EMSL

THE MOLECULAR BOND

SCIENTIFIC INNOVATION THROUGH INTEGRATION

JUNE 2014

THE SECRET LIFE OF AEROSOLS

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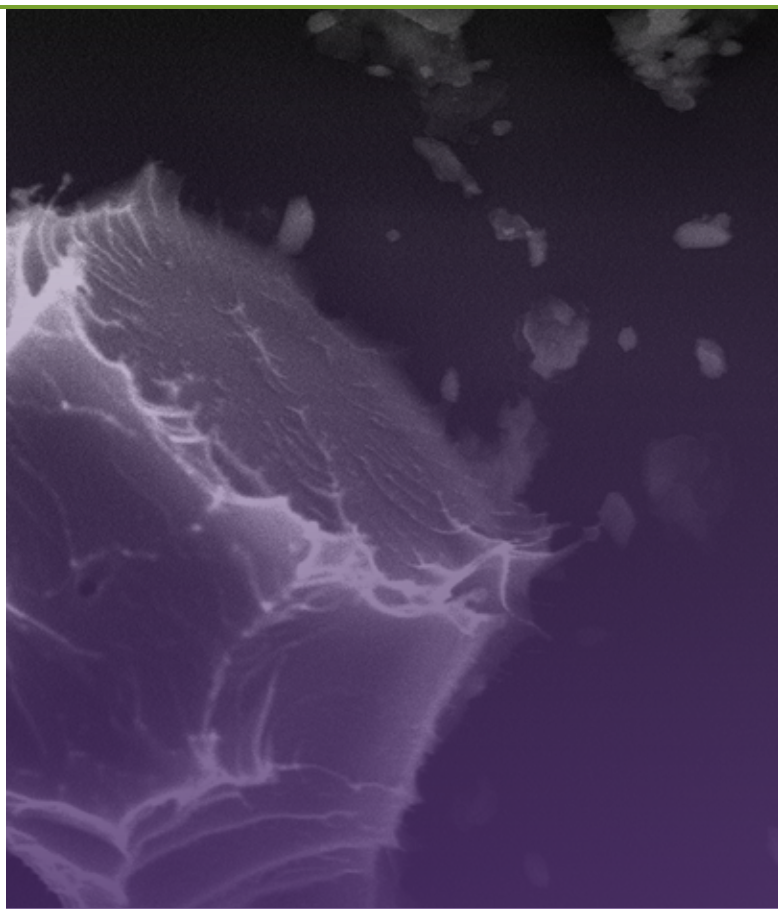
About the Cover

Atmospheric aerosols play an important role in cloud formation. Understanding the creation and lifecycle of aerosol particles and their role in cloud formation is central to improving climate models. Sophisticated instruments, including many available at EMSL, provide scientists with new information about how aerosols form. But a better understanding about the chemical transformations that create aerosols is needed.

The cover shows an environmental scanning electron microscopy image of an ice crystal nucleated at minus 37 C over a sample of mineral dust particles imaged in-situ using an experimental platform being developed by Bingbing Wang, an EMSL postdoc, to visualize ice nucleation. *(A non-colorized image of this ice crystal is shown on page 7. This image is colorized.)*



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 emslcom@pnnl.gov

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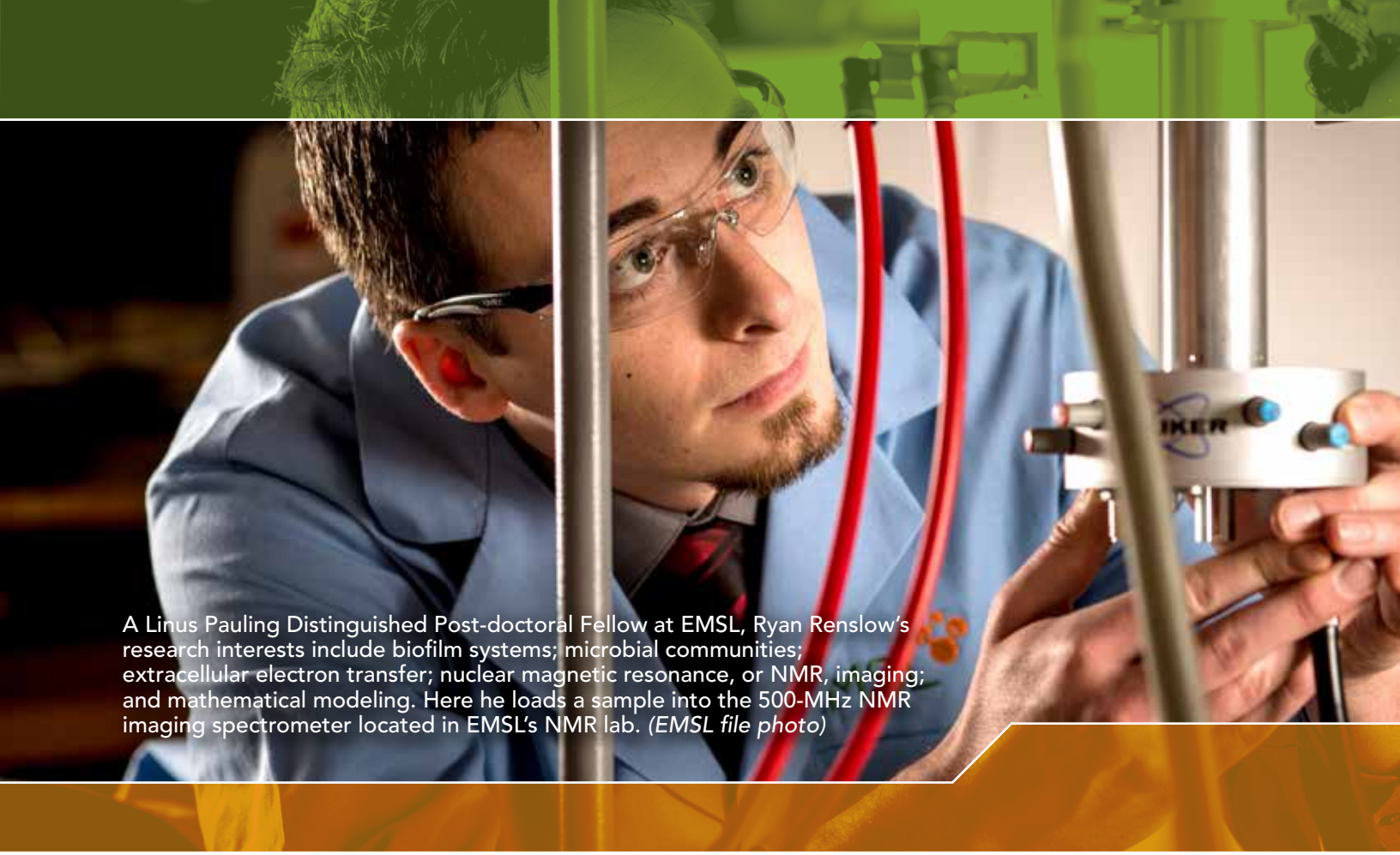

A Linus Pauling Distinguished Post-doctoral Fellow at EMSL, Ryan Renslow's research interests include biofilm systems; microbial communities; extracellular electron transfer; nuclear magnetic resonance, or NMR, imaging; and mathematical modeling. Here he loads a sample into the 500-MHz NMR imaging spectrometer located in EMSL's NMR lab. *(EMSL file photo)*

