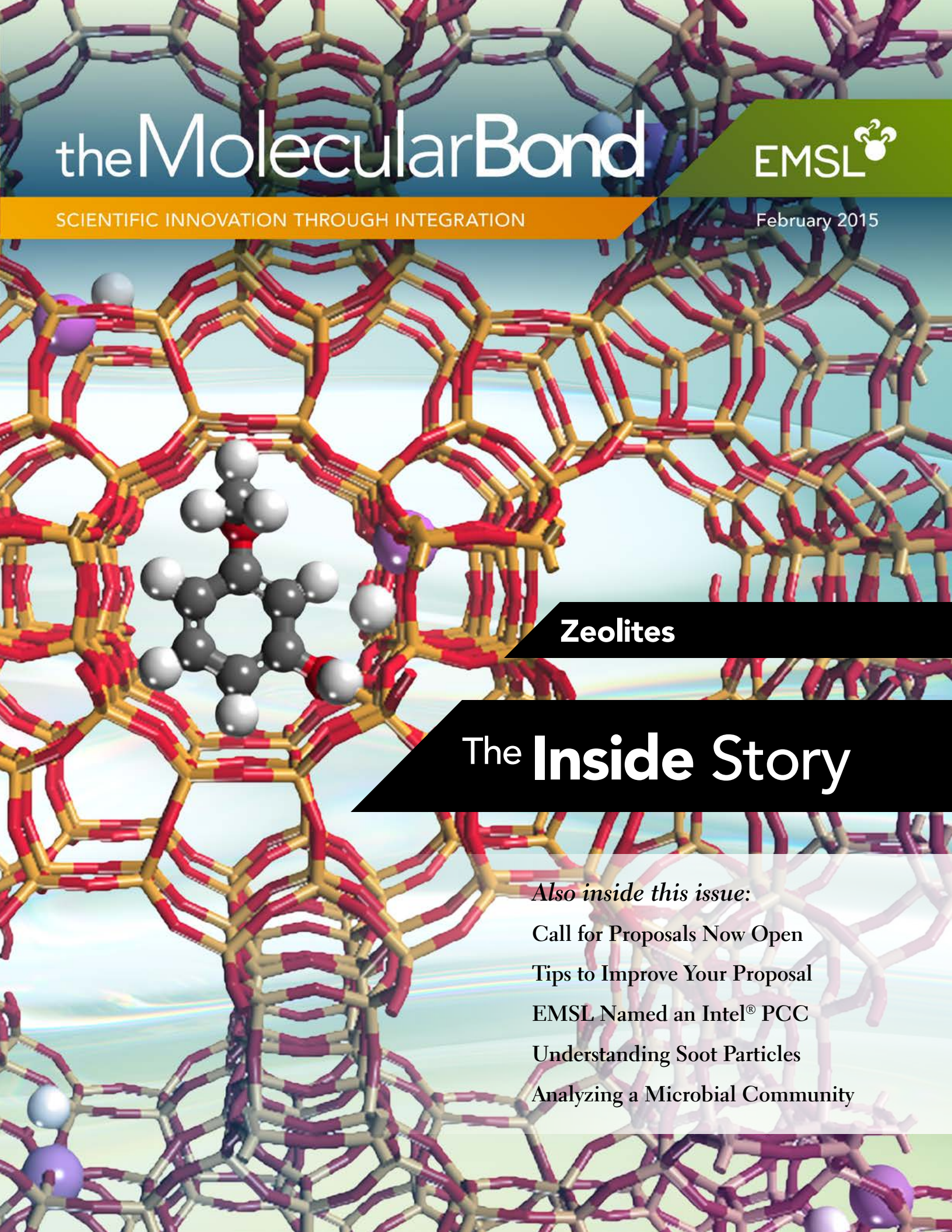
the Molecular Bond

EMSL

SCIENTIFIC INNOVATION THROUGH INTEGRATION

February 2015



Zeolites

The Inside Story

Also inside this issue:

Call for Proposals Now Open

Tips to Improve Your Proposal

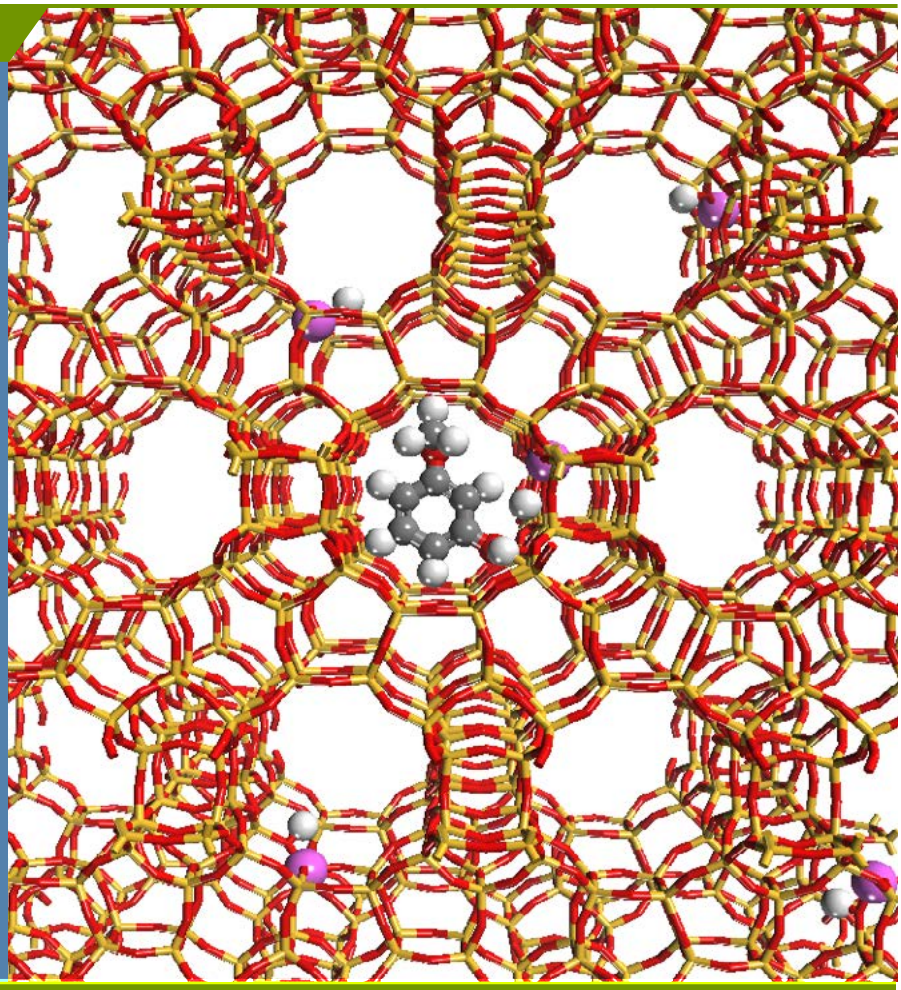
EMSL Named an Intel® PCC

Understanding Soot Particles

Analyzing a Microbial Community

About the Cover

A zeolite is a crystalline, porous aluminosilicate commonly used in catalytic operations. The zeolitic channels, or pores, are microscopic. This model represents a low aluminum H-BEA zeolite pore system with a phenolic molecule inside, such as a lignin-derived phenolic monomer, for biomass-derived renewable fuel production. (Image created by Amity Andersen, EMSL scientist.)



About *The Molecular Bond*

The Molecular Bond is EMSL's bimonthly newsletter for users, potential users and other interested individuals. EMSL Communications oversees the production of *The Molecular Bond*.

