plant level. Ferrieri's research interests focus on explaining behavioral patterns in higher plants by elucidating their molecular, biochemical and physiological mechanisms in response to environmental stimuli. She is currently a Humboldt Postdoctoral Research Fellow at Max Planck Institute for Chemical Ecology in Jena, Germany. Ferrieri arrives at EMSL in the fall and will be working in EMSL's mass spectrometry group.

The Wiley fellowship is named after William R. Wiley, a former director of Pacific Northwest National Laboratory.

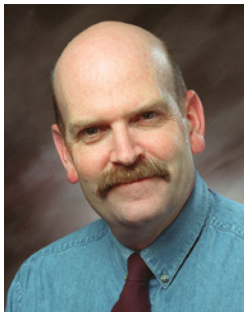
EMSL awards the fellowships to candidates who display superb ability in scientific research and show promise to become outstanding leaders in their research field. The fellowship's purpose is to attract high-performing, newly graduated PhD scientists with the potential to become full-time scientific staff at EMSL. Fellowships are awarded for a one-year term, with the possibility of renewing up to three years. Read more about the Wiley fellowship.

Lercher and Peden Selected as Wiley Research Fellows

Johannes Lercher

EMSL has appointed Johannes Lercher and Charles H.F. Peden Wiley Research Fellows in recognition of the role they will play in EMSL's Energy Materials and Processes Science Theme, and their proven record of generating highly impactful science.

Lercher is the director of the Pacific Northwest National Laboratory Institute for Integrated Catalysis, a Battelle Fellow and professor of chemistry at Technische Universität München, Germany. He is internationally renowned for his work on the fundamental aspects of industrially relevant catalyzed reactions. His research includes low-temperature acid-base catalyzed activation, functionalization and transformation of alkanes; the oxidation of light alkanes including methane; and the hydrodefunctionalization of heavy biogenic and fossil molecules.



Charles H.F. Peden

Peden is a Laboratory Fellow at PNNL and associate director of the Institute for Integrated Catalysis. Peden has an international reputation for his research studies aimed at the development of structure/function relationships and reaction mechanisms of automobile exhaust catalytic reactions. His current research programs address numerous aspects of the physical and chemical properties of oxide-based catalytic materials, including zeolites for diesel vehicle emission control.

Wiley Research Fellows contribute to the success of EMSL as a user facility by supporting the user program beyond their own specific research projects. Examples of these contributions include participation on EMSL advisory committees and partner proposals for development of new capabilities, acting as a scientific consultant for users, advocacy for EMSL and its capabilities in the scientific community, and assistance and support of a broad range of EMSL user activities.

EMSL Holds First "Science Slam"

EMSL Science Theme Lead Nancy Hess presents an overview of her Leadership Science Acceleration project at EMSL's first Science Slam.

EMSL held its inaugural Science Slam on July 21 to promote interest in the Leadership Science Acceleration projects. Karl Mueller, interim EMSL chief science officer, organized the event.

Leadership Science Acceleration projects are short-term research ventures that were funded in April 2014. The projects are meant to accelerate research in science areas identified by EMSL's chief science officer, chief technology officer and science theme leads as relevant to EMSL's new science themes and science leadership areas.

A Science Slam is an informational brown bag session. During the event, the presenters, usually the lead or sub-task lead on a Leadership Science Acceleration project, each have five minutes and no more than two PowerPoint slides to describe their projects.

Kramer Named New EMSL Visiting Scientist

Marc Kramer

Marc Kramer has been selected as a 2014 EMSL Wiley Visiting Scientist. He is an associate professor of environmental pedology and biogeochemistry at the University of Florida, Gainesville.

While at EMSL, Kramer will conduct fundamental research on terrestrial and subsurface ecosystem processes using EMSL's analytic capabilities. He will also focus on select low-throughput testing of emerging technologies and analytic capabilities using well-characterized terrestrial samples that can be used to benchmark, validate and verify new instrument capabilities and possibly result in novel discovery. He will be working with EMSL Terrestrial and Subsurface Ecosystem Science Theme Lead Nancy Hess.

In addition to his research activities, Kramer will collaborate with EMSL staff to write proposals and develop new projects. As a visiting scientist he will contribute to capabilities in the EMSL user program and provide tactical and strategic input related to terrestrial ecosystems. He will also assist in peer reviews of Department of Energy proposals and projects.

Kramer holds a Master of Science from Montana State University in Bozeman and a PhD. from Oregon State University in Corvallis. He was an American Academy of Science Postdoctoral Fellow at NASA Ames Research Center.

MSA Recognizes Dohnalkova for her Service

MSA presented EMSL's Alice Dohnalkova with two awards for her years of service to the society. "It's been my pleasure and privilege to serve the society at the national level," she said.

The Microscopy Society of America honored EMSL's Alice Dohnalkova at its recent annual meeting in Hartford, Conn.

MSA President Jeanette Killius presented Dohnalkova, an EMSL senior research scientist, with two awards following completion of her three-year term of service. The first was as an outgoing member of the MSA Council, and the second was as an outgoing committee chair of local affiliated societies.