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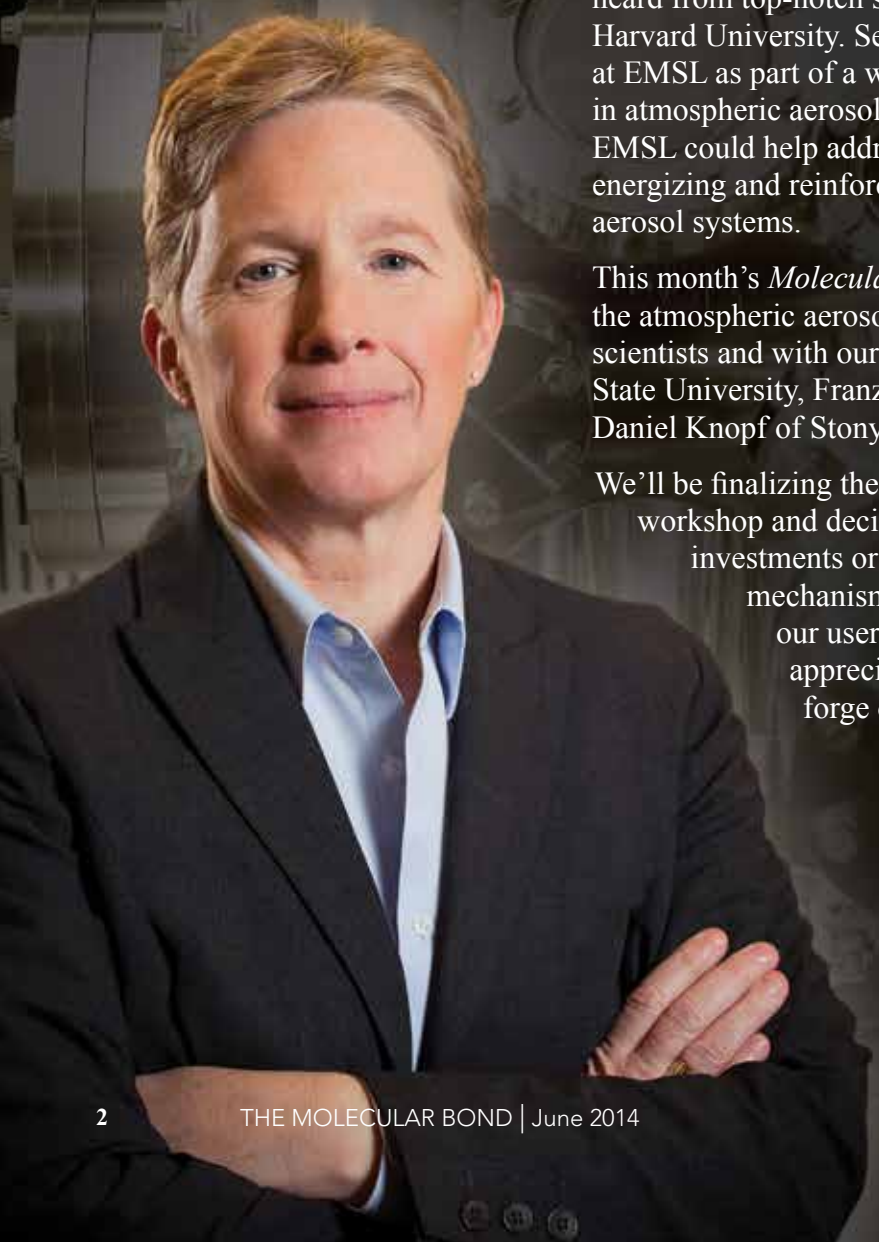
FROM THE DIRECTOR

Allison Campbell



It's been exciting to watch EMSL's Atmospheric Aerosol Systems Science Theme grow over the last two years. We created this new science theme area after building a critical mass of experts, facilities and instrumentation we knew could help advance climate science and we knew the community needed.

Last month, we held our annual user meeting. This year's theme was the Science of Atmospheric Organics. Nearly 100 attendees heard from top-notch scientists, including Scot Martin of Harvard University. Several of the speakers spent an extra day at EMSL as part of a workshop to discuss the critical challenges in atmospheric aerosol systems over the next 10 years and how EMSL could help address those challenges. The dialogue was energizing and reinforced EMSL's vision for atmospheric aerosol systems.

This month's *Molecular Bond* cover story focuses on some of the atmospheric aerosol research going on at EMSL – by our scientists and with our users, including Peter Buseck of Arizona State University, Franz Geiger of Northwestern University and Daniel Knopf of Stony Brook University, among others.

We'll be finalizing the recommendations elicited during the workshop and deciding how we want to follow up, through investments or new programs. These workshops are one mechanism for soliciting the input and expertise of our users and the broader community. We appreciate their time and energy in helping us forge our new vision.

—Allison

Designed for the study of biological samples at high-resolution, the liquid helium cryogenic transmission electron microscope, or LHe cryo-TEM, is housed in EMSL's Quiet Wing. The superior stability and specimen preservation capabilities of the LHe cryo-TEM create an optimal high-resolution imaging platform for biological samples such as two-dimensional protein crystals and single particles. The only one of its kind currently operational within the United States, the LHe cryo-TEM is one of the instruments available through EMSL's Special Science Call for Proposals. *(EMSL file photo)*

NEWS & KUDOS

Special Science Call for Proposals Continues

EMSL's Special Science Call for Proposals is open until Sept. 15 for high-impact research that advances the Department of Energy's Office of Biological & 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

More information about this call is available at **http://www.emsl.pnnl.gov/access/calls/2014/science_theme.jsp**

Jansson Named EMSL Director for Plant Sciences

Christer Jansson

Christer Jansson has been selected as director for Plant Sciences at EMSL. He will lead the development of a vision and strategy for Pacific Northwest National Laboratory and EMSL in plant sciences and bioenergy.

Jansson has been a senior staff scientist and bioenergy program lead at Lawrence Berkeley National Laboratory for the past six years. He has more than 30 years of experience with Department of Energy research programs. His research focuses on bioengineering of plants and cyanobacteria with an emphasis on understanding and exploiting photosynthesis, lipid and carbohydrate metabolism and source-sink interactions.

Viewing Biology in Action

James Evans

EMSL received first-year funding of almost $1M for a pilot program to develop imaging approaches to understand how Department of Energy-relevant microbes sense and respond to their environment on the molecular to cellular scale. The goal of a multi-institutional team led by EMSL Scientist James Evans is to build a general-purpose platform that will generate multi-dimensional imaging data to inform predictive biology through a tight coupling of experimental observations, models and theories.

The pilot program is the result of a proposal to DOE's Office of Biological and Environmental Research to create new technologies to observe the multiple mechanisms cells use for communication and regulation. The research team includes scientists from EMSL, Pacific Northwest National Laboratory, the University of New Mexico and Massachusetts Institute of Technology. This platform will ultimately be made available to BER researchers through the EMSL user program.

The team includes James Evans, Scott Baker, Ryan Kelly, Galya Orr, Ljiljana Paša-Tolić, Steven Wiley and Zihua Zhu (EMSL); Bill Cannon, Ziyu Dai, Matt Marshall and Aaron Wright (PNNL); Diane Lidke and Keith Lidke (UNM); and Mark Bathe (MIT).

EMSL Participates in NUFO's Congressional Science Expo

EMSL joined with other national user facilities in the 4th annual congressional science expo organized by the National User Facility Organization, or NUFO, on June 10 in Washington, D.C.

Kristyn Roscioli, an EMSL postdoctoral research assistant, discusses her joint JGI/EMSL biofuel demonstration with Dan Drell, DOE Biological Systems Science Division program manager.

