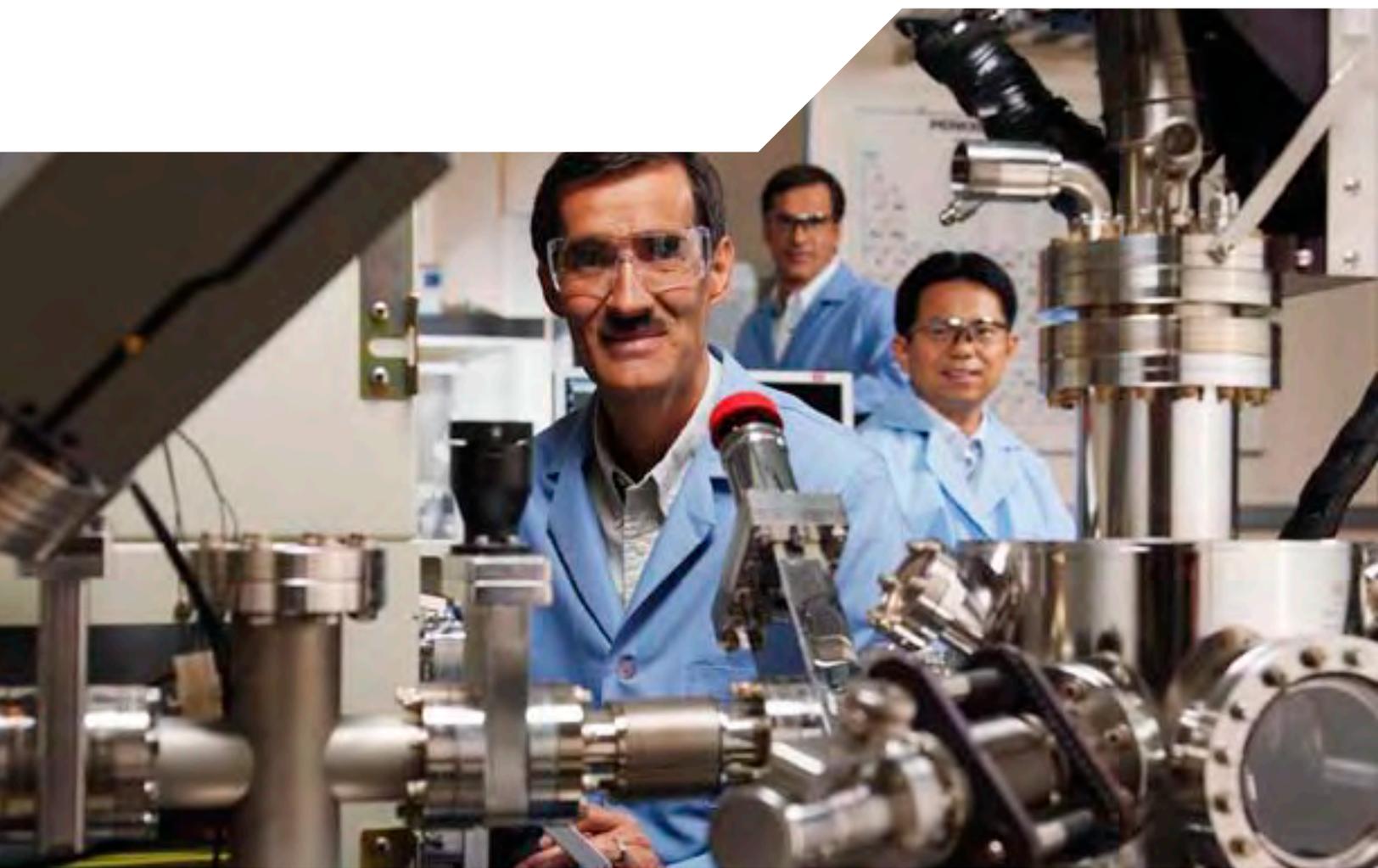


# State-of-the-Art Capabilities



## EMSL's Mission

EMSL, a U.S. Department of Energy national scientific user facility located at Pacific Northwest National Laboratory in Richland, Washington, provides integrated experimental and computational resources for discovery and technological innovation in the environmental molecular sciences to support the needs of DOE and the nation.

## Overview

EMSL's distinctive focus on integrating computational and experimental capabilities as well as collaborating among disciplines yields a strong, synergistic scientific environment. Bringing together experts and state-of-the-art instruments critical to their research under one roof, EMSL has helped thousands of researchers use a multidisciplinary, collaborative approach to solve some of the most important national challenges in energy, environmental sciences, and human health. EMSL houses an unparalleled collection of state-of-the-art capabilities used to address complex scientific challenges. Researchers from around the world are encouraged to use EMSL's unique capabilities in combination with each other with an emphasis on merging computational and experimental instruments.