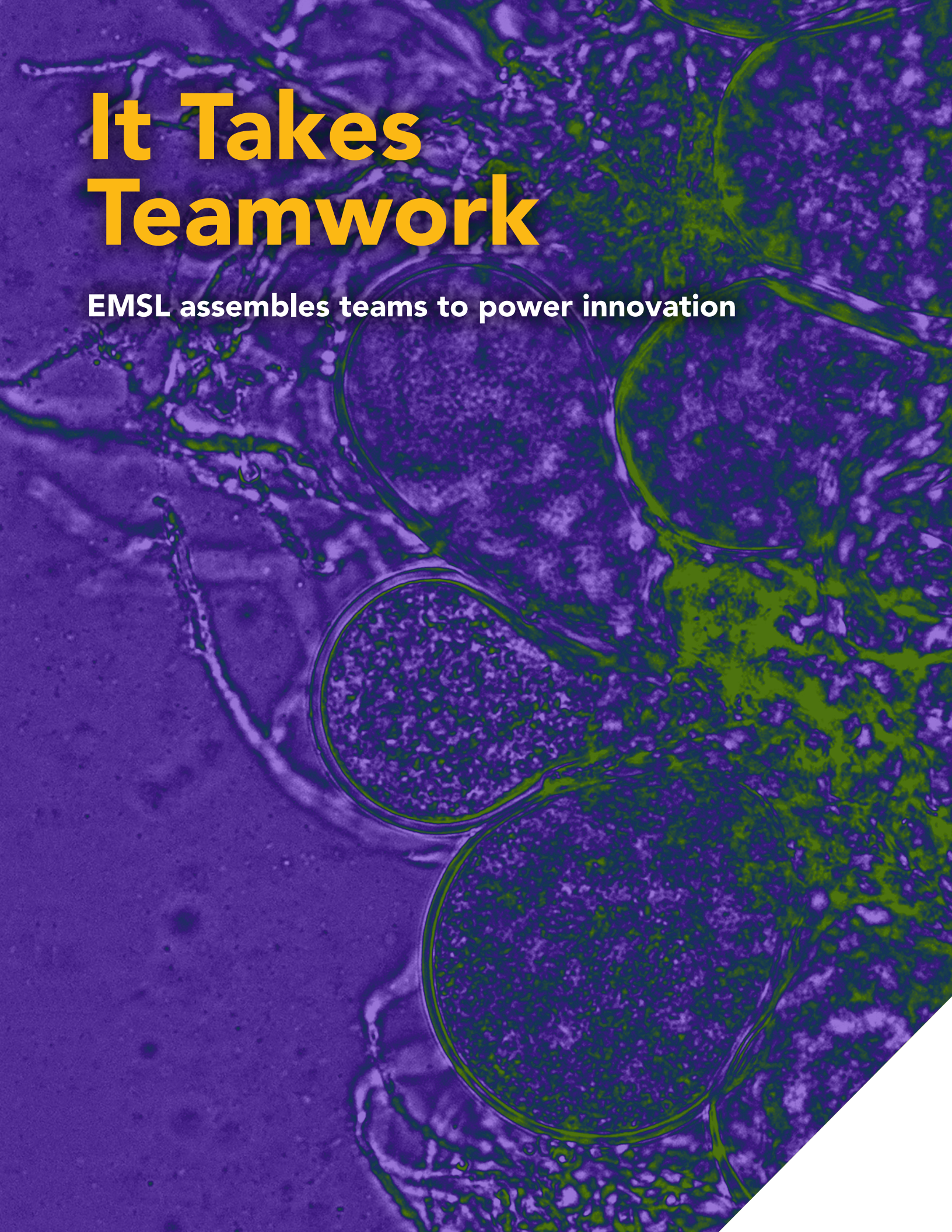
"It's been my pleasure and privilege to serve the society at the national level," said Dohnalkova, who is a member of EMSL's microscopy group. "It gave me a great perspective and appreciation of the incredible amount of work behind every successful conference, where volunteers direct most of the activities in this non-profit organization. I have come across an amazing network of microscopy professionals, and I'm looking forward to participating in the planning and preparation of the next national MSA meeting."

MSA's next national meeting, Microscopy and Micro-analysis, will be held Aug. 2-6, 2015, in Portland, Ore.

MSA is a non-profit organization dedicated to the promotion and advancement of techniques and applications of microscopy and microanalysis in all relevant scientific disciplines.

It Takes Teamwork

EMSL assembles teams to power innovation



Even before Dr. William R. Wiley started planning the brick and mortar version of the Environmental Molecular Sciences Laboratory, he was paving the way for the team-based research campaigns that draw scientists to the national user facility today. The former director of Pacific Northwest National Laboratory was known for dropping in to see scientists in their labs, starting conversations and collaborations. But Wiley would have to walk much farther than a few hallways to visit with all the researchers working with EMSL now.

EMSL's genesis can be tracked back to a discussion in 1986 between William R. Wiley, then director of Pacific Northwest National Laboratory, and his senior leaders.

In the last decade EMSL has spread the science around, calling for interdisciplinary teams of scientists to tackle complex scientific questions at the Richland, Wash., campus. Taking that approach a step further in the past two years, EMSL launched joint campaigns with other national laboratories. A 2013 call issued with the Department of Energy Joint Genome Institute, or DOE JGI, spawned eight collaborative studies that include hundreds of scientists from across the country. Another combo-campaign call went out earlier this year.