EMSL, the Environmental Molecular Sciences Laboratory, is a national scientific user facility sponsored by the Department of Energy's Office of Biological and Environmental Research in the Office of Science. Located at Pacific Northwest National Laboratory in Richland, Wash., EMSL offers an open, collaborative environment for scientific discovery to researchers around the world. Its integrated computational and experimental resources enable researchers to realize important scientific insights and create new technologies. More information about EMSL is available at: www.emsl.pnnl.gov

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

EMSL

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Alice Dohnalkova, EMSL senior research scientist, was a member of the research team studying how the presence and distribution of carbon within the root zone impacts the diversity and function of the rhizosphere microbial community featured on the inside back cover. In this photograph, Dohnalkova is using EMSL's cryogenic transmission electron microscope. The cryo-TEM is primarily devoted to biological samples involving morphological and immuno-cyto chemistry studies, but it also supports imaging of samples such as soft materials and polymers. (EMSL file photo)

INSIDE THIS ISSUE

From the Director 2

Allison Campbell

News & Kudos 3

EMSL Now Accepting FY2016 Proposals

12 Tips for a Successful User Proposal

EMSL Named an Intel® Parallel Computing Center

EMSL Scientist on Team Winning Technology Transfer Award

Baer Elected APS Fellow

Cliff Named EMSL's New NanoSIMS Expert

Breaking News: EMSL's 21 T Mass Spectrometer at Field

Feature 6

Zeolites: The Inside Story

Science Highlights 11

Integrated Omics Opportunity

Better Battery Performance

Unified Multiscale Model

Soot Science

EMSL

FROM THE DIRECTOR

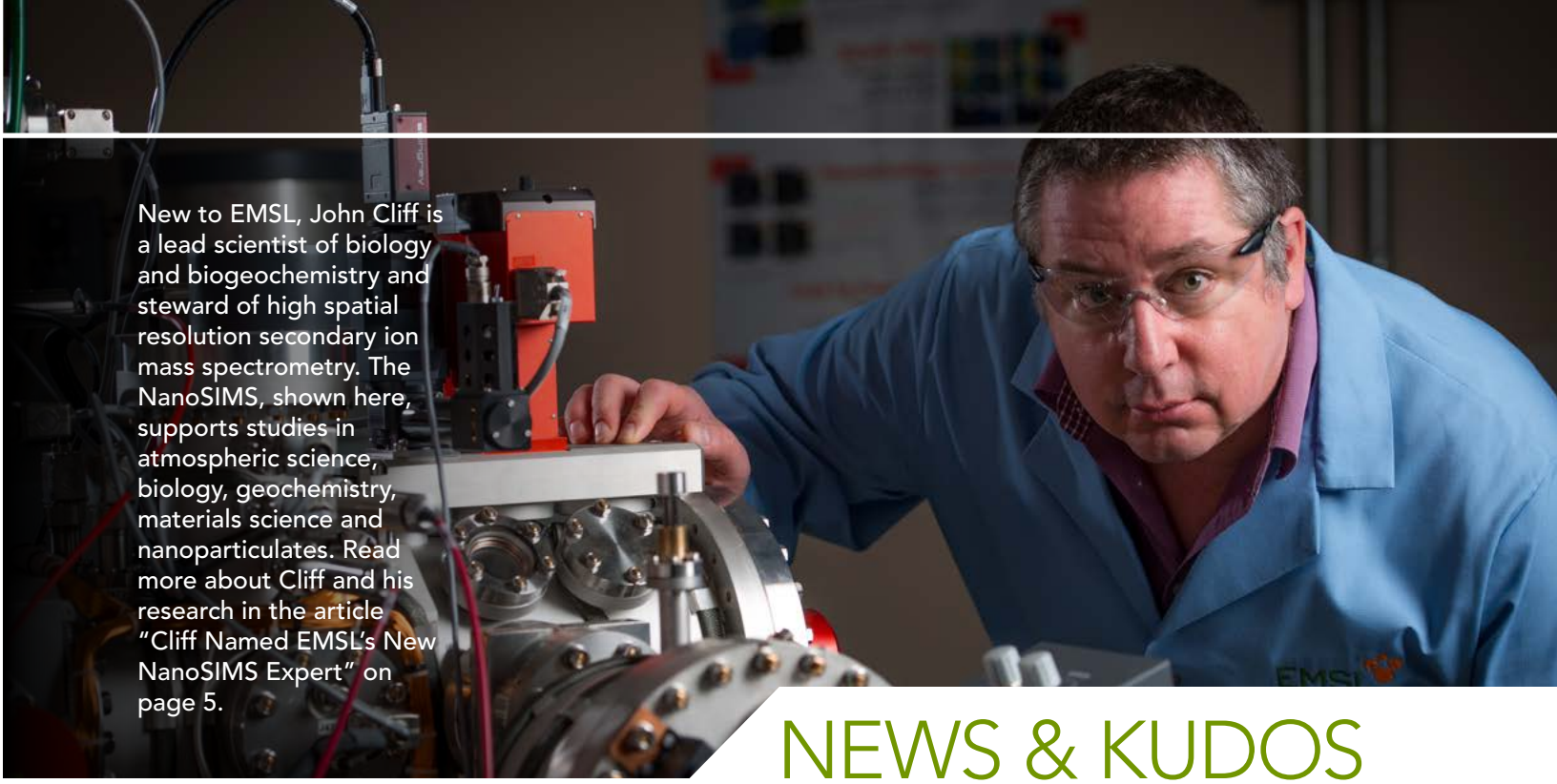
Allison Campbell

I'm pleased to bring you this issue focused on zeolites and catalysis – an important area for the Department of Energy as it looks to new catalysts for clean transportation and energy storage. Catalysis and related oxide surface chemistry research were part of the initial foundation of EMSL and remain highly successful components of our research. Growth of catalysis research activities within EMSL and other parts of the Pacific Northwest National Laboratory, EMSL's host laboratory, contributed to the formation of PNNL's Institute for Integrated Catalysis in 2005. EMSL users and staff members have advanced the understanding of catalysis and oxide surfaces in part through the development and application of novel approaches to examine and model surface reactions in realistic conditions. This expertise lies at the heart of our contributions with zeolites, a mineral often targeted for catalysis applications. As you'll read in this issue, we're collaborating with industry, academia and international organizations to advance this area of science – leveraging our staff's expertise and our advanced instrumentation.

In mid-September, we'll host our annual user meeting focused on energy materials and processes, including battery studies and catalysis. Don Baer, our Science Theme lead in this area, is developing a 'boot camp' that will provide collaborators with a unique opportunity to access our expertise and instrumentation for studying specific questions related to advanced batteries for energy storage. We're still finalizing our plans but watch for registration opening in the next couple of months.

I'm also excited that we've recently hired John Cliff to lead the research and application of EMSL's NanoSIMS system, which provides high spatial resolution of extremely small areas and volumes with high sensitivity. We expect he'll progress our ability to study environmental microbiology, cell biology, atmospheric research and materials sciences with the NanoSIMS. I encourage our users to consider how John and the NanoSIMS could help advance your research.

—Allison



New to EMSL, John Cliff is a lead scientist of biology and biogeochemistry and steward of high spatial resolution secondary ion mass spectrometry. The NanoSIMS, shown here, supports studies in atmospheric science, biology, geochemistry, materials science and nanoparticulates. Read more about Cliff and his research in the article "Cliff Named EMSL's New NanoSIMS Expert" on page 5.

NEWS & KUDOS

EMSL Now Accepting FY2016 Proposals

EMSL's call for fiscal year 2016 proposals is open and offers two opportunities for submitting research projects – Science Theme Research and DOE JGI/EMSL Collaborative Science Initiative. Applicants may apply to either or both calls, but should be aware of the differences in schedules and due dates.

Award decisions for both calls will be made by July 31, and approved proposals will be granted access to EMSL resources beginning Oct. 1.

Science Theme Applications

EMSL will accept proposals for its annual Science Theme Research Call until March 2 at 11 p.m. PST. Proposals can be submitted at any time through the EMSL User Portal until the deadline.

Researchers should submit proposals for molecular-scale research that address specific selected topics in EMSL's Science Themes to accelerate results in emerging science areas of interest to EMSL, the Department of Energy's Office of Biological and Environmental Research and the DOE. The Call for FY2016 Science Theme Research webpage at http://www.emsl.pnl.gov/emslweb/call-fy16-science-theme-research provides more information.

DOE JGI/EMSL Collaborative Science Applications

Letters of intent for the DOE Joint Genome Institute/EMSL Collaborative Science Initiative will be accepted until April 6 at 11 p.m. PDT. Proposals can be submitted at any time through the EMSL User Portal until the deadline.