Representing EMSL with demonstrations were Kristyn Roscioli, a postdoctoral research assistant in EMSL's Mass Spectrometry Group, and EMSL Scientist Arun Devaraj. Also representing EMSL were Director Allison Campbell and User Program Services Manager Terry Law.

Roscioli's exhibit was a collaborative effort by EMSL and the DOE-Joint Genome Institute using "omics" resources to better understand microbial communities for biofuel production. Devaraj's exhibit built onto the omics demonstration to describe how reducing the weight of vehicles through new lightweight alloys of titanium, aluminum and magnesium could improve gas mileage and help reduce carbon dioxide emissions.

Entitled "Science Works for America," the event was hosted by the U.S. House of Representatives' Science and National Labs Caucus. Co-chairs of the caucus include Rep. Chakah Fattah of Pennsylvania, Rep. Randy Hultgren of Illinois, Rep. Ben Ray Lujan of New Mexico and Rep. Alan Nunnelee of Mississippi.

EMSL Expertise Featured in Special Issue of *Proteomics*

A special issue of *Proteomics* journal highlighted EMSL's top down proteomics expertise.

Ljiljana Paša-Tolić, EMSL's lead scientist for mass spectroscopy, co-edited the special issue with Christophe Masselon, CEA Grenoble. Paša-Tolić and Masselon also co-authored the publication's editorial entitled "Shining a spotlight on intact proteins."

Ljiljana Paša-Tolić

Paša-Tolić was a contributor to three of the articles featured in the special issue. Other EMSL scientists co-authoring articles in the journal were Rosalie Chu, Nikola Tolić, Si Wu, Haizhan Zhang (now at Fred Hutchinson Cancer Research Center) and Rui Zhao.

The cover art for the special issue featured the first research project for the Consortium for Top Down Proteomics; the resulting article was co-authored by Wu, Chu, Tolić and Paša-Tolić.

The May 2014 *Proteomics* top down proteomics special edition is volume 14, issue 10, pages 1125-130, DOI: 10.1002/pmic.2014700700.

Baer Receives 2014 ASTM International Award of Merit

Don Baer

ASTM International Board of Directors has selected EMSL's Don Baer to receive the 2014 Award of Merit. The award and its accompanying title of fellow is ASTM's highest organizational recognition for individual contributions to standards activities.

Baer garnered the award "For his exceptional service to ASTM International Committee E42 on Surface Analysis, innovations in the development of standards for surface analysis and development of new information resources for surface analysis." His ASTM activities focused on improving the reliability of the surface sensitive tools important to the success of his research.

A PNNL Laboratory Fellow, Baer is the lead for EMSL's Energy Materials and Processes Science Theme. Baer is internationally known for the application of surface analysis methods to examine behaviors of nanoparticles, corrosion processes and the reactive properties of oxide and mineral surfaces.

ASTM International is a globally recognized leader in the development and delivery of international voluntary consensus standards.

Creating Cascade's Secure Computing Platform

EMSL's supercomputer Cascade before installation included 1,400 commodity servers unpacked and staged for set up.

EMSL's Molecular Science Computing Operations team developed a process to manage and customize high-performance computing operating systems during the setup of the new Cascade supercomputer. The phased process was featured in the cover story in a special high-performance computing issue of *LINUX Journal*.

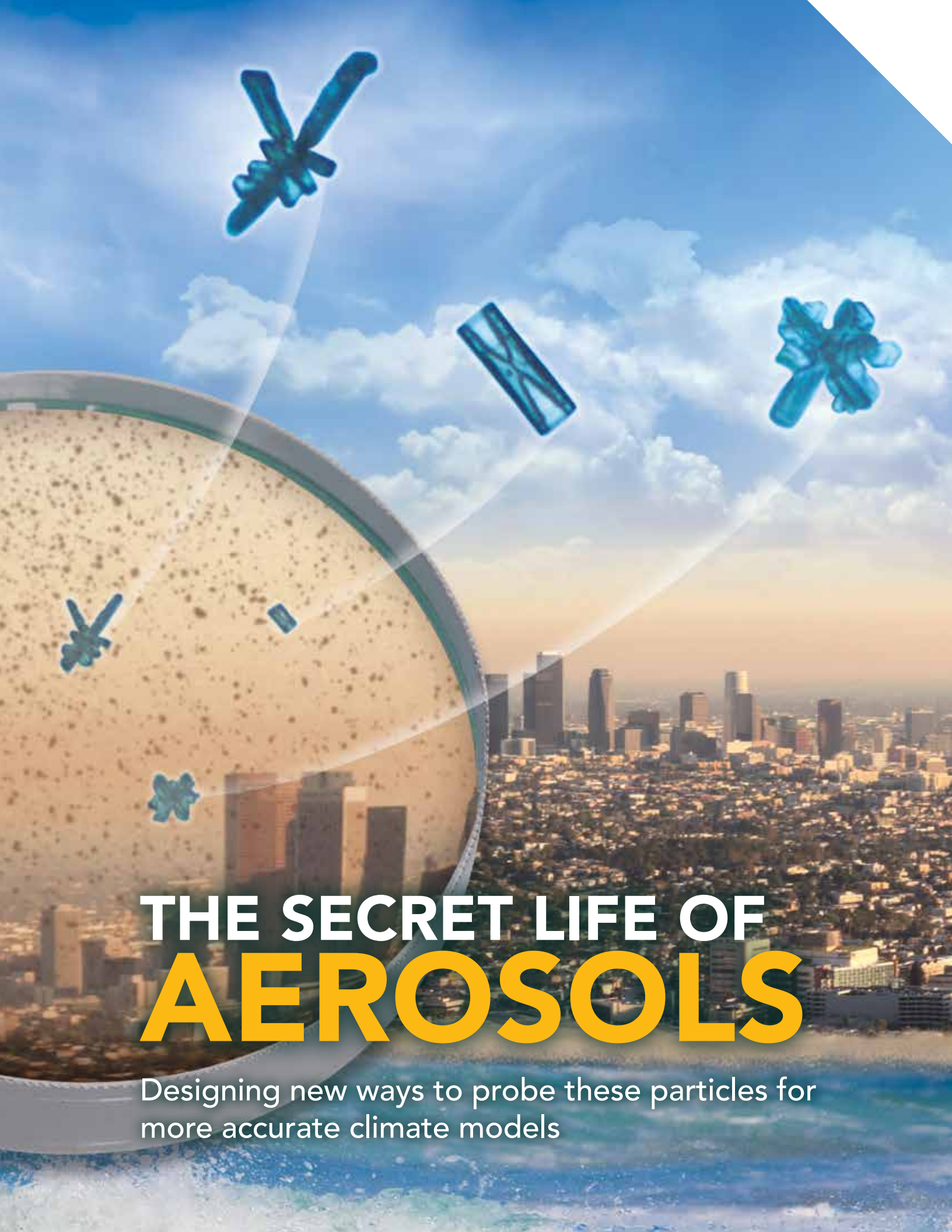
The team's disciplined approach was essential for moving from the old Chinook supercomputer to the new Cascade supercomputer. The MSC Operations team turned 1,400 commodity servers into a secure platform for experimental and high performance computing.

Today, Cascade runs computationally intensive climate and biological simulations and provides experimental and high-performance computing to scientists across the country on environmental and energy challenges through molecular-level theory and experiment.

The article, "A Process for Managing and Customizing HPC Operating Systems" written by David Brown, MSC Operations, appeared in *LINUX Journal*, April 2014.