"It was also successful as a way of going forward into the future; a deepening understanding of each other's science."

"The joining of expertise and capabilities from EMSL and DOE JGI brings together sets of cutting-edge or unique instrumentation from two DOE Office of Biological and Environmental Research-sponsored user facilities, as well as the combined expertise and knowledge of an expanded group of scientific staff, to attack truly complex and grand challenges," said Karl Mueller, the interim chief science officer at EMSL. "The directed efforts of users and staff at two major national user facilities elevates and accelerates the potential for impactful science."

Involving a wide range of people in problem solving has always been at the core of EMSL's mission. Even at EMSL's inception, Wiley brainstormed with a team of up to 50 scientists to create the national user facility. But effectively bringing these large, interdisciplinary teams of scientists together can be as complex as the problems they're trying to solve.

◀ **Micrographs of anaerobic gut fungi (Neocallimastix sp S3) isolated from a sheep used in Michelle O'Malley's research.**

Grand Experiments

"When you bring together scientists, who are each really excellent in their own field, the concept of a team has more of what I call a human social experiment to it. And it's not always a given that these experiments will be successful," said Himadri Pakrasi, director of the International Center for Advanced Renewable Energy and Sustainability at Washington University in St. Louis, or WUSTL, who led EMSL's inaugural "Membrane Biology Grand Challenge" campaign in 2004.

Pakrasi was the first principal investigator to come from outside EMSL's ranks and lead an interdisciplinary team. Their mission? To discover how cyanobacteria, a blue-green algae, managed the complexities of carbon and nitrogen cycling during photosynthesis, with an eye toward learning how to more efficiently engineer that process for human energy needs. The innovative technology at EMSL enabled Pakrasi, and about 60 other scientists working on the 5-year grand challenge, to uncover key details about the night-and-day timing mechanisms that cyanobacteria use to regulate their photosynthesis.

William R. Wiley (center left) and dignitaries at the groundbreaking ceremony for EMSL in 1994.

The project was enormously successful, but not just in terms of scientific papers and knowledge gained. "It was also successful as a way of going forward into the future; a deepening understanding of each other's science," Pakrasi said. "The scientists understood the value of these kinds of interactions; how important it is to be able to do something as a team that one group or one scientist can never imagine can be done."

Now Pakrasi is working on the synthetic biology campaign. Again, he's working with co-principal investigator David Koppenaal, the chief technology officer at EMSL with whom he teamed up for the first grand challenge. This time, they're taking a 'tag team' approach to investigate ways to get antenna proteins on cyanobacteria membranes to capture light more efficiently than nature intended.

Pakrasi receives funding, through the DOE, from the Photosynthetic Antenna Research Center at WUSTL to lead about 100-odd scientists in 20 different labs. But he relies on EMSL for transcriptomics, proteomics, metabolomics and imaging of these proteins. For example, Pakrasi anticipates getting "detailed imaging that is unprecedented in biology" with EMSL's helium-ion microscopy to get a much better idea about how antenna-protein complexes are organized on the membrane; this is important to figure out how energy gets captured by these antenna, and then flows into photosynthetic "reaction centers" of the bacteria.

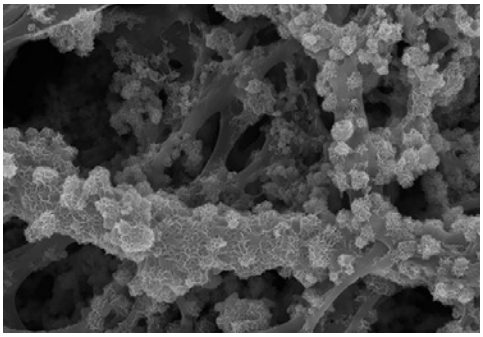
Photosynthetic bacteria with modified light-harvesting antenna show dramatic color changes used in Himadri Pakrasi's research.

"Researchers have learned that science moves faster when you compartmentalize efforts that feed into a much larger collaboration."

Picking up the Pace

Although large collaborative efforts weren't common when Pakrasi led EMSL's grand challenge, team-building approaches are more familiar to researchers coming up the ranks today.

"It used to be possible – for better or worse – for people to do good science in an ivory tower. But it's no longer possible due to the division of expertise, how fast the technology moves and extremely large datasets," said Michelle O'Malley, an assistant professor of chemical engineering at the University of California, Santa Barbara. "Researchers have learned that science moves faster when you compartmentalize efforts that feed into a much larger collaboration," she added.



Scanning electron microscopy image of manganese oxide minerals coating fungal hyphae used in Colleen Hansel's research.

O'Malley was already leveraging an Early Career Award from the DOE when the EMSL-DOE JGI joint call went out. She collaborated with scientists at Argonne National Laboratory and the National Renewable Energy Lab to study how microbial enzymes break down plant fiber in the rumen of cows. Then EMSL-DOE JGI accepted her proposal to search for powerful new enzymes made by fungi found in the gut of other herbivores (think: sheep, elephants and giraffes) that are also really good at processing tough, woody cellulose into sugars that can later become alcohol-containing biofuels.