This initiative represents a unique opportunity for researchers to combine the power of genomics at the DOE JGI and molecular characterization at EMSL into one proposed research project. Both user facilities, stewarded by BER, play critical roles in supporting DOE energy, environment and basic research missions. Applications should focus on high risk/high payoff projects that can be completed on an accelerated timeline. Proposed projects should utilize a broad range of the capabilities of each facility, and generate datasets beyond what each facility could generate by itself.

Applications for this collaborative initiative will follow a proposal package, schedule and review process tailored to meet both EMSL and DOE JGI requirements. The DOE JGI/EMSL Collaborative Science Initiative webpage at http://www.emsl.pnnl.gov/emslweb/jgi_initiative_call has more information.

Questions regarding EMSL's user program or specifics about the calls may be directed to the User Support Office at emsl@pnnl.gov or 509-371-6003.

12 Tips for a Successful User Proposal

EMSL's call for fiscal year 2016 proposals opened Jan. 7. Access to use EMSL capabilities continues to be competitive, and it's even more important to make sure your submission stands out from the other proposals. Here's how:

1. Contact an EMSL capability lead or Science Theme lead prior to starting your proposal to talk about your research ideas and what instruments you are planning to use. The leads can help you develop a much stronger submission.

2. Requirements change – carefully read the proposal guidance for the call, and fully understand what should be included in your submission.

3. Follow the guidance on the recommended number of words per section. A successful proposal can be, and has been, written within the prescribed limits.

4. Ensure your proposal is concise and well written. For those who may be submitting a proposal someone else authored, carefully review it and put your personal stamp on it.

5. Have clear definable hypotheses and specific science objectives.

6. Provide a measured assessment of the benefits of your research. Overstatements of benefits harm a proposal.

7. Clearly explain how your research addresses specific mission areas and advances the science pertinent to the Department of Energy's Office of Biological and Environmental Research. Just stating there is a linkage is not enough; you need to describe the linkage in detail.

8. Have an explicit research approach – clearly state what steps you are going to follow, such as why you want to use a particular instrument, how many samples you have and when they'll be ready, and what you are going to do with the data.

9. State the role of each key contributor on the project. If aspects of the study are outside your areas of expertise, indicate who and how others will support those science areas.

10. Explain why you need to do your research at EMSL and link those reasons to specific instruments. Make a strong case why you should be selected to use national user facility capabilities. Just stating an interest in using a specific instrument isn't as compelling.

11. State if your proposal is part of a phased project. Make sure the reviewers know there will be more phases in this project.

12. Don't cut and paste your proposal from previous documents. Take the time to write an integrated proposal for each call. Proposals that are cut and pasted are often disjointed and are noticed by the peer reviewers.

The peer reviewers will be looking at many proposals. Don't make them labor to understand your request. Make sure your submission stands out with clear and concise writing, strong ideas and impactful science. Good luck.

The principal investigators on the project are EMSL scientists (from left to right) Niri Govind, Eric Bylaska, Karol Kowalski and Edoardo Apra. Not shown is Hubertus van Dam.

EMSL Named an Intel® Parallel Computing Center

Intel has named EMSL an Intel® Parallel Computing Center. As an Intel® PCC, EMSL's scientific computing team will work with Intel to modernize the codes of NWChem to take advantage of technological advancements in computers. NWChem is one of the Department of Energy's premier open-source computational chemistry software suites and has been developed at EMSL.

Updating NWChem codes will allow it to more effectively utilize the emergent hybrid parallel computer systems based on the Intel® Many Integrated Core Architecture technology.

The modernized codes will be applicable to several science drivers including studies of aerosol particles, soil chemistry, biosystems, hormone-cofactor functionality in proteins, ionic liquids in cells, spectroscopies, new materials and large-scale reaction mechanisms.

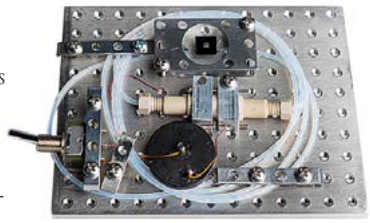
The investigators on the project are EMSL scientists Karol Kowalski, Edoardo Apra, Eric Bylaska, Niri Govind and Hubertus van Dam.

The Intel® PCC program provides funding to universities, institutions and research labs to modernize key community codes used across a wide range of disciplines to run on current state-of-the-art parallel architectures.

EMSL Scientist on Team Winning Technology Transfer Award

A team of Pacific Northwest National Laboratory and EMSL scientists working at EMSL received a prestigious Excellence in Technology Transfer Award in 2015 from the Federal Laboratory Consortium for Technology Transfer for development of SALVI. The award recognizes outstanding work in transferring U.S. government-sponsored technologies to the public and private sector.

Short for System for Analysis at the Liquid Vacuum Interface, SALVI allows instruments such as mass spectrometer and scanning electron microscopes to image liquid samples in real-time and space. With SALVI, scientists can gain new insights into nanoparticles, bacteria, cells, batteries and more.



SALVI, short for System for Analysis at the Liquid Vacuum Interface, allows solid-liquid interface observation while imaging with mass spectrometers or scanning electron microscopes.

Xiao-Ying Yu was the PNNL lead scientist for the project. Zihua Zhu, an EMSL scientist who works with a time-of-flight secondary ion mass spectrometer, led the ToF-SIMS measurement and data analysis portion of the project. The other team members recognized for transferring SALVI to the market are PNNL's Bruce Harrer and Li Yang, a former PNNL scientist. Gene Rodek of Structure Probe Inc. also played an important role in bringing the technology to the commercial market.

Some of Cliff's recent research includes the transfer of plant photosynthate to soil microbes; sulfur isotope fractionations associated with microbial sulfate reductions; sulfur isotope evolution in sulfide ores; and a chemical, isotopic and microstructural study of pyrite from uranium deposits.

Prior to EMSL, Cliff was an assistant professor at the Centre for Microscopy, Characterisation and Analysis at The University of Western Australia in Perth. At the Centre he was facility manager of an IMS 1280, a high mass resolution high transmission SIMS, and used a NanoSIMS extensively.

Don Baer

Baer Elected 2015 APS Fellow

The American Physical Society has chosen Don Baer a 2015 Division of Chemical Physics Fellow. A PNNL Laboratory Fellow, Baer is the lead for EMSL's Energy Materials and Processes Science Theme.

The APS Council elected Baer to Fellowship for his "research and capability development that significantly advanced molecular-level understanding of environmentally important interfacial processes relevant to nanoparticle reactivity, mineral dissolution and stress corrosion cracking."

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. Among his numerous awards and honors, he was recently elected to the Washington State Academy of Sciences, named an AVS trustee and received an ASTM International Award of Merit. He has authored or co-authored more than 250 peer-reviewed journal articles and book chapters.

Baer will be formally recognized at the APS March Meeting 2015 in San Antonio.

John Cliff

Cliff Named EMSL's New NanoSIMS Expert

John Cliff has joined EMSL as a lead scientist of biology and biogeochemistry and steward of high spatial resolution secondary ion mass spectrometry, or NanoSIMS. Among his duties are development and implementation of techniques for chemical imaging and isotopic characterizations of environmental samples using SIMS.

BREAKING NEWS!

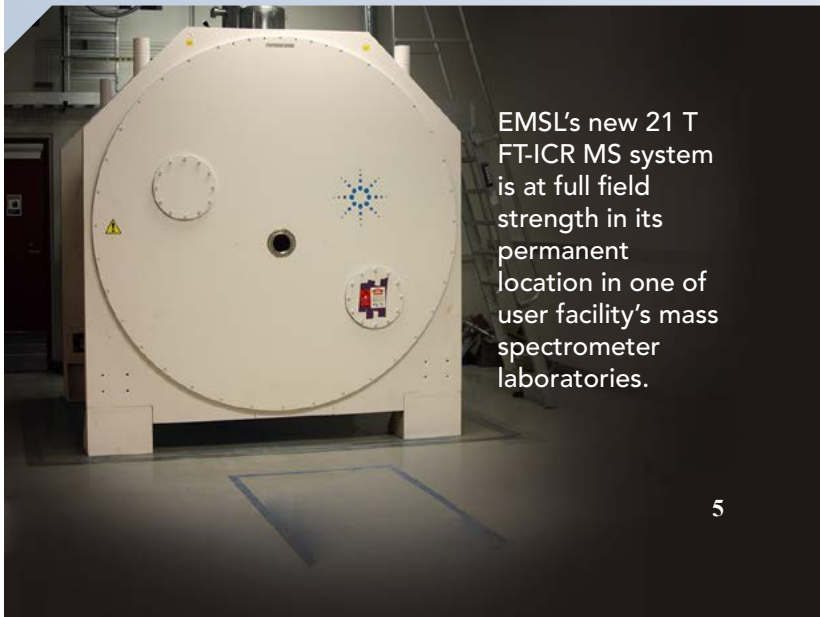
EMSL's 21 T Mass Spectrometer at Field

EMSL's new 21 Tesla Fourier Transform Ion Cyclotron Resonance Mass Spectrometer is now at its full magnetic field of 21 Tesla.

