

# DISCOVERY IN ACTION



The Environmental Molecular Sciences Laboratory was dedicated in 1996 and opened its doors to the global research community in 1997. Since then, EMSL has welcomed more than 12,000 researchers to build cross-disciplinary teams as they tackle some of the most challenging scientific issues facing the nation.

## Opening doors to collaboration

*This is the ninth of a 12-part series that features some of the scientific challenges PNNL has tackled over its 50-year history and highlights its vision for the future. PNNL is one of 10 national laboratories overseen by the U.S. Department of Energy's Office of Science and has been managed by Battelle since its inception in 1965. Through this enduring partnership—and by working closely with sponsors and collaborators—PNNL builds upon its legacy to advance science and solutions that improve the lives of Tri-Citians and people around the world. This edition focuses on EMSL, or the Environmental Molecular Sciences Laboratory, a DOE national user facility on PNNL's campus that makes scientific capabilities—people, instruments and facilities—available to the global research community.*

### PACIFIC NORTHWEST NATIONAL LABORATORY

Solving scientific challenges often takes time, teams, tools and tenacity. Understanding the chemical nature of manmade soot particles, how they form and how they contribute to climate change is certainly no different.

A study by collaborators from several research institutions working together and using the unique tools of EMSL—a Department of Energy national user facility also known as the Environmental Molecular Sciences Laboratory—suggests that fundamental models of soot formation are not completely accurate.

Researchers from EMSL, the University of Dayton Research Institute, the University of Toronto and Stanford University examined the chemical composition of young soot particles in diffusion flames of a jet fuel surrogate blend. In diffusion flames, combustion takes place at the flame surface only and the interior of the flame contains unburnt fuel like that of a candle. The scientists relied upon EMSL's specialized instruments, including high-resolution spectrometers and a technique called nanospray desorption electrospray ionization, to conduct their study.

Their research could ultimately lead to improved climate-model representations of the chemical and physical properties of anthropogenic soot, greater insight into the role of soot in cloud formation and cleaner aviation engines through more accurate soot models.

Projects like this illustrate the collaborative research made possible by EMSL, which is located on Pacific Northwest National Laboratory's campus and funded and sponsored by the DOE's Office of Biological and Environmental Research.

"At the end of the day, our mission is scientific impact—to advance our understanding of the science of complex adaptive systems, whether biological, climate, soil or energy materials," said Allison Campbell, EMSL director. "We accomplish great impact by drawing together members of the scientific community and assembling the people, resources and facilities to solve problems. And we've proven it works."

### From the beginning

EMSL's vision is to pioneer discoveries and effectively mobilize the scientific community to provide the molecular science foundations for DOE's research priorities and our nation's critical biological, environmental and energy challenges. It enables groundbreaking research by connecting the scientific user community to extensive scientific expertise and capabilities, as well as providing an operational environment that supports problem solving beyond what is possible in a typical university, industrial, or even single national laboratory setting.

In the 1980s, William Wiley began articulating the need to create a user facility that would "facilitate

integration between the physical, mathematical and life sciences." Wiley, who was PNNL director from 1984 to 1994, and his team proposed a center for molecular science that would bring together theoreticians with experience in computing modeling of molecular processes and experimentalists from the physical and life scientists.

The team recognized that the ability to characterize, manipulate and create molecules would enable scientific advancements. They helped pioneer the establishment of a user facility that would provide researchers across the nation with advanced instrumentation for molecular-level chemistry with a focus on developing the science and technology necessary to clean up environmental problems at government sites such as Hanford.

EMSL was dedicated in Wiley's honor in October 1996, a few months after he unexpectedly passed away. His wife, Gus, cut the ribbon at the ceremony. The facility began operation about a year later. Since then, scientists from all 50 states and more than 35 countries have used EMSL to support their scientific efforts.

### Come collaborate

EMSL makes its nearly 200 staff members, 150 experimental instruments and a high-performance supercomputer available to the international research community, typically at no cost, through a variety of proposal opportunities. Some of these cutting-edge instruments are truly one-of-a-kind; others are only available at a few research institutions around the world. They include mass spectrometers, microscopes, nuclear magnetic resonance spectrometers, surface characterization tools and more.

PNNL and EMSL staff members work with nearly 700 scientists a year to advance their research in support of DOE's mission to provide innovative solutions to the nation's environmental and energy challenges. Collaborators come from academia, other national laboratories and industry.

### EMSL examples

As a user facility, EMSL provides the scientific expertise and instruments to give researchers a deeper understanding of molecular-level processes. This knowledge helps predict how aerosols and terrestrial systems affect climate; makes possible new clean, affordable and abundant energy; and supports legacy waste cleanup—among other things.

Owned by the U.S. Department of Energy; operated by Battelle; and supported by academic, industrial and governmental collaborators, Pacific Northwest National Laboratory is celebrating 50 years of inspiring and enabling the world to live prosperously, safely and securely. Interdisciplinary teams at PNNL address many of America's most pressing issues in energy, the environment and national security through advances in basic and applied science. With an annual budget of about \$1 billion and nearly 4,300 staff members, Battelle is the largest employer in the Tri-Cities.

Learn more about PNNL at [www.pnnl.gov](http://www.pnnl.gov) and through stories to commemorate 50 years of scientific discovery contributed by employees, retirees and the community at [www.celebrate.pnnl.gov](http://www.celebrate.pnnl.gov).