Watch EMSL's iDirector on YouTube

EMSL Director Allison Campbell interviews Malak Tfaily, a post doc in EMSL's Mass Spectrometry group. Tfaily is EMSL's first postdoctoral researcher funded by the Department of Energy's Office of Biological and Environmental Research Terrestrial Ecosystem Science program. Campbell talked with Tfaily as part of her monthly iDirector interview series available on EMSL's YouTube channel at **www.youtube.com/user/EMSLatPNNL**.



THE SECRET LIFE OF AEROSOLS

Designing new ways to probe these particles for more accurate climate models

Dust storms, volcanic eruptions and hurricanes are tangible events that send particles of sand, soot and salt into the atmosphere. These particles can alter the climate cycles that heat and cool the Earth. Less obvious sources of aerosols affect these cycles, too; the sea salt sprayed off breaking waves or volatile organic compounds emitted from trees. But nearly untraceable chemical transformations also lead to the birth of new atmospheric particles. Accounting for these newborn particles and their role in cloud formation is key to improving climate models. Scientists recently gathered at EMSL to discuss ways to more accurately chronicle the clandestine lives of these aerosols in the lab and the field.

The precise processes that govern how new particles are created out of vapor, then grow and nucleate clouds – enticing other organic molecules into chemical reactions – largely remains a mystery. Increasingly sophisticated instruments provide scientists with new details about these transformations; they also point out big gaps between theoretical models and field findings.

"We discovered nucleation is an important source of atmospheric particles more than 20 years ago. And ever since we've been trying to figure out the chemical and physical processes that lead to their creation," says Peter McMurry, a professor at the University of Minnesota. "The goal is to achieve closure between the rates observed in the atmosphere and those predicted by models. This will lead to more credible climate models. Right now we can't do that."

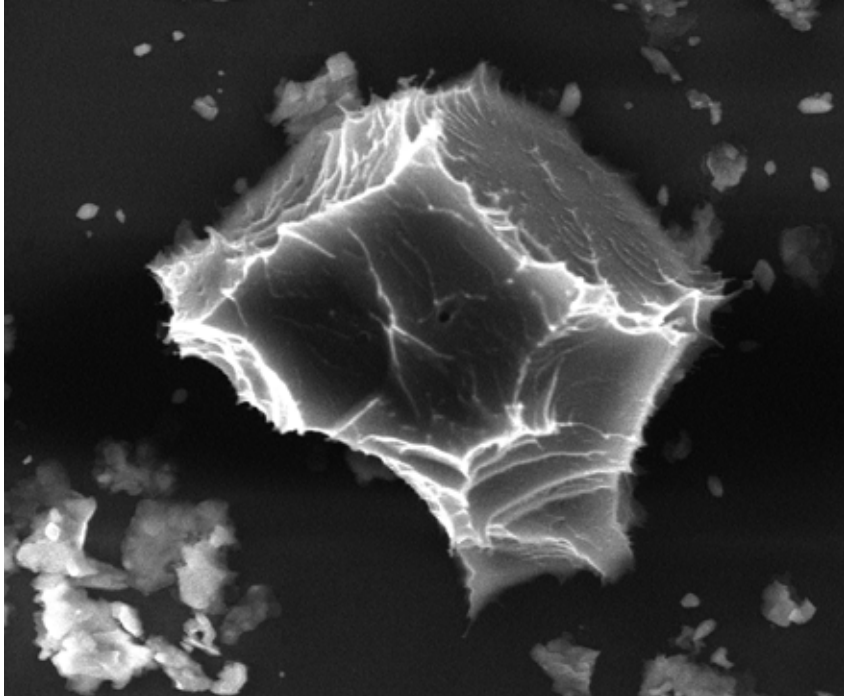
In the Beginning

Part of the problem is catching the particles in the act of doing whatever it is they do. Researchers spend weeks in the field stalking new particle formation events. With little lead time the particles are born. Within a few hours they grow to sizes large enough to serve as cloud condensation nuclei, sending a brief bloom of data across suites of specialized sampling instruments. "It's a challenge," says McMurry. "Some of the species that lead to particle formation are found in almost unimaginably low concentrations. Sometimes it's like trying to pick out one person in a thousand or a million Earths."

From Field to Lab: An Inside Job

For the last 15 years Alexander Laskin, an atmospheric aerosol chemist at EMSL, and collaborators have been using the unique analytical chemistry capabilities of EMSL on particle samples collected from test facilities, laboratory studies and far-flung field sites. A variety of off-line chemical imaging techniques have been advanced at EMSL – including mass spectrometry, spectroscopy, microscopy and microanalysis methods – to probe the composition and properties of these particles. "But there's no single technique in existence that gives us all the information we need to know," says Laskin.

◀ Conceptual artwork illustrating an ice nucleation experimental platform under development by Bingbing Wang, an EMSL postdoctoral researcher.



An environmental scanning electron microscopy image of an ice crystal (center) nucleated at minus 37 C over a sample of mineral dust particles imaged in-situ using an experimental platform being developed by Bingbing Wang, an EMSL postdoctoral researcher, to visualize ice nucleation. *(A colorized version of this image was used on the cover.)*

The ability to run multi-modal analyses on the same sample is a particular strength at EMSL. But even interrogating particles with multiple techniques can't answer some of the pressing questions. So EMSL researchers are devising new strategies in collaboration with scientists across the country.

Laskin and his colleagues want to understand the physical and chemical properties of aerosols that nucleate ice clouds. Although ice nucleation has been studied for more than two decades, much about the process remains unknown.

"But there's no single technique in existence that gives us all the information we need to know."

"In the traditional view of ice nucleation events, there are very few particles in the atmosphere with the right properties to become ice nuclei," says Laskin. "But now there's growing evidence that's not always case," he says. "Particles with mediocre ice nucleation propensity – but

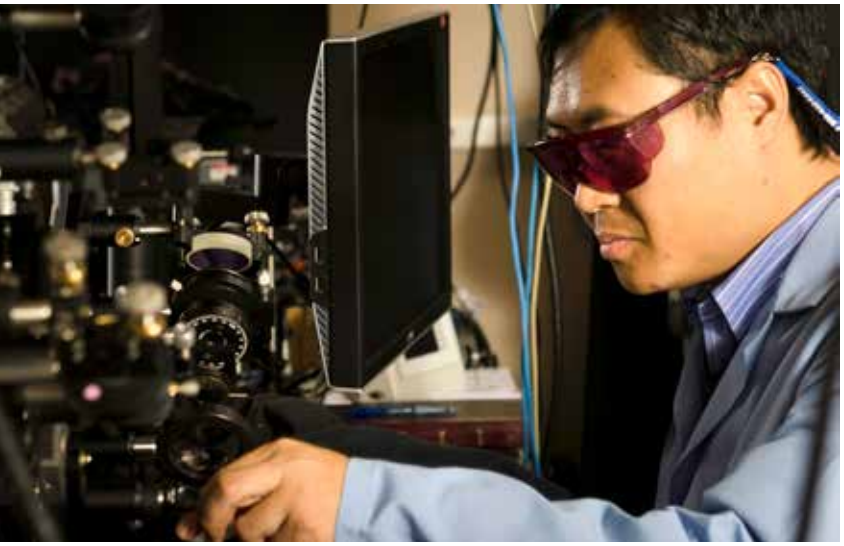
present at high number concentrations – can play an equivalently important role. So the big question is how to delineate the two scenarios: Under which conditions would different nucleation particles prevail?"

It would be easier to figure out if they could visualize nucleation events, says Bingbing Wang, a postdoctoral researcher at EMSL. To see which individual particles nucleate ice first, he started a project coupling ice nucleation experiments with scanning electron microscopy, complemented with particle spectro-microscopy. Then he can probe the composition of the instigating particles. "From that knowledge we can achieve better understanding of heterogeneous ice nucleation. Then with further data analysis we can provide better parameterizations for cloud and climate models," says B. Wang.