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

EMSL anticipates the capability will be ready for its first scientific studies this summer.

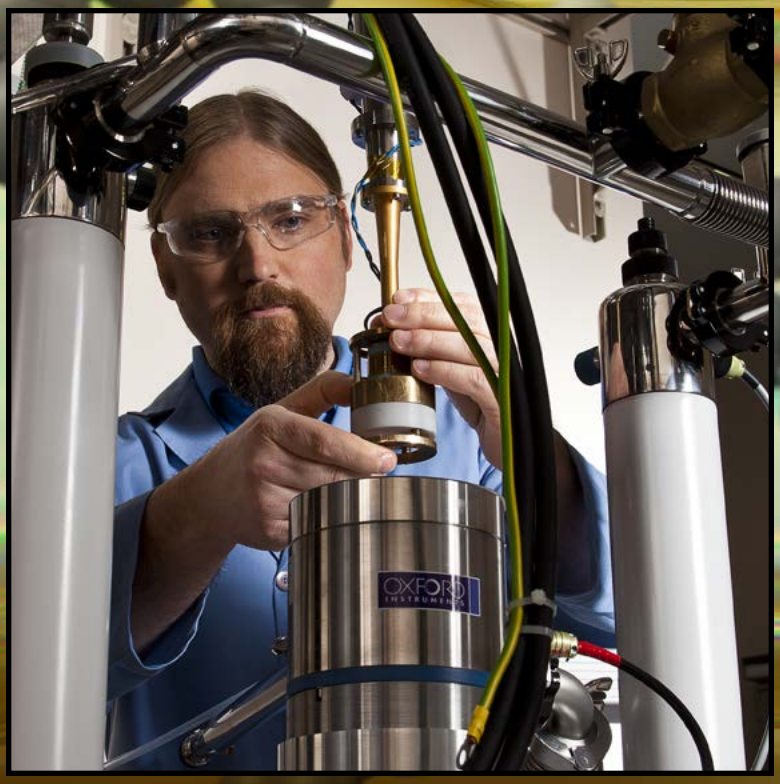
The system was developed to advance the science mission of the Department of Energy's Office of Biological and Environmental Research, and was funded as a Major Item of Equipment by BER.



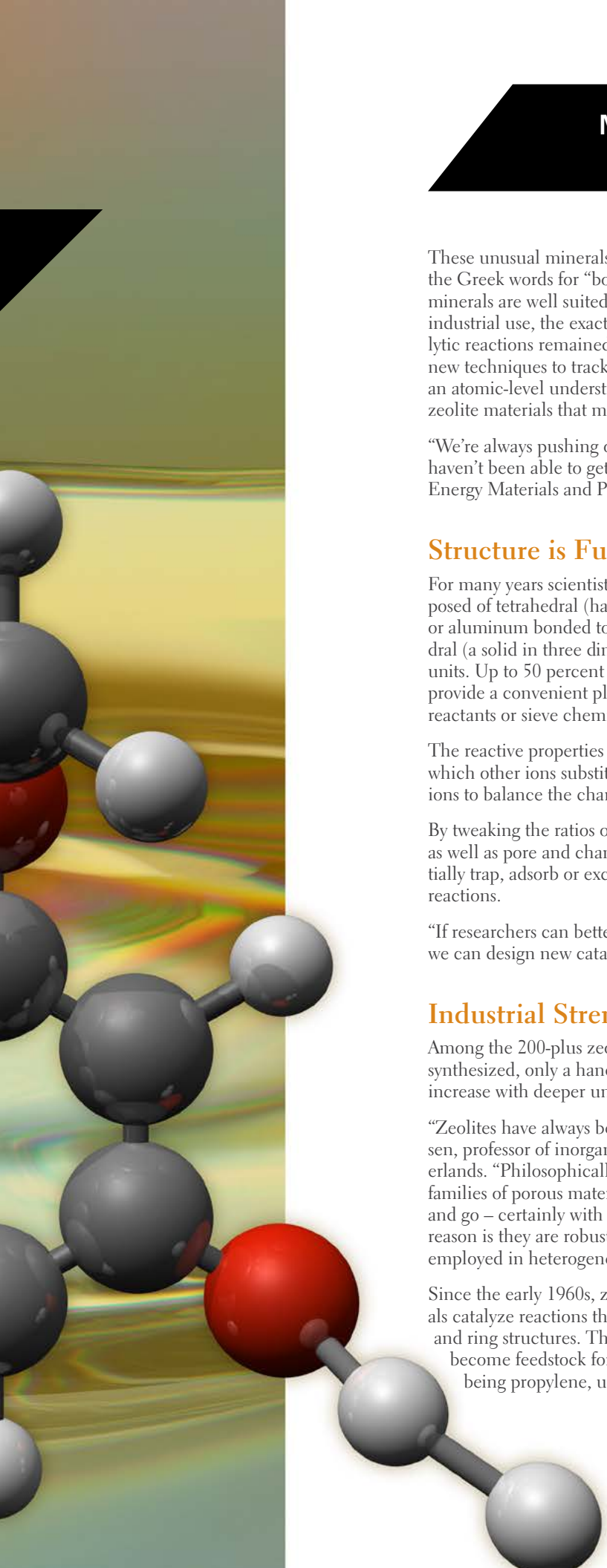
EMSL's new 21 T FT-ICR MS system is at full field strength in its permanent location in one of user facility's mass spectrometer laboratories.

The Inside Story

EMSL users find new ways to probe centuries-old catalysts



Senior Research Scientist Eric Walter is characterizing the catalytic nature of zeolites under varying conditions using EMSL's high-field electron paramagnetic resonance capability system. (EMSL file photo)



More than 200 years ago, a Swiss mineralogist discovered zeolites.

These unusual minerals emitted steam when heated, garnering a name based on the Greek words for "boiling stones." Since then, scientists have found these porous minerals are well suited for catalysis, among other applications. Despite decades of industrial use, the exact transformations occurring within the minerals during catalytic reactions remained poorly understood. Now researchers at EMSL are applying new techniques to track molecular action inside these lattice-like structures. With an atomic-level understanding of these catalysts, scientists can design more efficient zeolite materials that may lead to new resources for energy and the environment.

"We're always pushing our capabilities to get scientifically important information we haven't been able to get before," said Don Baer, EMSL Science Theme lead for Energy Materials and Processes.

Structure is Function

For many years scientists have known zeolites have a crystalline framework composed of tetrahedral (having four triangular faces) patterns made primarily of silicon or aluminum bonded to oxygen. These lattices form sheets, chains or other polyhedral (a solid in three dimensions with flat faces, straight edges and sharp corners) units. Up to 50 percent of these structures are voids, with pores and channels that provide a convenient place – for industrial purposes – to collect contaminants, stow reactants or sieve chemical products after reactions.

The reactive properties of a zeolite vary depending upon the nature and degree to which other ions substitute for silicon. For chemical stability, the zeolite seeks other ions to balance the charge forming a solid acid site.

By tweaking the ratios of aluminum (or other charged molecules or ions) to silicon, as well as pore and channel sizes, scientists can synthesize zeolites that preferentially trap, adsorb or exchange with other molecules or ions to speed up specific reactions.