With the combined resources of EMSL and DOE JGI, O'Malley reported they've identified more than 300 novel enzymes from just one gut fungus. Once they figure out which enzymes are the most efficient, the goal is to produce these enzymes at industrial scale to turn biomass into biofuels. Then they'll use this understanding to metabolically re-engineer the behavior of anaerobic fungi.

"In this age of sequestration it's harder for young scientists to succeed. It can be intimidating," O'Malley said. "Getting 'into the fold' is hard, but linking up with the DOE has made that possible."

Banding Together

"Connections" may be one of the words most frequently used by scientists when they talk about working on these large research campaigns.

Colleen Hansel, an associate scientist of marine chemistry and geochemistry at the Woods Hole Oceanographic Institution in Massachusetts, or WHOI, was already hooked into the EMSL network after working on other mineral-based projects with microscopy expert Alice Dohnalkova. When EMSL issued the 2013 joint call, David Hoyt, EMSL scientist, contacted Hansel about expanding her research to other facilities in the national lab.

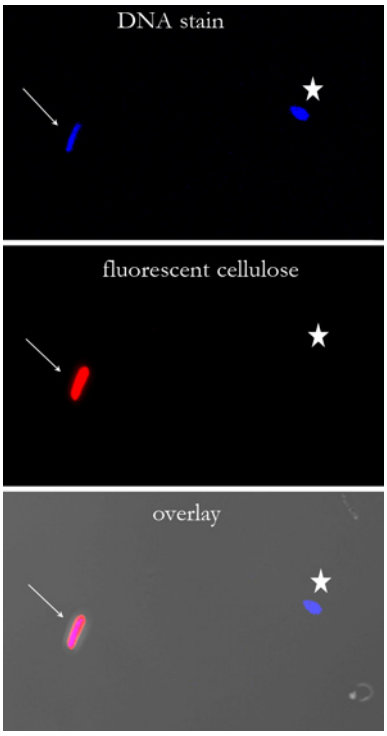
Now Hansel has teamed up with EMSL, DOE JGI, colleagues in her WHOI lab and at the Smithsonian Institute, to study how *Ascomycetes* fungi can cycle and degrade 'recalcitrant carbon' – so called for its resistance to enzymatic breakdown. The fungi can oxidize manganese to form manganese oxides, a mineral that's one of the strongest natural oxidants on our planet. This mineral also possesses the ability to oxidize and degrade carbon. So, indirectly, *Ascomycetes* can play an important role in carbon cycling.

With sequenced fungal genomes from the DOE JGI collaboration, Hansel's group is querying proteomic and

metabolomic data acquired at EMSL to identify the biochemical pathways these fungi use to degrade carbon indirectly through the production of both manganese oxides and reactive oxygen species, or ROS.

One year into the 18-month timeframe of this research campaign, they have draft genomes of two fungi of interest and a host of proteome samples analyzed. With new *in situ* mass spectrometer imaging techniques they've also discovered that manganese oxide and ROS generation varies by fungal interactions. Eventually, they aim to have the proteomes and genomes of six to eight fungal species grown in the presence of different carbon sources and ecological conditions.

"Working in these joint campaigns is different from collaborations among academic institutions," said Hansel. "In the academic world, projects tend to get divvied up, and you try to bring it all back together at the end. In this case, we're all working on one problem together, which requires constant coordination and communication."



Certain bacterial cells, detected by the DNA-specific fluorescent probe (Hoecsht, blue), can become associated or internalize fluorescent cellulose (Alexa 546, red), as determined by the colocalization of the two dyes (magenta, arrow). Other bacteria l cells remain unassociated with the cellulose (star).

Key Communications

It's no surprise that good communication skills are critical to making—and keeping—collaborations effective. But, as Wiley understood, those skills are also essential to foster those partnerships in the first place.

No one knows that better than Kirsten Hofmockel, a biogeochemist at Iowa State University. She's a veteran of simultaneous collaborations with other national laboratories, including a 4-year carbon cycling grant shared between DOE research facilities, NASA and the USDA. But she'd never met anyone from EMSL until a chance meeting at a conference led to an introduction to Nancy Hess, Science Theme lead for EMSL's Terrestrial and Subsurface Ecosystems Science Theme.

> ***"It's a big challenge to do open science. But it creates new opportunities to connect and do bigger science."***

Hofmockel credits Hess with having the communication and collaborative skills to parlay their meeting into a scientific partnership. "She [Nancy Hess] 'got' my science and was clearly able to communicate with me," Hofmockel said. "That's not native to a lot of us. We're scientists and we – myself included – don't always have great communication skills."

Through further discussions Hofmockel learned that EMSL's unique fluorescent cell-sorting technology might help her studies on carbon cycling in the microbial communities of soil where crops are grown for biofuels. These are important because they churn out the enzymes that digest plant cellulose, which then affects how much carbon and nitrogen stay stored in the dirt or become available for cycling into the atmosphere.

Now, Hofmockel and her colleagues are coaxing microbes to eat cellulose labelled with fluorescent crystals. Then, with EMSL's cell sorter, they'll pick out which soil microbes make cellulose-digesting enzymes under varying crop and soil conditions. At the same time, with metatranscriptome capabilities from DOE JGI, they'll parse which soil organisms directly digest plant fiber from ones making enzymes that indirectly contribute to the process. In biofuel reactors, only one or two microbes are used, but Hofmockel's research may show that microbial communities are more effective.

