William R. Wiley
EMSL
Environmental Molecular Sciences Laboratory

A NATIONAL USER FACILITY FOR THE SCIENTIFIC COMMUNITY

The William R. Wiley Environmental Molecular Sciences Laboratory (EMSL) is the cornerstone of the U.S. Department of Energy's commitment to provide world-class research capabilities for enabling fundamental research on the physical, chemical, and biological processes. A more thorough understanding of these processes lays the foundation for new solutions to environmental problems and other critical issues.

Equipped with over 100 major instrument systems for use by the research community, EMSL facilitates multidisciplinary approaches to complex scientific problems and provides a climate for advancement and education in the molecular and computational sciences. As a national scientific user facility and research organization, EMSL's mission is to

- Provide innovative experimental and computational resources to scientists engaged in fundamental research on key physical, chemical, and biological processes.
- Conduct fundamental research in molecular and computational sciences, through the user program, to meet DOE's missions and support other government agencies.
- Educate students and scientists to meet the demanding multidisciplinary challenges of the future.

EMSL offers, at one location, a comprehensive array of leading-edge resources available on a peer-reviewed proposal basis. To best meet their own special needs, users may define combinations of equipment and capabilities from six research facilities. Staff members work with users to expedite access to the facilities and enhance the user's experience. Researchers from around the world who share their results from their selected proposals in the open literature are given access to the EMSL – at no cost.

The William R. Wiley Environmental Molecular Sciences Laboratory is operated by Pacific Northwest National Laboratory for the U.S. Department of Energy (DOE) Office of Biological and Environmental Research. EMSL is located in Richland, Washington.






CHEMISTRY AND PHYSICS OF COMPLEX SYSTEMS FACILITY

fosters fundamental research in the natural sciences to provide the basis for new and improved energy technologies and for understanding and mitigating the environmental impacts of energy use and contaminant releases.

Representative Research Activities

Researchers develop molecular information about processes occurring at the interface among environmentally important liquids, solids, and gases. In addition, they work to obtain a mechanistic understanding of chemical transformations of molecules and materials driven by thermal, radioactive, or optical sources. Additional themes of research within this facility include providing a molecular-level understanding of solvation and subsequent reactions in simple and complex systems related to the chemistry of complex wastes, contaminated solids and groundwater, and other natural systems; single-molecule spectroscopy and high-resolution imaging techniques for studying biological systems; and development of instrumentation for real-time analyses of chemical and biological natural or human-made species.

Instrumentation:

- High-intensity and high-sensitivity surface chemistry systems
- Systems for thermal and non-thermal interfacial chemistry research
- Single-molecule and non-linear imaging microscopy systems
- Systems for molecular-scale synthesis and characterization of model materials
- Electron microbeam for live cell radiation biology research
- Environmental scanning electron microscope

ENVIRONMENTAL SPECTROSCOPY AND BIOGEOCHEMISTRY FACILITY

is involved in experimental and modeling studies of chemical phenomena and mechanisms on mineral and microbe surfaces and on complex heterogeneous environmental materials from soils, sediments, and groundwater zones.

Representative Research Activities

The research performed in this facility results in improved microscopic models of environmental processes that can be applied to the real world. Research capabilities include materials characterization, aqueous-phase and solid-phase speciation and reaction/kinetic measurements, analytical environmental chemistry, modeling of molecular and thermodynamic geochemical processes, and large-scale reactive-transport studies. A research staff with broad interests in mineral surface chemistry, biogeochemistry, thermodynamics, environmental spectroscopy, and molecular modeling use the facility and are available for collaborative research and to assist users in integrating results of experiments and modeling. Some of the equipment used to further the research within this facility is as follows:

Instrumentation:

- Laser-induced fluorescence, nonlinear, photoacoustic, Raman, and ultraviolet-visible spectrometers, streak camera, confocal microscope, and lasers
- Near-mid-far Fourier transform infrared spectrometer/microscope
- Mossbauer and electron paramagnetic resonance spectrometers
- Scanning tunneling and atomic force microscopes
- Multi-fluid flow/transport cells
- Geochemistry molecular modeling software
- General analytical equipment

HIGH-FIELD MAGNETIC RESONANCE FACILITY

provides state-of-the-art nuclear magnetic resonance (NMR) and electron paramagnetic resonance (EPR) instrumentation for determining molecular structures that impact environmental remediation and biological health effects.

Representative Research Activities

Staff within this facility offer expertise in the areas of structural biology, solid-state materials/catalyst characterization, magnetic resonance imaging (MRI) techniques, and high-resolution spectroscopy of biological objects using a slow (1-100 Hz) magic angle spinning. Research activities include structure determination of large molecular assemblies such as protein, DNA (normal and damaged), and RNA complexes as a cellular response to chemical or radiological insults; conformational changes in membrane protein complexes involving metal clusters as followed by pulsed EPR; NMR-based structural and functional genomics; materials and catalyst characterization via solid-state techniques; non-invasive biological imaging, integrated magnetic resonance and confocal microscopy and slow spinning NMR to study cell systems.

Instrumentation:

- Twelve NMR spectrometers (ranging from 300 to 900 MHz) and one pulsed EPR spectrometer, with capabilities in high-field liquid-state, solid-state and micro-imaging techniques
- Combined optical and magnetic resonance microscope
- Low temperature probes for metallo-protein chemistry and structure
- Virtual NMR capability to enable use and collaboration with EMSL scientists for remote users via secure shell over the internet







HIGH-PERFORMANCE MASS SPECTROMETRY FACILITY

provides cutting-edge mass spectrometry capabilities that focus on global proteomics research and allow visualization and analyses of proteins of a cell in greater detail than before.