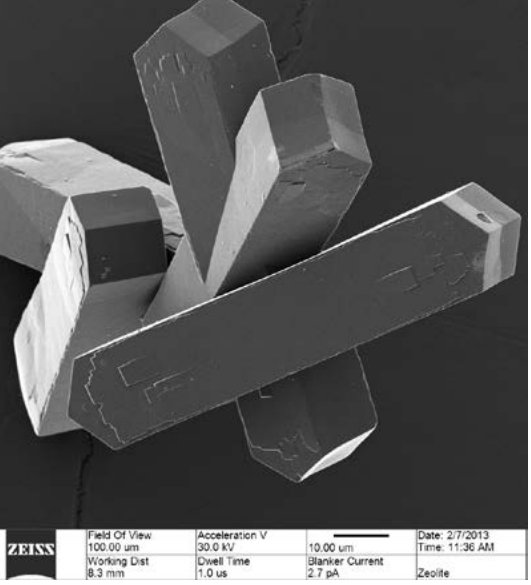
"If researchers can better understand reaction sites and how to stabilize the zeolites, we can design new catalysts with longer lifetimes and at lower costs," Baer said.

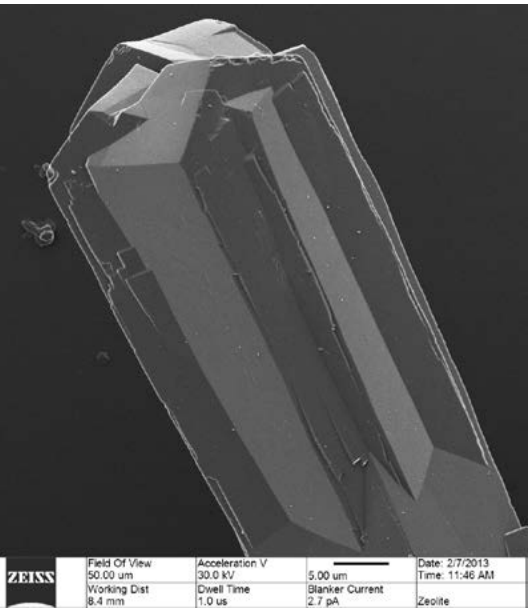
Industrial Strength

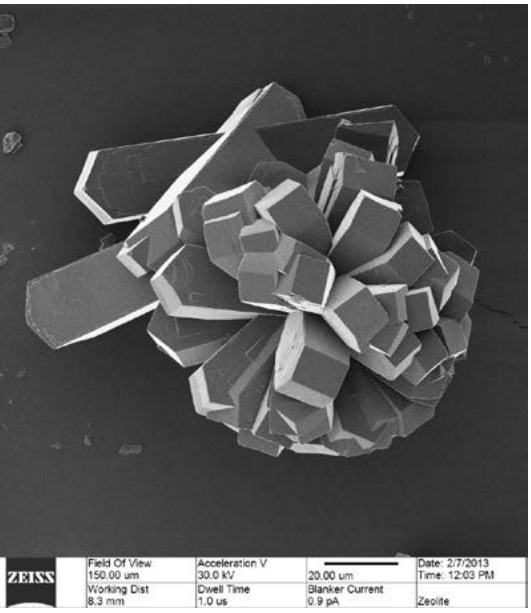
Among the 200-plus zeolite structures known today, both naturally occurring and synthesized, only a handful find regular industrial application. That number could increase with deeper understanding of the catalytic performance of zeolites.

"Zeolites have always been very intriguing catalytic materials," said Bert Weckhuysen, professor of inorganic chemistry and catalysis at Utrecht University in the Netherlands. "Philosophically it's important to realize that every year one or two new families of porous materials are discovered. Waves of new porous materials come and go – certainly with promising applications – but the zeolites stick around. One reason is they are robust, solid materials that can survive the harsh conditions often employed in heterogeneous catalysis."

Since the early 1960s, zeolites have been a workhorse for oil refineries. The minerals catalyze reactions that "crack" long chains of hydrocarbons into shorter chains and ring structures. These smaller products can then be converted to gasoline or become feedstock for other petrochemical reactions; an example of the latter being propylene, used for making plastics. (continued on page 8)







Simon R. Bare, Bert Weckhuysen and Daniel Perea's zeolite research used EMSL's helium ion microscope in the Quiet Wing to image the ZSM-5 zeolite crystal morphology prior to specimen preparation for atom probe tomography. (Images taken by Bruce Arey, EMSL technologist.)

Zeolites have now found steady work in the automobile industry, too. Catalytic converters for gasoline engines typically use precious metal-based catalysts to convert unburned hydrocarbons – as well as carbon monoxide and nitrogen oxide, or NOx – into carbon dioxide, water, nitrogen and oxygen.

Demand for more fuel-efficient diesel engines has driven the search for new catalysts. In lean-burning engines (more air, less fuel), excess oxygen accumulates in the exhaust. In that chemical environment, the removal of NOx emissions wasn't so favorable using precious metal-based catalysts.

To solve that problem, scientists discovered zeolite-based catalysts could remove NOx – even with the oxygen excess – via selective catalytic reduction. This process introduces ammonia into the exhaust system as a "selective" reductant for converting the NOx into nitrogen. Although plenty of zeolites were quite active for the selective catalytic reduction reaction, a big stumbling block to developing this new approach was that none of those catalysts were stable enough to last the 200,000-mile lifespan of a car, explained Charles Peden, a Laboratory Fellow at Pacific Northwest National Laboratory, or PNNL, and associate director of PNNL's Institute for Integrated Catalysis.

By the late 2000s, scientists identified small pore zeolites that provided the major breakthrough to solve this problem. In particular, Cu-SSZ-13, a zeolite containing ion-exchanged copper ions, had the smaller pores necessary for preventing unburned hydrocarbons from poisoning the catalyst. Furthermore, this zeolite was much more thermally stable in the vehicle exhaust environment than others that had been tried.

"It was an unusual situation," Peden said. "They started commercializing these new emission control catalysts when the community, as a whole, didn't know exactly what the material was."

When scientists added copper ions to zeolite SSZ-13, they surmised where copper was located based on chemical properties and molecular structure; however, they were not sure where the atoms were exchanged in these frameworks. Nor did they know the position of reactive sites. To learn more about Cu-SSZ-13 catalysis, Peden and his colleagues used a combination of EMSL's instrumentation, such as electron paramagnetic resonance, or EPR, X-ray diffraction and computational modeling.

"One of the real surprises was how much the copper seems to move under reaction conditions," Peden said of their findings. "You couldn't learn that by taking just one measurement. But under reaction conditions, copper moves maybe 5-10 ångstroms. That doesn't sound like much, but that's significant for changing the zeolite catalyst's nature."

To further characterize the catalyst's nature, scientists followed the distribution of copper ions in SSZ-13 while the catalytic reaction progressed under different conditions. To do this, Eric Walter, an EPR expert and senior research scientist at EMSL, engineered a special cell to control reactant gas flow conditions in the EPR spectrometer. When varying amounts of copper were added to the catalyst, scientists correlated changes in performance and molecular properties with the changing conditions.

In the future, fuel economy standards will require vehicles with much higher mile-per-gallon numbers. When that happens, scientists will have a new problem to solve: Increasing fuel efficiency means more heat will be captured in the engine, resulting in exhaust temperatures too low for the current crop of catalysts to work well. (continued on page 9)

"We're looking for new catalyst materials, or something that significantly enhances what we've got now," Peden said.

Researchers are building dossiers on different zeolites to determine which ones might perform best in these new engine environments using sophisticated instruments at EMSL. In the past eight months, Peden and his colleagues have used EMSL's Mössbauer spectroscopy to study zeolite catalysts that contain iron ions rather than copper.

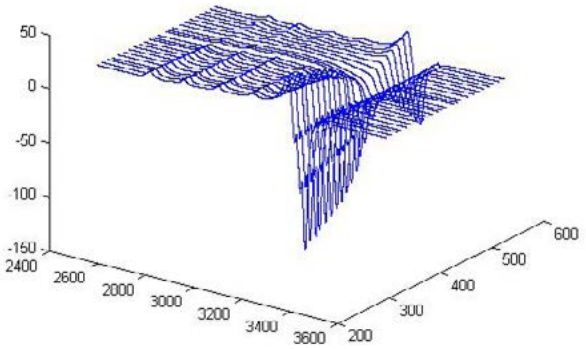
Probing Further

Scientists prefer to synthesize zeolites, because naturally occurring minerals often contain impurities that interfere with intended reactions. But synthesizing these structures with specific geometries, under readily reproducible conditions, presents an ongoing challenge.