Big Science

For Hofmockel, the teamwork approach is changing the way she's doing science on all of her research projects. Her increasing familiarity with EMSL's technology, and the kinds of science questions that national laboratories want answered, has helped her find opportunities to make datasets available for colleagues that want to pursue scientific questions outside of her domain.

"Many of the fundamental questions we are asking are applicable to other projects on carbon cycling. Microbes in ruminant guts could be using enzyme pathways similar to soil microbes. So an investment in one experiment can blossom into many others," Hofmockel said. "It's a big challenge to do open science. But it creates new opportunities to connect and do bigger science."

That sounds like what Dr. Wiley planned about all those years ago. ■

Elizabeth Devitt is a science journalist and freelance writer.

DEVELOPING BETTER BIOMASS FEEDSTOCK

Researchers collect samples of mutant poplars to undergo multi-omics analysis to determine if the genetic changes affect other pathways and functions in the tree.

Biomass holds great promise as a fuel source to generate renewable energy to help the United States achieve energy independence. Kim Hixson is applying what she's learned from a lowly weed to bioengineer better biomass feedstock.

Kim Hixson

Hixson, an EMSL senior research scientist, is collaborating with Norman Lewis, a regents professor and director of the Institute of Biological Chemistry at Washington State University in Pullman. Together they are using EMSL's multi-omics capabilities to better understand how manipulating the genes in one plant can be applied to other plants to improve their potential as biofuel and biochemical feedstock.

"Our research is hypothesis driven, but there's also a lot of discovery," says Hixson. "The more we study biology, the more we see how interconnected things are in nature."

More Than a Weed

Central to this research is *Arabidopsis*, a model plant system. A small flowering plant related to cabbage, *Arabidopsis* makes for an ideal plant model. Its genome has been sequenced and is easy to genetically modify. Hixson calls it the "lab rat of the plant world."

Arabidopsis has a six-member isoenzyme family of arogenate dehydratases, or ADTs. These enzymes are involved in the catalytic reactions that turn arogenic acid, a metabolite, into phenylalanine, an essential metabolite which is incorporated directly into proteins or is further modified into other chemicals such as flavonoids, coumarins, anthocyanins and lignin.

Hixson's research found hundreds of different changes occurring in the plant due to the modifications in the ADT composition. The collaborators at WSU discovered that out of the six ADTs in *Arabidopsis*, five ADTs are seemingly linked to the production of phenylalanine utilized in the phenylpropanoid pathway, which is involved in lignin production. Lignin gives plants their recalcitrance; it's hydrophobic and difficult to degrade. Lignin is the structural material that makes the sugars in plants difficult to extract when making biofuels.

"It is well known that a significant amount of the carbon dioxide that *Arabidopsis* fixes goes into the phenylpropanoid pathway and ultimately ends up as lignin," says Hixson. "This is very important from the perspective of turning plant material into biofuel."

Hixson's *Arabidopsis* studies earned her an American Chemical Society Withycombe-Charalambous Graduate Student Symposium Award. At the symposium she presented some of her findings from the multi-omics analysis of the gene knockouts conducted at EMSL. The researchers analyzed several knockout mutants of ADTs, including single, double, triple and quadruple knockout

Scientists are studying poplars, a deciduous tree native to the Northern Hemisphere, as a possible biomass feedstock.

mutants, with each mutant strain producing varying degrees of lignin reduction. They found that knocking out multiple ADTs and specific ADTs leads to a measured reduction of lignin in the plants.

By knocking out different combinations of the ADT-related genes, the researchers produced plants with various levels of lignin. In the most extreme case where they knocked out four ADT-related genes, the plant was unable to hold its own weight and became vine-like.

"We knew there were a lot of changes going on in this plant, but we didn't know at the molecular level what those changes were," says Hixson. "The questions about what pathways are being changed and what potential points of regulation are being up-regulated or repressed are precisely what transcriptomics coupled with proteomics can answer."

Other findings from Hixson's research showed knocking out ADT genes alters the photosynthesis machinery and pathways in the mutant plants. For reasons not completely understood, knocking out ADT genes causes the mutant plant systems to produce more photosynthetic machinery, potentially fixing more carbon, but an overall increase in plant mass was not observed. Using transcriptomics and proteomics techniques at EMSL, the researchers were able to look at the other pathways and genes that were changed in the mutant plants. They found the photorespiration pathways were also up-regulated. While more carbon was potentially being fixed, more of it was likely being lost or released back into the atmosphere through the photorespiration pathways.

***Arabidopsis* is a small flowering plant related to cabbage and a model organism used to research plant biology. The plant on the top is wild-type *Arabidopsis* at five weeks. The plant on the bottom is *Arabidopsis* at five weeks with ADT-related genes knocked out, reducing the levels of lignin.**

"This is potentially a very useful discovery," says Hixson. "In future bioengineering attempts we may need to incorporate strategies to counteract carbon loss via photorespiration which would potentially improve the rates of biomass growth in ADT-altered plants used for biofuels or biochemicals."