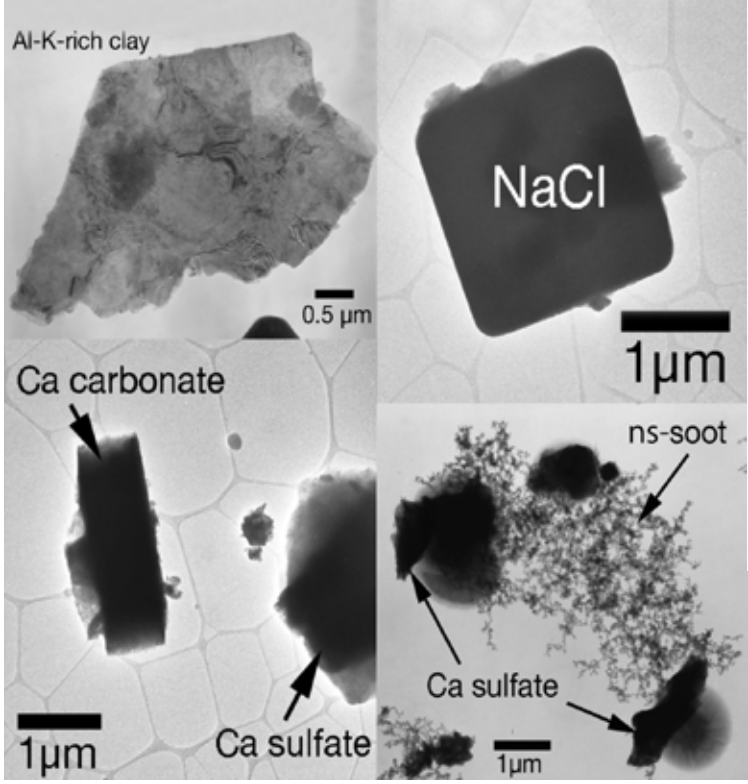
The study involves a group of Pacific Northwest National Laboratory experts in collaboration with Daniel Knopf of Stony Brook University and Mary Gilles at Lawrence Berkeley National Laboratory.

An Outside Approach

Another way to analyze these perplexing particles is to look at them one by one. To accomplish this, transmission electron microscopy, or TEM, is the technique of choice for Peter Buseck, a professor at Arizona State University who attended the recent user meeting at EMSL. "We want to know the intimate details about these aerosol particles," he says. "TEM has been used on a larger scale, but now the technique is needed on a nanometer scale because there's a whole range of particle sizes in the atmosphere."



EMSL Chief Scientist Hongfei Wang studies complex surface interactions using EMSL's high-resolution sum frequency generation spectrometer, or HR-SFG, which he and others developed at EMSL. The HR-SFG is capable of providing greater levels of detail about complex particle structure and reactions on surfaces.



Aerosol particles occur in many shapes and mixing states. These particles were imaged at the electron microscopy facility at Arizona State University at Tempe. *(Images provided by Peter Buseck, Arizona State University)*

Although Buseck already has the TEM capabilities he needs, EMSL could devise novel ways to combine electron microscopy with instruments such as the helium ion microscope in EMSL's Quiet Wing. No one's doing that now with aerosols, says Buseck.

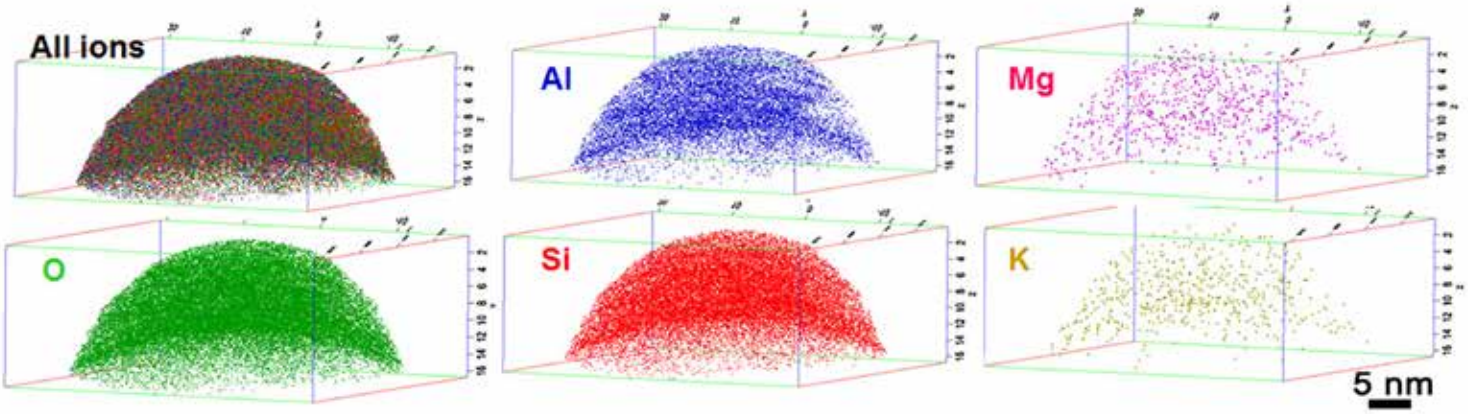
Probing the Surface

It's not just the particles that need to be accounted for.

"An intrinsic scientific problem is how reactions occur and the particle surface is key for those. From mass spectrometry you can find out what kind of molecules are in aerosols, but you don't know how they are arranged on the particle surface," says Hongfei Wang, a chief scientist at EMSL.

To get at the structure of the surface, in 2011 H. Wang and his colleagues developed a unique high-resolution sum frequency generation, or HR-SFG, spectrometer to discern surface particle reactions with a resolution 10 times better than any other instruments out there. That kind of resolution was critical for Sergey Nizkorodov who studies aerosol photochemistry in his laboratory at the University of California at Irvine and then sends samples to H. Wang for high-resolution studies at the surface.

"We want to be able to detect minor species that might be important for controlling reactions," says H. Wang. "We've improved resolution, but the sensitivity of the signal needs to be improved for field measurements. It's possible – but will take at least several years. It will be a real milestone to do this."



This is an atom probe tomography, or APT, analysis result showing the sub-nanoscale elemental distribution within a single aerosol particle. *(Image by Arun Devaraj, EMSL)*

Another pioneer in applying SFG spectroscopy to aerosol particles is Franz Geiger of Northwestern University. After meeting H. Wang at an American Chemical Society conference two years ago, he started using the high-resolution instrument to study alpha-pinene, one of the main components of secondary organic aerosol particles. EMSL's HR-SFG gave Geiger a significant improvement in his analytics, getting resolution from standard values of about 10 wave numbers down to 0.6 wave numbers.

To bridge the gap between particle analysis in the lab and the field, Geiger is working with Northwestern colleague Regan Thomson, Victor Batista of Yale University and Scot Martin at Harvard University on an EMSL user project and with matching funds from Northwestern (and he hopes, the National Science Foundation).

"There's no silver bullet. But more current tools will give us a more complete understanding."

Geiger is focused on the organic emissions of trees, namely pinene, that react with ozone at the ground level. The resulting cascades of reactions create aerosols that can interact with water vapor and ultimately make clouds. The questions he wants to answer are: Will future, possibly warmer, climates lead to faster emission rates of pinene over the Northern hemisphere? And if more organic particles form, potentially leading to more clouds, would this cause a negative feedback mechanism to cool our planet?