One technology that pushed zeolite work forward was the development of bubbling reactor technology at EMSL. This allowed researchers to quickly (within two hours) synthesize large quantities of stable zeolite MFI suspensions, with controllable pore size and silicon-to-aluminum ratios. Among its many uses, zeolites with MFI structure are commonly the catalyst of choice for processes that lead to the formation of paraxylene, the raw material for manufacturing plastics products such as beverage containers.

Zeolites are also attractive acid catalyst candidates for converting biomass into diesel-range biofuels. Lignin is the main component of abundant, woody biomass. If scientists can design catalysts that efficiently break down this tough, long-chain polymer, then the resulting smaller components can be readily degraded into biofuels.

The slowest step in the overall chemical breakdown sequence for lignin is the alcohol dehydration reaction. To model ways to accelerate that rate-limiting step, Aleksei Vjunov, a research associate at PNNL, used zeolite H-BEA to catalyze the dehydration of cyclohexanol in water, at high temperature and pressure. Using EMSL's high-resolutions magic angle spinning nuclear magnetic resonance, or NMR, spectroscopy and isotope labeling of the alcohol molecules, he followed the chemical transformations and the associated



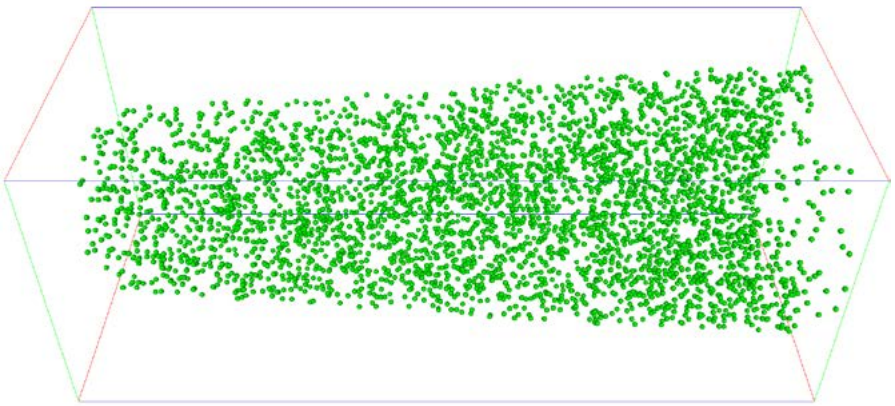
Charles Peden and Eric Walter's catalysis research on Cu-SSZ-13 zeolite used EMSL's electron paramagnetic resonance capability system to create a plot showing how the spectrum changes with temperature. (Image provided by Eric Walter, EMSL senior research scientist.)

redistribution of the 13C labels in the products and reactants during the reaction.

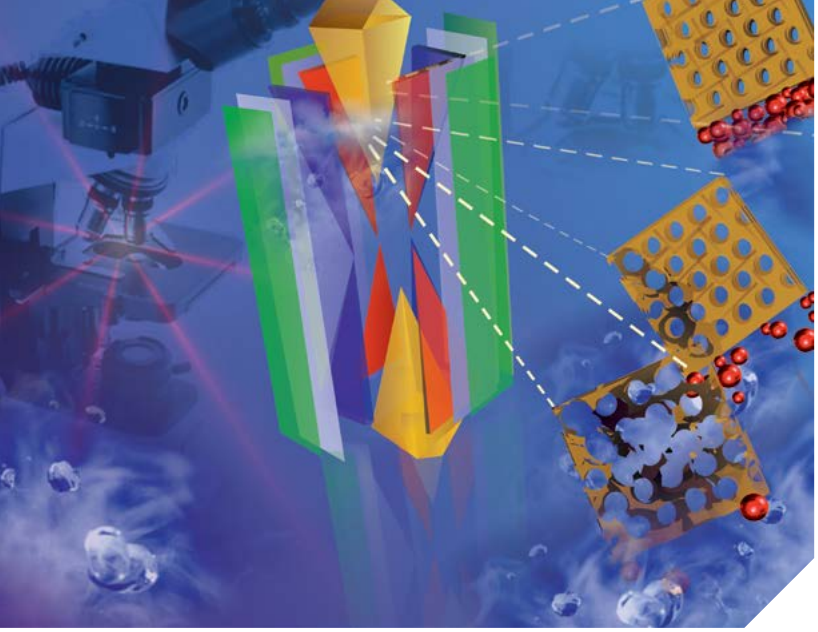
"If you want to improve the reaction, you need to know the exact mechanisms by which it takes place," Vjunov said. This novel approach nailed down the mechanism of this critical step.

To further study the structure of H-BEA catalysts, Vjunov and colleagues analyzed aluminum positioning among the nine tetrahedral sites in the silicate-zeolite structure. Their novel approach to this combined extended X-ray absorption fine-structure spectroscopy, performed at the Swiss Light Source in Switzerland, with NMR spectroscopy that was supported by theoretical calculations using EMSL's NWChem software package. As a result, researchers discovered aluminum atoms preferentially populate the tetrahedral sites located in particular ring–structures of the framework.

"Next we'll look at catalyst stability at high temperatures, and estimate the impact of structural degradation on the zeolite's catalytic performance," Vjunov said. (continued on page 10)



The distribution of aluminum atoms within a ZSM-5 zeolite sample imaged using EMSL's atom probe tomography capability as part of Simon R. Bare, Bert Weckhuysen and Daniel Perea's zeolite research. (Images created by Daniel Perea, EMSL senior research scientist.)



This image illustrates the use of advanced micro-spectroscopy to gain insight about zeolite ZSM-5 at the single particle level. Different regions in the zeolite crystal show zoning in elements, such as aluminum, as well as differences in the type and accessibility of micropores, and the generation of mesopores. It is this complex interplay between local chemical composition and accessibility that determines the overall performance of zeolite materials. Key to the understanding of these materials is insight into the local chemical composition and accessibility, and linking it to catalytic performance. (Image provided by Bert Weckhuysen, professor at Utrecht University.)

EMSL Senior Research Scientist Daniel Perea imaged the distribution of aluminum atoms in a zeolite structures using EMSL's atom probe tomography system. The instrument is among the first of its kind available to the global scientific community through a user facility. (EMSL file photo)

Another innovative way to follow aluminum atoms inside zeolites is with atom probe tomography, or APT. The technique has been used for more than 50 years to visualize three-dimensional structures of metals at the atomic level. But the tiny, needle-tip sample, and high electrical potential needed to vaporize individual atoms made it a challenge to apply this technology to zeolites. To address the challenge, EMSL scientists developed new ways to work with the porous, highly insulated zeolites and then track aluminum atoms inside a prototypical zeolite structure.

With APT, research collaborators, including Simon R. Bare, a senior scientist at UOP, LLC, as well as Weckhuysen, wanted to know: How are aluminum atoms bonded in the structure? Where do aluminum ions distribute? Furthermore, can aluminum ion distribution be correlated with catalytic properties, so more efficient materials can be designed?

Similar to the work performed using zeolite H-BEA, the APT indicated preferential aluminum clustering at specific sites inside the MFI zeolite particle.

"We're leading the effort using APT in this area," said Daniel Perea, an EMSL senior research scientist. "We can position ourselves to be world leaders in this because of our expertise and very unique tools," he said.

Accelerating Ahead

With a 50-year history on the catalytic scene, zeolites have already made a huge impact, said Baer.

"We now need catalysts that will turn the messy soup of biology into simple products that have the right form and structure to be a fuel or a valuable chemical," he said. "Once we understand these catalysts, we can have a whole new generation of products that can help us make the most of our resources." ■

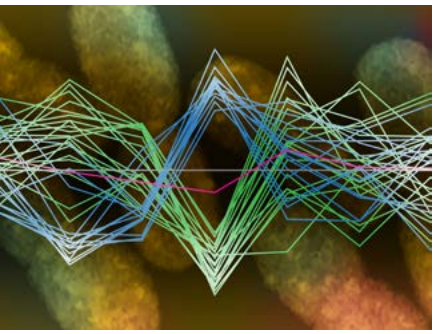
The research highlighted in this article received funding from a variety of sources. Funding for the various projects came from the Department of Energy's Office of Biological and Environmental Research, DOE's Office of Basic Energy Sciences, Pacific Northwest National Laboratory's Laboratory Directed Research and Development fund, the Netherlands Research School Combination-Catalysis, and the Netherlands Research Council.