## Kinetics and Reactions



EMSL's kinetics and reactions capabilities are designed for a research focus on surface processes as well as gas-phase cluster and solution-phase studies. Specific capabilities include photoelectron spectroscopy, catalysis, desorption, molecular beam kinetics tools, high-pressure catalysis reaction chambers attached to ultra-high vacuum instruments and Fourier Transform Infrared spectroscopy, high-resolution electron energy loss spectroscopy, and transient kinetic analyses.

These capabilities enable EMSL users to study the dynamics and kinetics of molecular interactions at a variety of surfaces and interfaces with exceptional resolution.

## Deposition and Microfabrication



EMSL offers deposition and microfabrication tools that can be used to tailor surfaces, atom by atom. With an emphasis on oxide mineral films and interfaces, users apply these tools to design and construct materials of various size distributions, ranging from high-quality, single-crystal thin films to nanostructures, with real-world applications. These materials are subsequently characterized and studied in detail using EMSL's mass spectrometry, microscopy, as well as spectroscopy and diffraction capabilities.

## Computing

EMSL's flagship computing resources include a high-performance, massively parallel supercomputer; premiere computational chemistry software; and graphics and visualization capabilities. These computational tools support a wide range of experimental activities in environmental molecular research—such as benchmark calculations on small molecules, reliable calculations on large molecules and solids, simulations of large biomolecules, and reactive chemical transport modeling.





## Subsurface Flow and Transport

EMSL users can employ subsurface flow and transport capabilities to focus on the application of fundamental physical chemistry concepts to the study of chemical reactions in heterogeneous natural material, with an emphasis on soil and subsurface systems. EMSL's approach to subsurface flow and transport studies is holistic, integrating flow cells, analytical tools, and predictive modeling capabilities to study the fate and transport of environmental contaminants, including metals, radionuclides, and chemicals.

## Microscopy



EMSL houses a wide variety of sophisticated microscopy instruments, including electron microscopes, optical microscopes, scanning probe microscopes, and computer-controlled microscopes for automated particle analysis. These tools are used to image a range of sample types with nanoscale—and even atomic—resolution with applications to surface, environmental, biogeochemical, atmospheric, and biological science.

## NMR and EPR



EMSL houses NMR instruments with frequencies up to 900 MHz, as well as an electron paramagnetic resonance spectrometer. EMSL staff are active in developing a variety of probes and techniques to complement their collection of state-of-the-art magnets. Research areas within this capability group involve interfacial and in situ chemistry and biology, environmental chemistry, and metallocomplexes.

## Spectroscopy and Diffraction



A suite of spectroscopy and diffraction instruments in EMSL allow users to study solid-, liquid-, and gas-phase sample structure and composition with remarkable resolution. Ideal for integrated studies, spectrometers and diffractometers are easily coupled with EMSL's computational and modeling capabilities, allowing EMSL users to apply a multifaceted research approach for experimental data interpretation and to gain a fundamental understanding of scientific problems.

## Mass Spectrometry

EMSL's mass spectrometry capabilities enable high-throughput, high-resolution analysis of complex mixtures. These resources are applied to a broad range of scientific problems from proteomics studies with applications to human health and environmental remediation to aerosol particle characterization, as well as fundamental studies of ion-surface collisions and preparatory mass spectrometry using ion soft-landing.



## About EMSL

EMSL offers researchers worldwide a comprehensive array of leading-edge resources – at one location – that are available on a peer-reviewed proposal basis. Proposals are encouraged to be submitted for research centered around EMSL's four science themes, which represent growing areas of research: Atmospheric Aerosol Chemistry, Biological Interactions and Dynamics, Geochemistry/Biogeochemistry and Subsurface Science, and Science of Interfacial Phenomena. Researchers may use EMSL's state-of-the-art instruments and world class experts at no cost if research results are shared in the open literature.



## Contact EMSL

**Nancy Hess**

Phone: 509-371-6385 | Email: [nancy.hess@pnl.gov](mailto:nancy.hess@pnl.gov)

**David Hoyt**

Phone: 509-371-6545 | Email: [david.hoyt@pnl.gov](mailto:david.hoyt@pnl.gov)

**Roy Gephart**

Phone: 509-371-6142 | Email: [roy.gephart@pnl.gov](mailto:roy.gephart@pnl.gov)

**Erich Vorpapel**

Phone: 509-371-6448 | Email: [erich.vorpapel@pnl.gov](mailto:erich.vorpapel@pnl.gov)

**Ljiljana Paša-Tolić**

Phone: 509-371-6585 | Email: [ljiljana.pasatolic@pnl.gov](mailto:ljiljana.pasatolic@pnl.gov)

**Theva Thevuthasan**

Phone: 509-376-1375 | Email: [theva@pnl.gov](mailto:theva@pnl.gov)

**Kevin Regimbal**

Phone: 509-371-6075 | Email: [kevin.regimbal@pnl.gov](mailto:kevin.regimbal@pnl.gov)

**Bert de Jong**

Phone: 509-371-6476 | Email: [wibe.dejong@pnl.gov](mailto:wibe.dejong@pnl.gov)