The answers to how these particles form will be found on their surfaces, thinks Geiger. But it's hard to analyze what's never been identified before. So the collaborators are creating synthetic compounds they surmise could be created when pinene reacts with ozone and are also surface reactive. By analyzing the chemical signatures of these lab-made components they'll build a reference library to help identify the unknown surface components they discover on these particles.

"There's no silver bullet," says Geiger. "But more current tools will give us a more complete understanding."

Helping Solve Problems

Aerosol research may also get a boost with instruments that haven't traditionally been used for studies in this field. In the past, the tiny sample sizes and filter collection methods for aerosol particles have hampered efforts to use analytic techniques such as nuclear magnetic resonance, or NMR, spectroscopy. But at the recent EMSL user meeting, NMR lead scientist Karl Mueller told researchers they're building smaller and better tools to aid aerosol research.

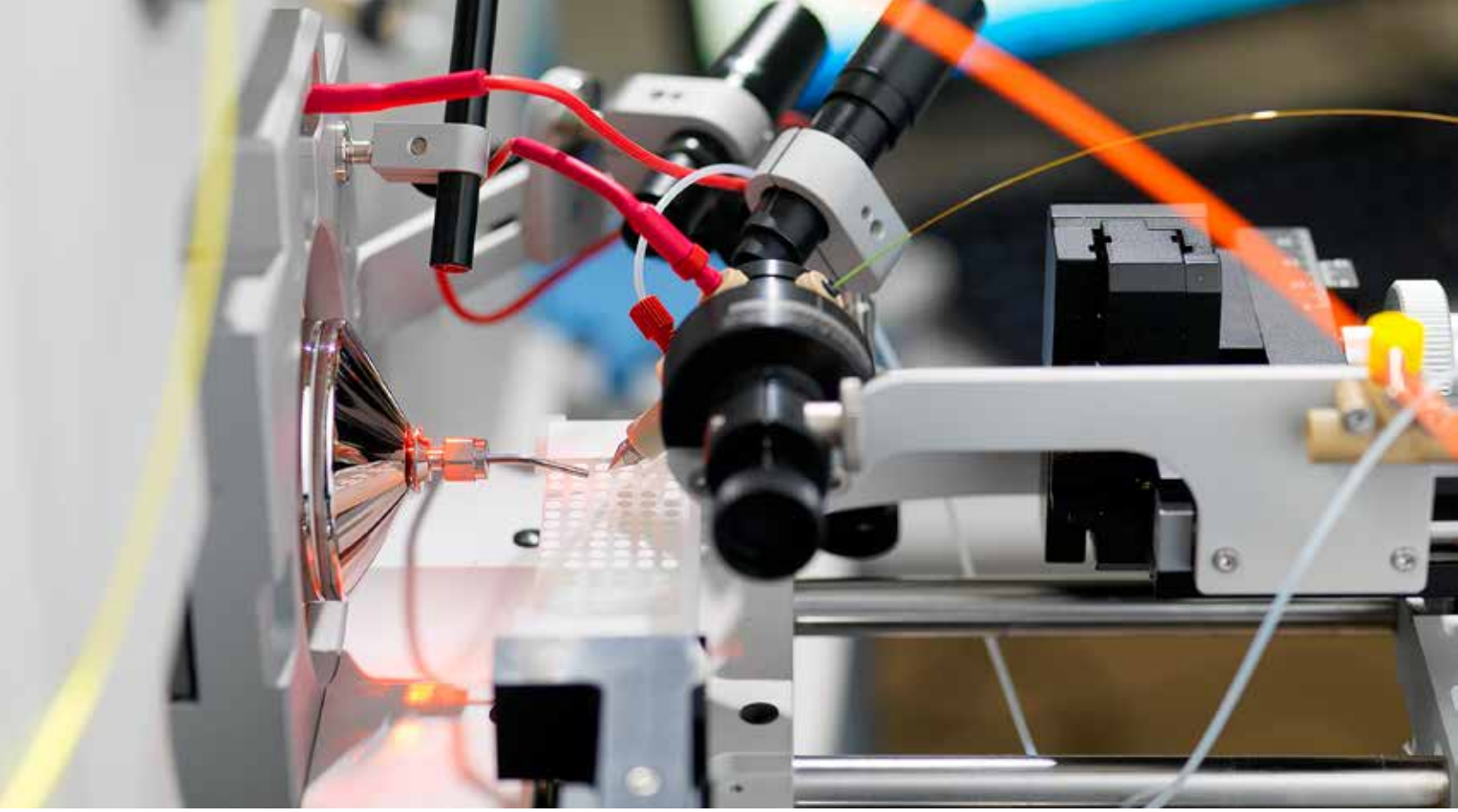
"NMR is phenomenal for determining chemical structure," says Nancy Washton, the capability lead for EMSL's NMR group. "But it's considered an insensitive technique because it requires such a large sample size – I want a vial full of stuff, about 20 milligrams."

Now Mueller and Washton are working with a team of scientists to make very small volume NMR detectors. "We're combining our abilities as 'spin jocks' with miniaturization and microfabrication capabilities to work with picoliter amounts more suitable for aerosol studies. Success here would be a real breakthrough," says Mueller.

Washton anticipates they'll be able to run aerosol samples within the year. The possibilities have already enticed collaborators to send samples and she thinks NMR will be very useful for scientists who are synthetically producing atmospheric molecules.

Another technique that might prove useful is atom probe tomography, or APT. EMSL Scientist Arun Devaraj thinks APT could provide a way to visualize the three-dimensional element distribution within a single aerosol particle at sub-nanometer spatial resolution.

"Even if a potential user doesn't quite know what capabilities they need, the staff at EMSL can discuss their



Researchers detect and characterize the molecular composition of organic constituents in aerosols using EMSL's high-resolution LTQ-Orbitrap mass spectrometer, which is configured for the analysis of environmental and atmospheric aerosol samples. This instrument is an advanced analytical platform that also provides a unique basis for closure studies aimed to reduce the uncertainty associated with the environmental effects of particulate organics in the atmosphere.

needs and provide guidance," says Alex Guenther, the lead scientist for atmospheric aerosol science at EMSL. The staff will make extraordinary efforts to understand what scientists need for their research and how the laboratory's capabilities can be applied to answer their scientific questions, he says.

Although new tools are nice, Nicole Riemer, a computer modeler at Illinois University, thinks researchers may squeeze more information out of the tools already on hand. "As modelers, we are using different tools from the researchers in the lab who measure these things," says Riemer. "But we're trying to solve the same problems."

The aerosols are really, really small. So it's difficult to develop equations that reflect the complexity of those minuscule – but critical – interactions without bogging down the ability to scale up to global proportions. Riemer believes careful, repeated experiments under varied conditions, using the equipment already in EMSL laboratories, can provide key details needed to derive more accurate aerosol predictions. For example, our models are based on particles with spherical shapes, says Riemer. Yet Laskin's work shows particle morphology changes. "Is that important?" she says. "If it is, we need to know how it changes over time so we can incorporate it into our equations."

"If there's a way to get those measurements in real time, that would be a big step forward."

Gathering Better Field Samples

But even the best available laboratory instruments don't really capture the conditions in the atmosphere. So, Guenther invited scientists to brainstorm better ways to get samples from the field. Among the more immediately feasible possibilities discussed were ways to build a better Orbitrap.

"I was excited to hear discussions about making a smaller high-resolution mass spectrometer to carry around in a truck or plane," says Nizkorodov. "If there's a way to get those measurements in real time, that would be a big step forward."