Elizabeth Devitt is a science journalist and freelance writer.

SCIENCE HIGHLIGHTS

Integrated Omics Opportunity

First study of its kind to analyze complex microbial community



Microbial communities respond to environmental perturbations through changes in the relative abundance of community members as well as changes in functional capacities of individual members. Although many studies have monitored changes in the structure of the microbial community, analysis has not kept pace with functional changes. This study is the first to use integrated omics to evaluate both membership and functional response of a complex community (i.e., cellulose-degrading microbes) to environmental perturbation.

Plant biomass is a promising and sustainable source of fuels and materials since cellulosic materials are plentiful with relative low cost, which makes them particularly attractive. Because cellulolytic microorganisms can break down tough material, their activity could be harnessed for efficient biofuel production. By shedding light on the structure and function of a complex cellulose-degrading microbial community, this research could improve predictive models of complex biological systems and pave the way for widespread use of plant biomass for biofuel production.

Funding: This research was partially funded by Pacific Northwest National Laboratory's Laboratory Directed Research and Development Program Microbial Communities Initiative and the Department of Energy's Office of Biological and Environmental Research and Genome Sciences Program Pan-omics Program.

Publication: Boaro A, Y-M Kim, A Konopka, S Callister and B Ahring. 2014, "Integrated 'omics Analysis for Studying the Microbial Community Response to a pH Perturbation of a Cellulose-Degrading Bioreactor Culture." *FEMS Microbiology Ecology*. DOI:10.1111/1574-6941.12435.

Participating Organizations: Washington State University Tri-Cities, PNNL and EMSL.

Better Battery Performance

Long-term performance possible for rechargeable batteries

Lithium metal has long been considered one of the most attractive anode materials, but large-scale application of high-energy rechargeable Li metal batteries still faces several barriers. One major hurdle is growth of Li dendrites – deposits that form on electrode surfaces during the charging process, causing batteries to short circuit and leading to serious safety hazards such as fires and explosions. This study evaluated the effect of an electrolyte additive that suppresses Li dendrite formation to stabilize Li metal.

The findings could help scientists design a safe and stable metallic Li anode: the Holy Grail of Li-based battery research. Ultimately, the study could pave the way for the practical application of several high-energy-density battery systems for powering electric vehicles and storing renewable energy on the grid.

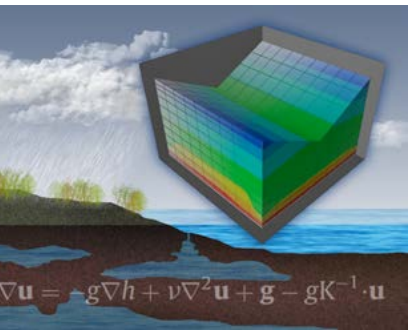
Funding: Portions of this research were supported by the Joint Center for Energy Storage Research, the Department of Energy's Office of Energy Efficiency and Renewable Energy, National Science Foundation of China, Linus Pauling Distinguished Postdoctoral Fellowship, Batteries for Advanced Transportation Technologies and US Army Research Laboratory Postdoctoral Fellowship.

Publication: Zhang Y, J Qian, W Xu, SM Russell, X Chen, E Nasybulin, P Bhattacharya, M Engelhard, D Mei, R Cao, F Ding, A Cresce, K Xu and J-G Zhang. 2014. "Dendrite-Free Lithium Deposition with Self-Aligned Nanorod Structure." *Nano Letters*. DOI:10.1021/nl5039117.

Participating Organizations: Harbin Institute of Technology; Wuhan University in Hubei, China; Tianjin Institute of Power Sources; US Army Research Laboratory; PNNL; and EMSL.

Unified Multiscale Model

Model simultaneously simulates flow in surface water and groundwater



Modeling hydrological processes in ecosystems containing both surface water and groundwater is crucial for understanding fluid flow, the transport of environmental contaminants, and nutrient supplies to microbes and plants. This understanding could potentially help control carbon and water cycles and remediate contaminants. But models traditionally use separate sets of equations to describe fluid flow in surface water and groundwater and thus require complex approaches to couple equations. This study presents a multiscale model that unifies physical theories governing water flow in pores and porous media, and demonstrates the unified theory to simultaneously simulate water flow in an ecosystem containing both surface water and groundwater.

The unified multiscale model significantly simplifies the simulation of hydrological processes in ecosystems, especially wetlands and other locations characterized by frequently changing interactions between surface water and groundwater. The model integrates hydrological processes across spatial scales – from the pore to the ecosystem – and across hydrological domains that are traditionally handled using different models. As a result, the approach can improve efficiency and accuracy of modeling the flow of contaminants, the transport of nutrient supplies to ecologically important microbes, and processes affecting production and release of greenhouse gases.

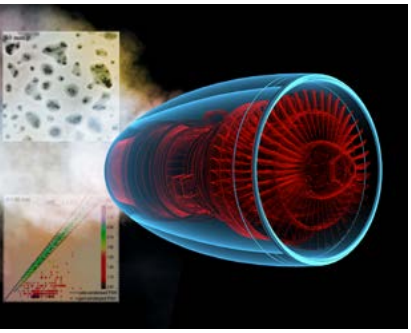
Funding: This research was supported by the Department of Energy's Office of Biological and Environmental Research.

Publication: Yang X, C Liu, Y Fang, R Hinkle, H-Y Li, V Bailey and B Bond-Lamberty. 2015. "Simulations of ecosystem hydrological processes using a unified multi-scale model." *Ecological Modelling* 296:93-101. DOI:10.1016/j.ecolmodel.2014.10.032.

Participating Organizations: University of Central Florida at Orlando, PNNL and EMSL.

Soot Science

New study of soot could improve climate models



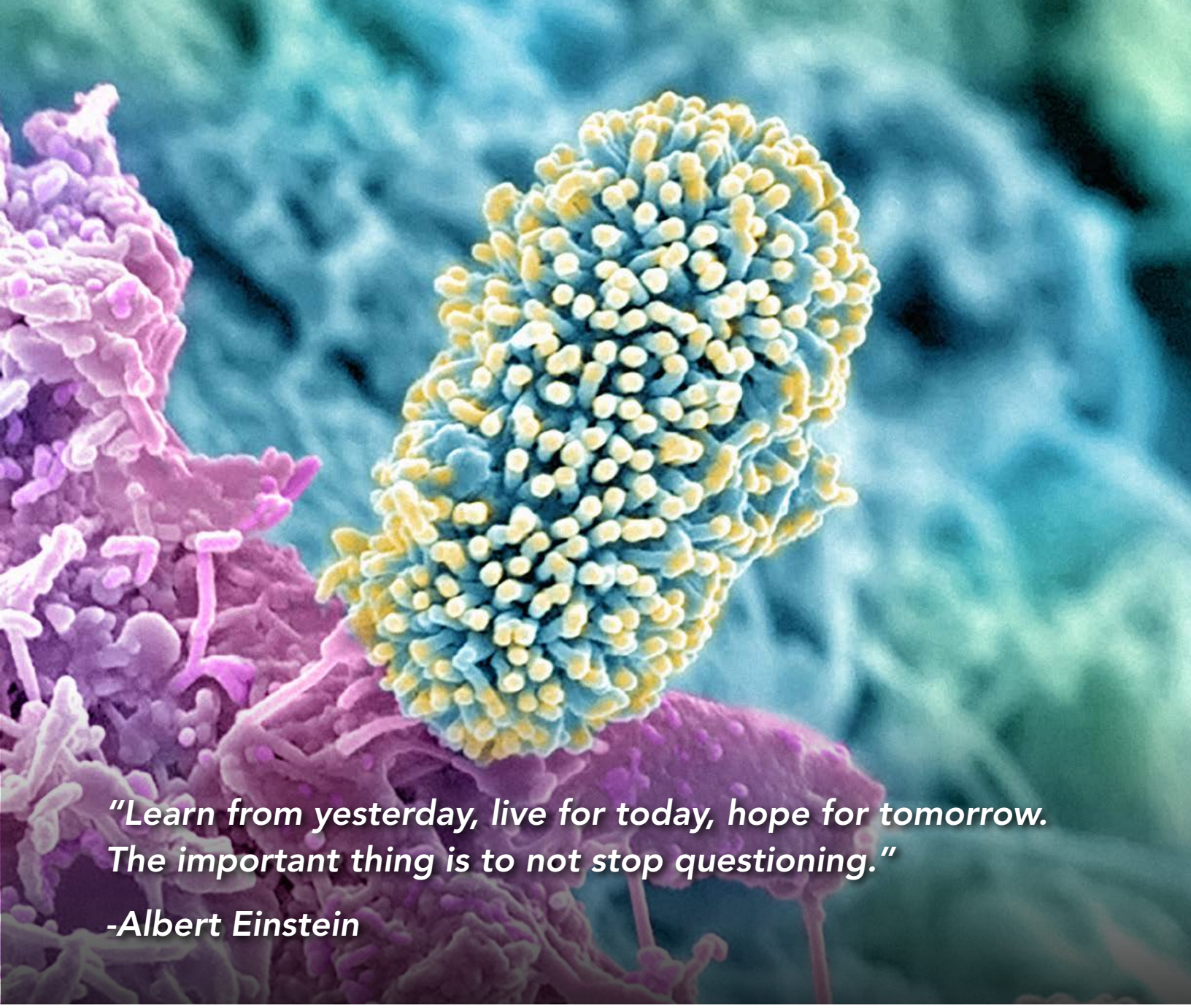
Soot is produced from incomplete combustion of hydrocarbon fuels. Because soot is an anthropogenic contaminant in the environment and an important contributor to climate change, it is necessary to understand how it forms. A recent study addressed this question by examining the chemical composition of soot particles sampled from a diffusion flame burning a jet fuel surrogate.