Applying Their Findings to Poplars

The research has developed several lines of mutant *Arabidopsis* by altering the composition of the ADT genes, which ultimately decreases the amount of lignin these plants produce. Questions arise about how much ADT can be lessened and thus how much lignin can be reduced before a plant in a real world setting shows detrimental growth affects. Additionally it is important to understand how these changes alter other pathways and other systems within the plant, and how the changes are altering the plant system as a whole.

"These are really important questions, not so much in *Arabidopsis*, which is just a little weed," says Hixson. "But we've

Red alder is a deciduous broadleaf tree native to western North America that holds promise as a source for biomass.

started to incorporate some of the same knockouts into poplar trees, which show good potential as a biofuel feedstock."

Poplar trees are native to the Pacific Northwest and widely used as a feedstock in the paper industry. The Department of Energy is interested in the poplar as a biofuel. Within the missions of EMSL and the DOE Office of Biological and Environmental Research is a charge to reduce the United States' dependence on foreign oil and to develop technology for alternative fuel and chemical options.

Hixson hopes the manipulations in the *Arabidopsis* translate to other plants, such as poplars. Poplar has a larger and more complex genome than *Arabidopsis*. She will test the altered poplars at EMSL with multi-omics analysis to see how the transcriptome and proteome changes and if she sees the same types of response in the tree as she saw in the *Arabidopsis*.

"Our end goal is to gather enough information throughout multi-omics evaluations to be able to bioengineer the ideal biofuel and biochemical feedstock."

"I expect a lot of things are going to be similar between the two plants," Hixson says. "But they are different systems and it will be interesting to see the changes in the poplar compared to the *Arabidopsis* at the molecular level."

The researchers have incorporated the ADT knockouts into poplar trees to test if the amount of lignin can be reduced and how far it can be reduced without damaging effects to the tree as a whole. Hixson recently collected samples of the mutant poplars from a test plot and greenhouse in western Washington. She will use EMSL's multi-omics capabilities to determine if a change to one pathway affects other pathways and functions in the tree. According to Hixson, proteomics and transcriptomics identity what genes are being affected, either positively or negatively. This information will be useful when bioengineering poplars as a feedstock. The data will also be incorporated into her dissertation for her doctorate in molecular plant sciences from WSU.

Other Proposals: Where few Have Gone Before

The study with the poplar trees is an approved EMSL user project. Lewis is the principal investigator and Hixson is a collaborator. Lewis is also Hixson's faculty advisor.

Hixson and Lewis have several research proposals they are hoping get approved. In collaboration with Mary Lipton, an integrative omics scientist at Pacific Northwest National Laboratory, and other scientists, they submitted a proposal to NASA. In this study several of the mutant *Arabidopsis* would be sent into outer space to test what happens to reduced-lignin plants in a microgravity environment.

"I really hope NASA approves it," Hixson says. "The findings could be very interesting."

In another submission, this one in response to an EMSL internal call, Hixson and Lewis are proposing to study red alder trees as an ideal biofuel source. A red alder grows almost as fast and dense as a poplar, but it forms specialized symbiotic relationships in its root system. These symbiotic relationships produce root nodules which can fix nitrogen, allowing red alders to thrive without added fertilizer and grow on marginal lands. Hixson believes red alder has the potential to be a highly valuable source for biomass feedstock or other wood-based materials.

For this study, they will apply what they learned from the *Arabidopsis* and poplar research. The proposal includes a full genetic characterization of the red alder and a multi-omics study of the tree's association with two ubiquitous root symbionts.

"Our end goal is to gather enough information throughout multi-omics evaluations to be able to bioengineer the ideal biofuel and biochemical feedstock," says Hixson. "We're not there yet, but we're working on it." ■

SCIENCE HIGHLIGHTS

Clouds up Close

Small-scale cloud processes improve projections

Predicting the types of clouds over the ocean is critical for climate projections. However, current climate models lack the spatial resolution necessary to accurately characterize low-altitude marine clouds and the physical processes that affect them. This study examines the impact of low spatial resolution on modeling the transition from stratocumulus clouds to cumulus clouds.

Using EMSL computing resources the study shows that current climate models lacking high spatial resolution are biased toward accelerating the transition from stratocumulus clouds to cumulus clouds. The findings could lead to more accurate climate projections and the development and implementation of better-informed policies related to climate change.

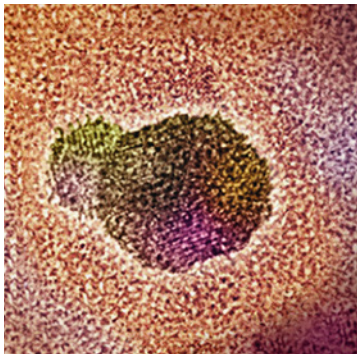
Funding: This research was supported by a U.S. Department of Energy Biological and Environmental Research Early Career grant award and the DOE Earth System Modeling Program.

Publication: Xiao, H., W Gustafson Jr. and H Wang 2014. "Impact of subgrid-scale radiative heating variability on the stratocumulus-to-trade cumulus transition in climate models." *J. Geophys. Res. Atmos.* DOI:10.1002/2013JD020999.