With that kind of innovation, Franz Geiger may one day realize a decades-old research dream: to analyze aerosol particle surfaces without plucking them out of the air. "People once said we couldn't study aerosols from ships or planes and now we do that all the time," he says. "It's not impossible." ■

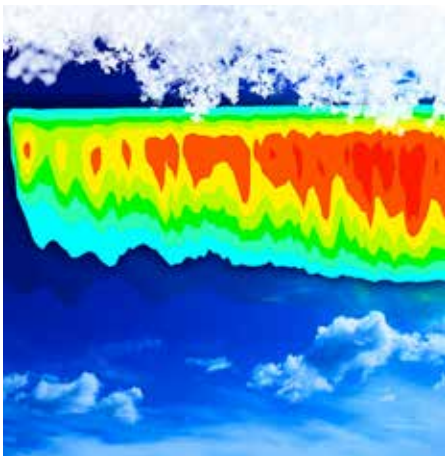
Elizabeth Devitt is a science journalist and freelance writer.

SCIENCE HIGHLIGHTS

Ice Particle Size Matters

Fine-tuning cloud models for improved climate predictions

Arctic clouds play an important role in climate, but different models have produced widely varying predictions about the properties of these clouds. This study using EMSL's supercomputer analyzes simulations of Arctic clouds by 11 different models and identifies the key factor responsible for the variable predictions.



The findings highlight the important role of ice particle size distribution in determining cloud evolution and suggest that adjustments of this parameter in climate models will reduce variability and improve accuracy. By enabling scientists to develop a better understanding of how clouds form and evolve, this study will improve climate predictions.

Funding: This work was supported by the DOE Office of Biological and Environmental Research as part of the Atmospheric System Research program.

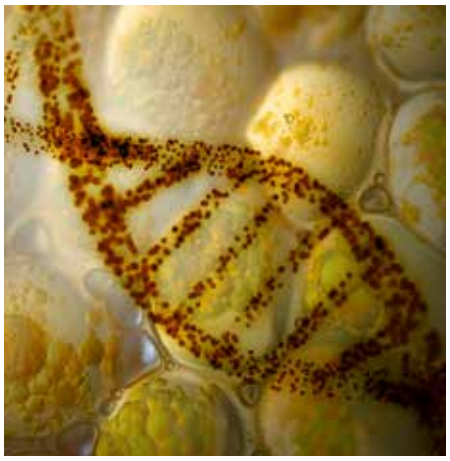
Publication: Ovchinnikov, M, et al. 2014. "Intercomparison of large-eddy simulations of Arctic mixed-phase clouds: Importance of ice size distribution assumptions." *J. Adv. Model. Earth Syst.* 6. DOI: 10.1002/2013MS000282.

Participating Institution: PNNL, NASA, MIT, Pennsylvania State University, Karlsruhe Institute of Technology, Environment Canada, University of Illinois at Urbana-Champaign, National Center for Atmospheric Research, Stockholm University, Met Office, University of Colorado/NOAA and Princeton University.

Bacterial Genes for Stress

Genes controlling cell division allow bacteria to adapt to stressful environmental conditions

Many bacterial species have genes called *mraZ* and *mraW*, which are located in a cluster of genes that regulate cell division and cell wall synthesis. Despite the prevalence of these two genes, little is known about their functions. Researchers using transcriptome analysis and bioinformatics resources at EMSL revealed that *mraZ* and *mraW* work in opposing ways to control cell growth and division, and that *mraZ* encodes a transcription factor that binds DNA to potentially regulate the activity of many other genes.



The findings shed light on a newly discovered mechanism that many bacteria may potentially use to adapt to suboptimal environments or growth conditions. Thus, this research contributes to the mission of the Department of Energy's Biological and Environmental Research program, which aims to define the principles that guide the translation of the genetic code into functional proteins and the metabolic/regulatory networks underlying the systems biology of plants and microbes as they respond to and modify their environments.

Funding: This research was supported by EMSL and the National Institutes of Health.

Publication: Eraso, J, L Markillie, H Mitchell, R Taylor, G Orr and W Margolin. 2014. "The highly conserved *MraZ* protein is a transcriptional regulator in *Escherichia coli*." *Journal of Bacteriology* 196. DOI:10.1128/JB.01370-13.

Participating Institutions: EMSL, PNNL and the University of Texas Medical School at Houston.

Chromium Detoxification

Iron-reducing bacteria could detoxify chromium

Hexavalent chromium is a major environmental contaminant at several Department of Energy sites as well as other sites around the world. Iron-reducing bacteria can convert the oxidized form of iron in clay minerals, called ferric iron, into the reduced form of iron, called ferrous iron, which can then reduce hexavalent chromium to trivalent chromium – the reduced, insoluble and less toxic form of the heavy metal that poses a lower risk of groundwater contamination. Using instruments in EMSL's Quiet Wing, researchers shed light on the poorly understood process by which iron-reducing bacteria reduce ferric iron in clay minerals, resulting in ferrous iron that could then immobilize and detoxify chromium.

The findings suggest that the iron-reducing activity of bacteria could be artificially stimulated to produce ferrous iron in clay minerals, which can then reduce hexavalent chromium to trivalent chromium. This promising strategy could potentially enable long-term remediation of heavy metal-contaminated sediments and groundwater aquifers worldwide.

Funding: This research was supported by the DOE Biological and Environmental Research Division through the Subsurface Biogeochemical Research Program.

Publication: Bishop, M, P Glasser, H Dong, B Arey, and L Kovarik. 2014. "Reduction and immobilization of hexavalent chromium by microbially reduced Fe-bearing clay minerals." *Geochimica et Cosmochimica Acta*. 133. DOI: 10.1016/j.gca.2014.02.040.

Participating Organizations: EMSL and Miami University, Oxford, Ohio.