Research findings suggest fundamental models of soot formation are not completely accurate. Molecular processes of soot formation in diffusion flames, when the oxidizer combines with the fuel by diffusion, may be more complex than previously thought. By providing a more complete understanding of the chemical nature of soot particles, this research could ultimately lead to improved climate-model representations of anthropogenic soot's chemical and physical properties, greater insight into the role of soot in cloud formation and cleaner aviation engines through more accurate soot models.

Funding: Portions of this research were funded by the Chemical Imaging Initiative, Laboratory Directed Research and Development Program at Pacific Northwest National Laboratory; the Department of Energy's Office of Biological and Environmental Research; National Research Council Research Associateship Award at Wright-Patterson Air Force Base; University of Dayton Research Institute Shock Tube Lab; Combustion Energy Frontier Research Center, an Energy Frontier Research Center funded by DOE's Office of Basic Energy Sciences; Natural Sciences and Engineering Research Council of Canada; and BioFuelNet Canada.

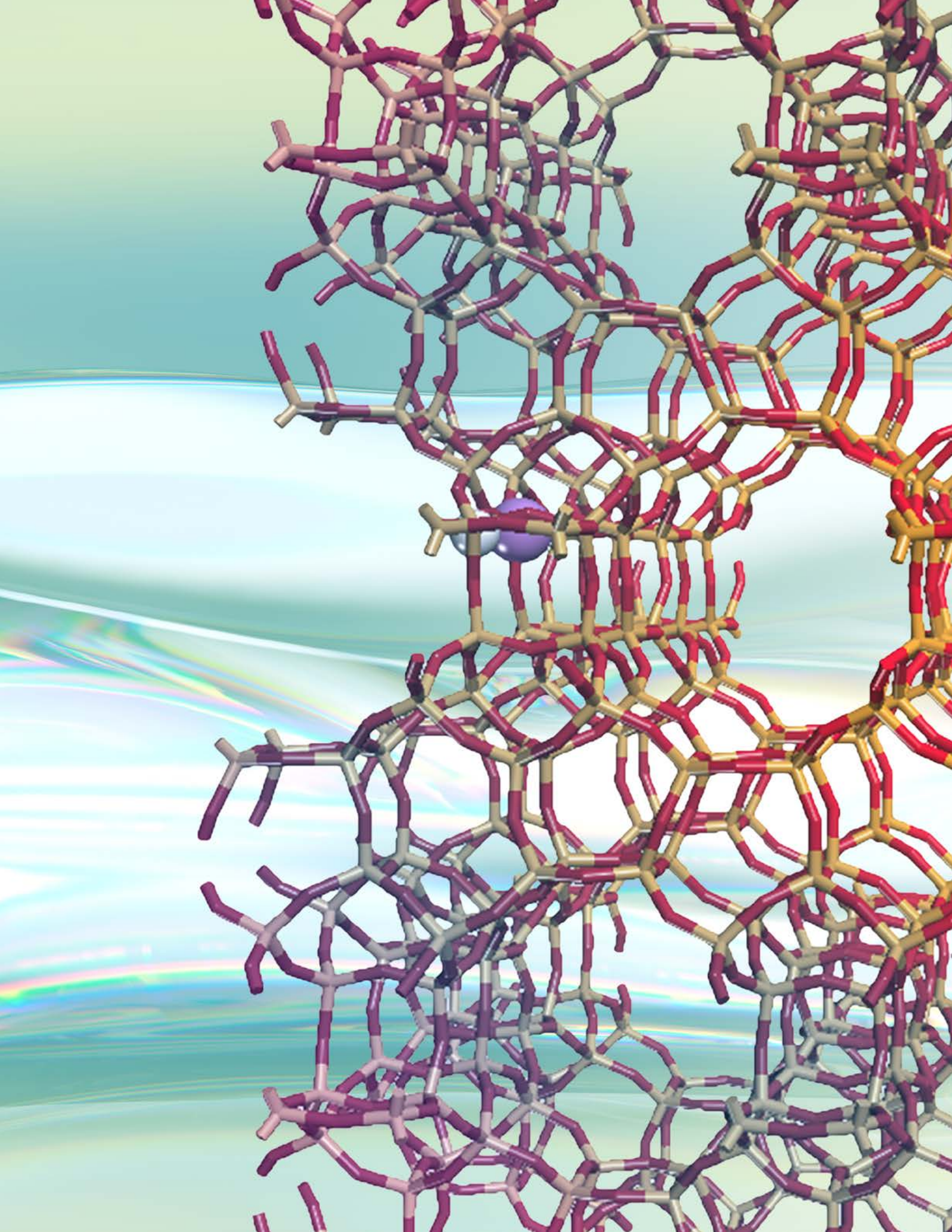
Publication: Cain J, A Laskin, M Kholghy, M Thomson and H Wang. 2014, "Molecular Characterization of Organic Content of Soot Along the Centerline of a Coflow Diffusion Flame." *Physical Chemistry Chemical Physics* 16:25862-75. DOI:10.1039/C4CP03330B.

Participating Organizations: University of Dayton Research Institute, University of Toronto, Stanford University, PNNL and EMSL.



About this Art

An intricately structured soil bacterium, less than a micron in size, makes its home on the root surface of an Arabidopsis plant. Much remains to be learned about the plant root zone – or rhizosphere – and its microbial communities and influence on environmental processes. A research campaign at EMSL is offering insights. The campaign includes scientists from EMSL, Pacific Northwest National Laboratory, the DOE Joint Genome Institute, Brookhaven National Laboratory, the University of Minnesota and the University of Missouri. The effort, funded by DOE's Office of Biological and Environmental Research, is focused on understanding how the presence and distribution of carbon within the root zone impacts the diversity and function of the rhizosphere microbial community. This soil bacterium was imaged using the Helios Nanolab dual-beam focused ion beam/scanning electron microscopy, or FIB/SEM, at EMSL.

Team members

Ljiljana Paša-Tolić, Alice Dohnalkova, Galya Orr, David Hoyt, Heather Brewer, Meng Markillie and Angela Norbeck of EMSL; Kevin Minard and Charles Ansong of PNNL; Susannah Green Tringe at DOE JGI; Richard Ferrieri at BNL; Mike Sadowsky and Chanlan Chun of the University of Minnesota; and Gary Stacey, Yaya Cui and Lihui Song of the University of Missouri. (Image colorized.)