Representative Research Activities

This facility provides state-of-the-art instrumentation for challenging research in areas such as proteomics, cell signaling, cellular molecular machines, and high-molecular weight systems, in general. The research activities conducted within this facility include proteomic analyses of whole cell lysates, analyses of organic macromolecules and protein complexes, quantitation using isotopically labeled growth media, targeted proteomics analyses of subcellular fractions, and nucleic acid analysis of RNA and DNA oligomers. The facility's capabilities of providing very high-sensitivity and high-resolution mass spectrometry and very high-resolution separations greatly benefit these areas of research and are enhanced by the equipment listed below.

Instrumentation:

- Four Fourier Transform Ion Cyclotron Resonance mass spectrometers, 3.5, 7, 9.4, and 11.5 tesla with electrospray ionization sources
- Sciex QSTARR quadrupole time-of-flight mass spectrometer
- Five Finnigan LCQ ion trap spectrometers
- Finnigan TSQ 7000 triple quadrupole spectrometer
- Ultra-high pressure liquid chromatographs

INTERFACIAL AND NANOSCALE SCIENCE FACILITY

is involved in researching a variety of oxide mineral films and interfaces, nanoscale materials, electronic and catalysis materials, microfabrication and microanalytical separations, and sensing.

Representative Research Activities

A unique environment is provided for research in areas such as nanoscience and nanotechnology; heterogeneous catalysis; environmental interfaces, including aerosols and minerals; materials interfaces and chemoselective interfaces; and areas within micronanalytical science, such as chemical sensing and microfluids. Portable deposition, electrochemical, and optical experimental stations located in this facility can be linked to analysis chambers to create unique experimental arrangements. Facilities are also available for material synthesis using thin film deposition and chemical synthesis, ion beam processing and analysis, surface and bulk characterization, catalytic reaction, microfabrication, electron microscopy and x-ray analysis, and microanalytical systems development and testing.

Instrumentation:

- Molecular beam epitaxy and chemical vapor and sputter deposition
- State-of-the-art surface science tools
- High-resolution electron microscopes and x-ray diffraction instrumentation
- Ultrahigh vacuum, liquid, and ambient environment scanning probes
- Gas chromatography, NO_x analyzer, and RX100 testing and characterizing system
- Research tools for microfabrication and clean-room capabilities

MOLECULAR SCIENCE COMPUTING FACILITY

provides a high-performance computer, using Intel Itanium2 processors Quadrics interconnect and HP RX2600 nodes, which supports a wide range of environmental molecular science.

Representative Research Activities

This facility provides capabilities for researchers at hundreds of sites across the world to use object-oriented, massively parallel and extremely scalable software developed by PNNL to conduct research and develop applications such as groundwater flow simulations; geochemical applications; modeling of chemistry on porous sites; heavy element chemistry; and molecular thermodynamics, kinetics, and prediction of excited states. Researchers are also developing models that approach nanosize particles (e.g., nanotubes) and examine biological systems. A Graphics and Visualization Laboratory within this facility provides researchers with visualization capabilities of large data sets generated by the facility's computing equipment. A web site detailing this facility's capabilities is available at http://mscf.emsl.pnl.gov/.

Instrumentation:

- 256-processor system with 1.5 terabytes of memory (Upgrade, summer of 2003, to a next-generation Intel processor based system with a peak performance of 11.4 teraflops and 6.8 TB of memory)
- Silicon Graphics 3400 graphics and visualization server with integrated video and audio editing system
- Molecular Science Software Suite, including NWChem, Extensible Computational Chemistry Environment, and ParSoft.

ACCESS TO EMSL

Researchers can request access to EMSL facilities by submitting proposals. The online proposal system is available at http://sos.emsl.pnl.gov:2080/EUS. Proposed research is peer-reviewed for

- Scientific merit and technical expertise of the investigators.
- Appropriateness for the facilities or capabilities being requested.
- Relevance to DOE missions.

A user agreement must be signed before access to the facility can be granted. Users must also abide by EMSL Standard Practices and Procedures while using the facility. EMSL staff members provide support and appropriate training and determine, in consultation with users, schedules for access to equipment and capabilities.

EMSL supports both open and proprietary research. Users engaged in open research are generally not charged for using EMSL facilities or equipment. A limited amount of proprietary research may be conducted in the EMSL and users engaged in proprietary research are obligated to pay the full cost recovery rate for use of the facility.

For questions about submitting proposals for accessing EMSL resources and capabilities, please contact EMSL User Services at 509-376-2553 or userservices@emsl.pnl.gov.

USER HOUSING

A User Housing Facility is open on the campus of the Pacific Northwest National Laboratory. The 28,000-square-foot building affords short/medium-term housing close to the PNNL campus for

- Visiting scientists, engineers, students, and faculty who use EMSL or other research facilities.
- Students and faculty who come to the Lab through our science education programs.

For further information about the User Housing Facility, see http://www.pnl.gov/uhf or, for local hotels visit the community website at http://www.visittri-cities.com/.

http://www.emsl.pnl.gov

CONTACTS

J.W. (Bill) Rogers, Jr.
Director
Telephone: 509-376-5328
Facsimile: 509-376-6742
Email: jw.rogers@pnl.gov

Allison A. Campbell
Associate Director
Telephone: 509-376-6688
Facsimile: 509-376-6742
Email: allison.campbell@pnl.gov

Marty Peterson
Associate Director
Telephone: 509-376-3797
Facsimile: 509-376-6742
Email: marty.peterson@pnl.gov

Pacific Northwest National Laboratory
Operated by Battelle for the U.S. Department of Energy

Office of Science
U.S. DEPARTMENT OF ENERGY