Slower as it Ages

Long-term study of uranium release could improve remediation strategies

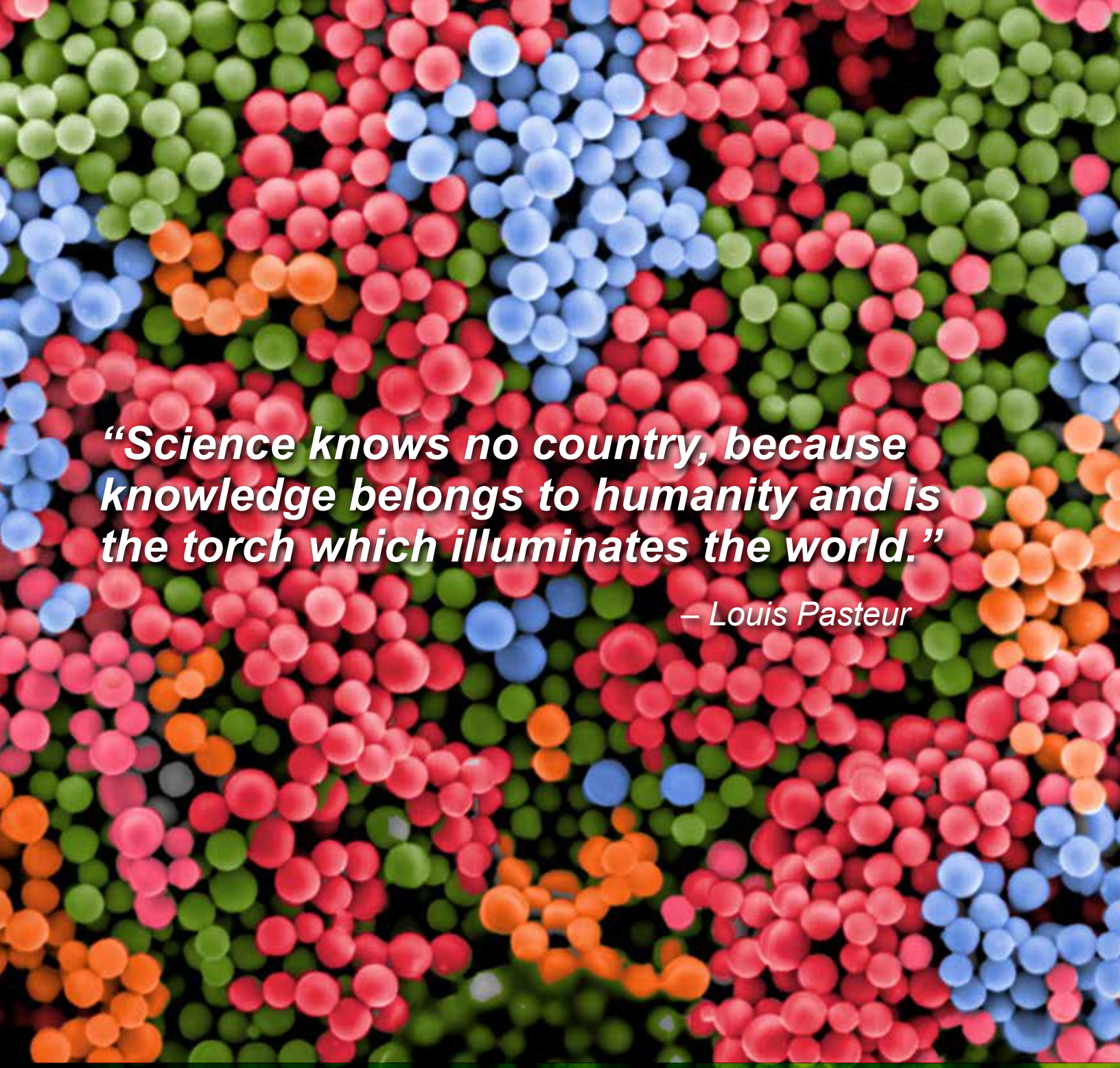
Uranium poses a serious risk of groundwater contamination at the Hanford Site. But most previous experimental studies addressing this important issue were performed over short time periods, focusing on the uranium that is quickly released from sediments to groundwater. This study, done in part at EMSL, combines modeling and laboratory experiments to assess uranium release under flow conditions over a time period long enough to evaluate the transport behavior of all of the uranium in sediment samples collected from the Hanford Site.

The study reveals fundamental processes and parameters controlling long-term uranium transport and shows that release of this contaminant slows down with time, suggesting that remediation strategies should take into account both short-term and long-term migration behavior. The findings will enable scientists to construct more accurate models for assessing the risk of groundwater contamination by uranium at the Hanford Site.

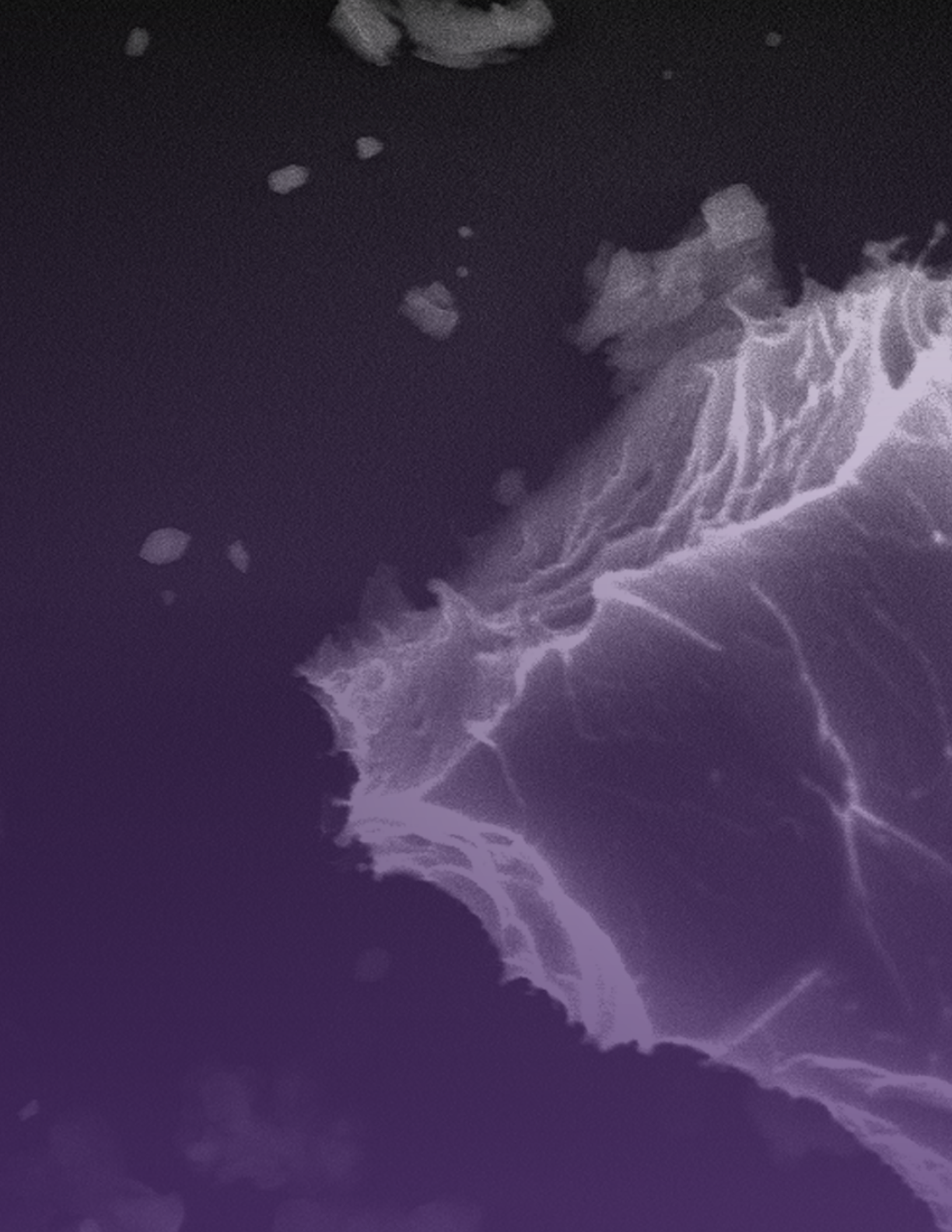
Funding: This research was supported by the DOE Biological and Environmental Research Division through the Subsurface Biogeochemical Research Program Science Focus Area at Pacific Northwest National Laboratory.

Publication: Shang J, C Liu, Z Wang and J Zachara. 2014. "Long-term kinetics of uranyl desorption from sediments under advective conditions." *Water Resour. Res*. 50. DOI: 10.1002/2013WR013949.

Participating Institution: PNNL



About this Art

Scientists at EMSL are studying the next generation of high capacity anode materials for lithium-ion batteries that could be used in electric vehicles and high performance consumer electronics. This scanning electron microscope image is of amorphous silicon balls being studied using multimodal chemical imaging capabilities, including *in situ* transmission electron microscope lithiation holder and atom probe tomography and computational simulations to understand the changes silicon undergoes during its usage as anode in a Li-ion battery. This image was also the 2014 Pacific Northwest National Laboratory Science as Art People's Choice winner.

The project team included Arun Devaraj, Chongmin Wang, Yang He, Meng Gu, Scott Alan Lea, Niri Govind, Amity Anderson, Daniel Perea and Suntharampillai Thevuthasan, all from EMSL; and Brian Korgel and Xiaotang Lu from The University of Texas at Austin. *(Image colorized)*