In the renewable energy arena, a project that included scientists from EMSL, PNNL and Washington University in St. Louis, Mo. is focused on the role of chemical reactions involving reduction and oxidization in blue-green algae called cyanobacteria, which could be used in producing chemicals and biofuels. With the help of EMSL's research capabilities, the team is learning about what causes these bacteria to start and stop photosynthesis and other important energy production functions so they can better use it to make renewable energy.

Recently, EMSL researchers have changed the scientific community's understanding of the behaviors of electrodes in rechargeable batteries, which can help address the need for efficient and reliable energy storage technologies. This advancement stemmed from multiple research efforts by EMSL's Chongmin Wang. In related efforts, scientists from Stanford University, Massachusetts Institute of Technology and Lawrence Berkeley National Laboratory along with EMSL observed the molecular and physical changes that occur during the batteries' actual charge-discharge cycle. Their results will help design new materials for high-capacity, low-cost, long-lasting and environmentally friendly batteries.

Other efforts are focused on understanding climate change, such as research that discovered tiny organic particles in the atmosphere that have been linked to air quality and climate change evaporate hundreds of times slower than was previously assumed. New information like this is helping scientists improve air quality and climate models.

EMSL scientists are helping uncover the processes of hydrology, biology and

chemistry occurring in the soil at a molecular level. They have identified thousands of molecules from organic matter that are present in as little as 100 milligrams, or one-fiftieth of a teaspoon, of soil. And they are developing an understanding of the chemical processes involved in the carbon that is underground and how its lifecycle can impact the atmosphere and, as a result, provide data for climate models in accurately predicting climate change.

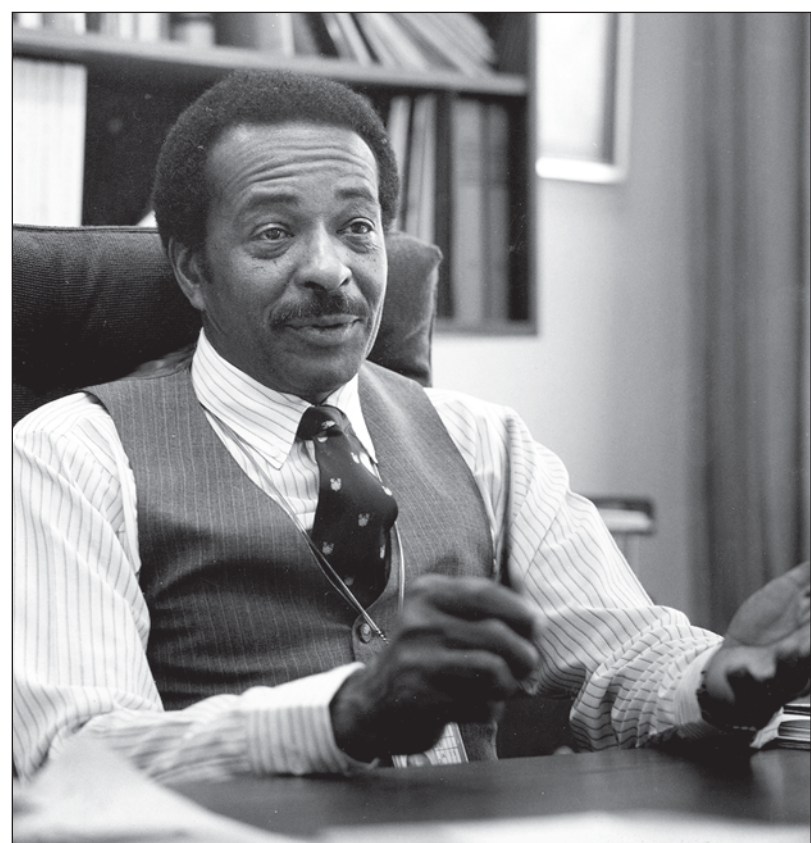
### New additions

In 2009, DOE announced a \$60 million investment in new capabilities for EMSL from the American Recovery and Reinvestment Act. These funds were used to upgrade existing capabilities as well as develop and deploy totally new systems and capabilities, including a Quiet Wing and a radiochemistry facility called RadEMSL.

The Quiet Wing is among the most advanced quiet laboratories in the world for high-resolution imaging capabilities and houses a suite of ultrasensitive microscopy and scanning instruments. RadEMSL opened in 2010 to accelerate scientific discovery and deepen the understanding of the chemical fate and transport of radionuclides in ecosystems at and below the surface.

### The future of science

Collaboration is the future of scientific understanding and innovation. "Team is in our DNA," Campbell said. "PNNL brings together the expertise, instruments, tools, computers and people at EMSL to make collaborations—and discoveries—possible."



The genesis for EMSL can be traced to 1986 when Lab Director William R. Wiley and a handful of his senior managers met to discuss how PNNL could respond to scientific challenges facing DOE, as identified in the National Academy of Sciences report entitled "Opportunities in Chemistry." Today, EMSL leads molecular-level discoveries for DOE that translate to predictive understanding and accelerated solutions for national energy and environmental challenges.



EMSL scientists collaborated with university researchers to study how one cyanobacterium performed photosynthesis during the day and nitrogen fixation at night. They characterized the cellular response network that governed bioenergy production in these cyanobacteria under different environmental conditions. (Image colorized.)



Scientists from around the world can advance their understanding of carbon cycling, microbial biology and climate change using a new 21 Tesla Fourier Transform Ion Cyclotron Resonance mass spectrometer, one of many specialized research instruments available to the research community at EMSL.