Participating Organization: PNNL

Improving Catalysts

Better bimetallic catalysts for fuel and chemical industries



Nanocatalysts consisting of two metals can offer superior performance compared with those made up of only one metal, so they are widely used for industrial processes that generate fuels and chemicals from natural gas, coal or plant biomass. However, complex interactions between the two metals during catalytic reactions can lower catalytic efficiency. This study addresses this issue by directly observing the changes of platinum-cobalt nanoparticles in operating conditions. Such particles are used as catalysts to convert carbon dioxide and hydrogen into long-chain carbon fuels and are important to the operation of low-temperature fuel cells.

The new insights on the transformations of multiple component catalysts gained from using environmental transmission electron microscopy, a specialized instrument housed in the Quiet Wing, will allow researchers to optimally design similar catalysts to improve their performance, extend their lifetime, and reduce their environmental impact. Moreover, this research could guide efforts to minimize the use of precious metal components such as platinum and therefore reduce the cost of catalysts and lead to a more economical product for consumers.

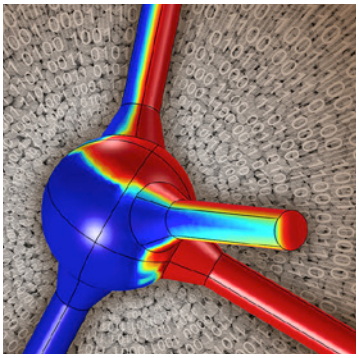
Funding: This research was supported by DOE's Office of Science and the Office of Basic Energy Sciences' Chemical Science Division, as well as the Chemical Imaging Initiative at Pacific Northwest National Laboratory through the Laboratory Directed Research and Development Programs at PNNL and Lawrence Berkeley National Laboratory.

Publication: Xin, H, S Alayoglu, R Tao, A Genc, C Wang, L Kovarik, E Stach, L Wang, M Salmeron, G Somorjai, and H Zheng. 2014. "Revealing the atomic restructuring of Pt–Co nanoparticles." *Nano Lett*. DOI: 10.1021/nl500553a.

Participating Organizations: LBNL, EMSL, PNNL, Brookhaven National Laboratory and FEI Company.

Pore Challenge

Research hones pore-scale models



The physical and chemical processes that occur at the scale of individual soil particles dictate the way fluids flow underground over much larger scales. To more accurately predict how plumes of subsurface fluids, such as those harboring contaminants, will spread underground, scientists design numerical models that simulate flow at the pore scale. However, linking these numerical models to tangible experimental data has been challenging. This study is the first of three responses to a challenge given to the pore-scale modeling community in 2011 to create models that more accurately predict subsurface flow.

Numerical simulations are required not only to model the way fluids move at the pore, or micron, scale, but also to extrapolate up to areas more expansive by several orders of magnitude, such as CO_2 sequestration sites, oil and gas reservoirs, or contaminated mining or nuclear disposal sites. This study allowed scientists from multiple institutions to hone their models on experimental data produced in EMSL's microfluidics laboratory, thus improving the predictive power of such models.

Funding: This research was supported by the DOE Offices of Biological and Environmental Research and Basic Energy Sciences, as well as by Laboratory-Directed Research and Development.

Publication: Oostrom, M, Y Mehmani, P Romero-Gomez, Y Tang, H Liu, H Yoon, Q Kang, V Joekar-Niasar, M Balhoff, T Dewers, T, G Tartakovsky, E Leist, N Hess, W Perkins, C Rakowski, M Richmond, J Serkowski, C Werth, A Valocchi, T Wietsma and C Zhang. 2014. "Pore-scale and continuum simulations of solute transport micromodel benchmark experiments." *Computational Geosciences*, DOI: 10.1007/s10596-014-9424-0.

Participating Organizations: EMSL; Los Alamos National Laboratory; University of Illinois at Urbana-Champaign; University of Texas, Austin; Sandia National Laboratory; Shell Global Solutions, Rijswijk, The Netherlands; and University of Strathclyde, Glasgow, Scotland.

Microbial Communication

Interpretation will crack the microbial language code

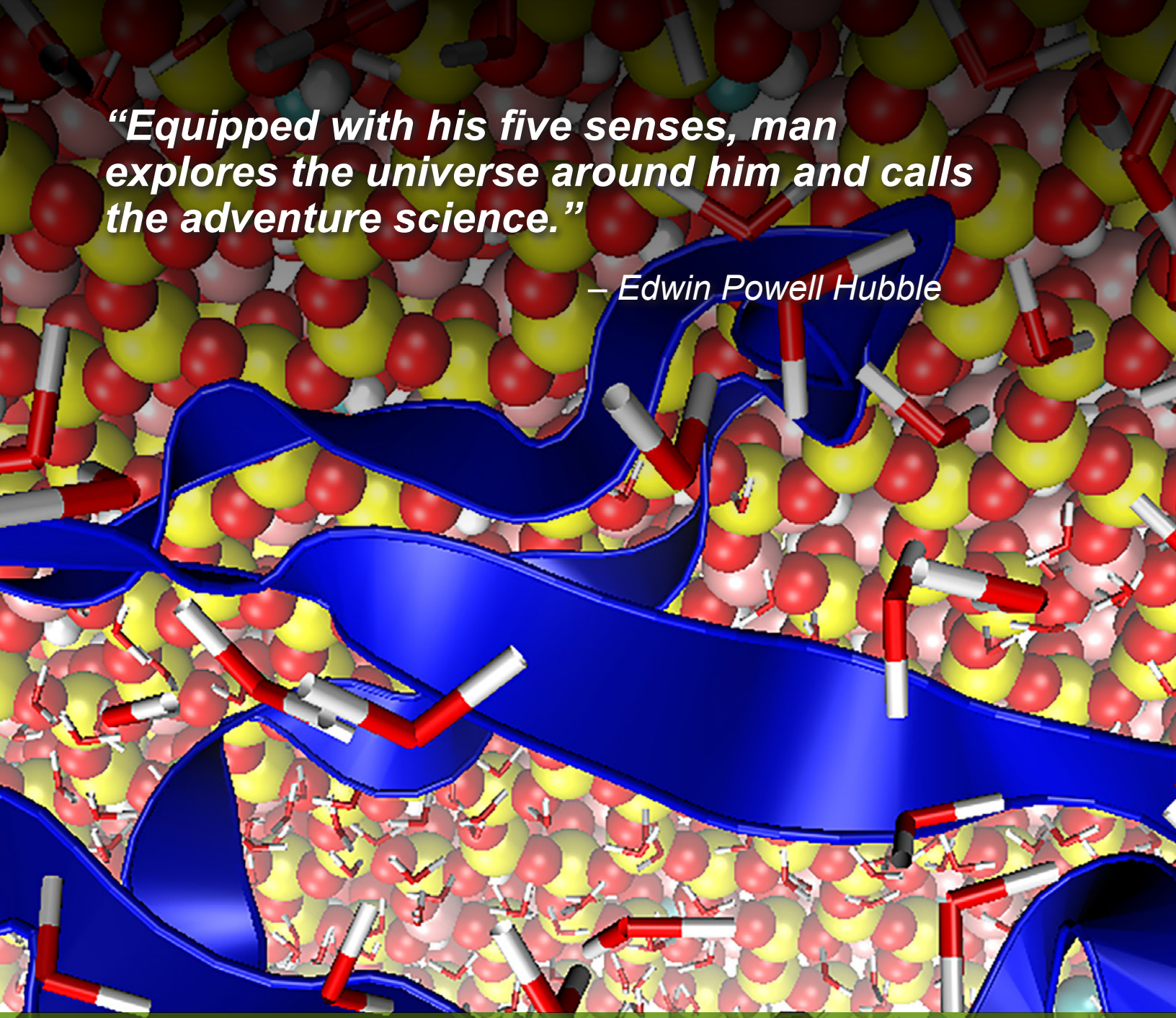
In the environment, microbes often communicate with each other using small molecules. Ribosomally synthesized and post-translationally modified peptides produced by microbes represent a class of metabolites that are ecologically important and potentially involved in microbial communication. Currently, there is a need for more automated computational tools that not only predict outcomes based on microbial genome sequences, but also connect that information to knowledge about the chemical properties of microbial metabolites. This study introduces the first genome-mining tool that automates both the prediction and connection steps for modified-peptide discovery.

The new open-access genome-mining tool, known as RiPPquest, can search mass spectrometry databases to identify and discover these microbial peptides. By combining genomics and proteomics, the automated computational tool will help scientists translate the chemical language of microbes into biological function. A portion of this research was performed using high-resolution mass spectrometry resources at EMSL.

Funding: This research was supported by the DOE Biological and Environmental Research Division through the Subsurface Biogeo-chemical Research Program Science Focus Area at Pacific Northwest National Laboratory.

Publication: Mohimani, H, R Kersten, W Liu, M Wang, S Purvine, S Wu, H Brewer, L Pasa-Tolic, N Bandeira, B Moore, P Pevzner and P Dorrestein. 2014. "Automated Genome Mining of Ribosomal Peptide Natural Products." *ACS Chem. Biol.* DOI: 10.1021/cb500199h.

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



"Equipped with his five senses, man explores the universe around him and calls the adventure science."

– Edwin Powell Hubble

About this Art

Proteins from microorganisms in the soil can bind to mineral surfaces. Scientists hypothesize soil organic carbon, or SOC, molecules can bind to minerals to stabilize carbon in soil. However, the modes of interaction between SOC molecules and mineral surfaces are largely unknown. To elucidate these interactions, scientists at EMSL are performing large-scale atomistic simulations with classical molecular dynamics on EMSL's Cascade supercomputer in tandem with nuclear magnetic resonance spectroscopy. This image shows protein 1gb1 (blue ribbon) adsorbed to the surface of montmorillonite clay (red, gold, white, pink and cyan balls) and solvated by water with solvated sodium and calcium ions.

This work is being performed as part of an internal EMSL research project entitled "Understanding molecular-scale complexity and interactions of soil organic matter." The computational part of the project is being led by Amity Andersen from EMSL. The other team members are Niranjan Govind, Nancy Washton, Patrick Reardon, Sarah Burton and Andrew Lipton, all from EMSL; Nikolla P. Qafoku, from PNNL; and Stephany Chaconan and Markus Kleber, both from Oregon State University, Corvallis.