William R. Wiley
EMSL
Environmental Molecular Sciences Laboratory

A DOE User Facility for the Scientific Community

I would like to introduce you to the William R. Wiley Environmental Molecular Sciences Laboratory (EMSL). EMSL is a U.S. Department of Energy (DOE) national scientific user facility and is the centerpiece of DOE's commitment to providing world-class experimental, theoretical, and computational capabilities for solving the nation's environmental problems. The facility is equipped with over 100 major instrument systems for use by the research community. In addition, our resident scientists conduct fundamental research in areas relevant to DOE missions and provide expert assistance to users.

EMSL capabilities are used to address the fundamental science that will be the basis for finding solutions to national environmental issues such as cleaning up contaminated areas at DOE sites across the country and developing "green" technologies to reduce or eliminate future pollution production. The capabilities also are used to further our understanding of global climate change and environmental issues relevant to energy production and use and health effects resulting from exposure to contaminated environments. The use of EMSL capabilities to address these issues is generally free of charge as long as the user intends to publish the results in the open literature.

If you are interested in collaborating with our scientists or using the facility's capabilities, please visit our web site or contact any of the individuals listed at the end of the brochure. More information and specific procedures for becoming an EMSL user can be found on our web site at http://www.emsl.pnl.gov.

My staff and I look forward to seeing you at the EMSL.

Jean H. Futrell

Jean H. Futrell, Ph.D.
Director

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

The EMSL is located at Pacific Northwest National Laboratory in Richland, Washington, adjacent to the DOE Hanford Site.

The Laboratory

The William R. Wiley Environmental Molecular Sciences Laboratory (EMSL) is a U.S. Department of Energy (DOE) scientific user facility and research organization that focuses on DOE and national issues. The facility is operated by Pacific Northwest National Laboratory (PNNL) for the DOE Office of Biological and Environmental Research (BER).

As a national scientific user facility and a research organization, the mission of EMSL is to:

- provide advanced resources to scientists engaged in research on critical environmental problems and other national issues, including health issues related to exposure to contaminated or hazardous environments
- conduct fundamental research on the physical, chemical, and biological processes that underpin critical environmental issues
- educate young scientists in the molecular sciences to meet the demanding environmental challenges of the future
- advance molecular science in support of DOE missions.

The Challenge

The environment is a coupled set of physical, chemical, and biological systems with complex, interrelated dynamics that determine the condition of the biosphere. An understanding of the fundamental processes that govern these systems is needed to help mitigate past mistakes, to anticipate the impact of current human activities, including human health, and to avoid further environmental insults in the future.

Specific environmental challenges that society must face include pollution from the production of toxic chemicals by industrial processes, clean up of contaminated groundwater and hazardous waste disposal sites, and understanding the implications of global climate change.

The Response

EMSL was created to generate the fundamental scientific knowledge needed to solve the complex environmental problems that are a legacy of the nation's nuclear weapons production activities. With its resident research staff and advanced capabilities, EMSL facilitates the multidisciplinary approaches needed to address complex scientific and technical phenomena relevant to DOE missions and the nation's environmental challenges.

EMSL Research

EMSL research focuses on attaining a molecular-level understanding of the physical, chemical, and biological processes that underlie the most critical environmental issues facing the DOE.

- *waste processing*—to provide a technical basis for retrieving, separating, converting, disposing, and minimizing waste streams ranging from DOE radioactive and hazardous wastes to industrial pollutants
- *contaminant fate and transport*—to understand the transformation and migration of contaminants in soils and groundwater, and to assist in developing innovative solutions for passive and active remediation of contaminated lands
- *cellular response to environmental contaminants*—to provide improved understanding of biomolecular structure, function, interaction, and response through development of new cellular characterization, analysis, and imaging approaches
- *atmospheric chemistry*—to provide insight into molecular processes in the gas phase and at gas/liquid and gas/solid interfaces, and to develop unique computational tools and experimental instruments for identifying and characterizing important tropospheric molecules and their reactions and the formation of aerosols.

The EMSL is a key player in national research programs focused on environmental issues, such as the Environmental Management Science Program and the Natural and Accelerated Bioremediation Research Project. Both programs are funded and managed by DOE.

The expertise of our staff and the facility's capabilities also are contributing to research undertaken in the Environmental Molecular Science Institutes (EMSI) funded at Columbia University and Northwestern University by the National Science Foundation and DOE. Each EMSI provides a unique program for academic scientists, engineers, and students to work with colleagues from industry and national laboratories to improve understanding of how nature and technology affect environmental systems at the molecular level.

800-MHz nuclear magnetic resonance spectrometer in the High Field Magnetic Resonance Facility

Research Facilities

EMSL offers at one location a comprehensive array of state-of-the-art equipment for research in the environmental molecular sciences. These capabilities can be integrated as needed by multidisciplinary teams of scientists to address complex problems. EMSL equipment and capabilities are grouped into seven facilities:

- High Field Magnetic Resonance Facility
- High Field Mass Spectrometry Facility
- Molecular Science Computing Facility
- Nanostructural Materials Facility
- Interfacial Structures and Compositions Facility
- Reactions at Interfaces Facility
- Gas- and Liquid-Phase Monitoring and Detection Facility.

The High Field Magnetic Resonance Facility, the High Field Mass Spectrometry Facility, and the Molecular Science Computing Facility house suites of specialized and unique capabilities. In contrast, the Nanostructural Materials Facility, the Interfacial Structures and Compositions Facility, the Reactions at Interfaces Facility, and the Gas- and Liquid-Phase Monitoring and Detection Facility are made up of unique or state-of-the-art capabilities and equipment from laboratories throughout the EMSL.

Descriptions of and the points-of-contact for these seven facilities follow.

High Field Magnetic Resonance Facility

Contact: David W. Koppenaal

Description. The High Field Magnetic Resonance Facility contains state-of-the-art nuclear magnetic resonance (NMR) and electron paramagnetic resonance (EPR) instrumentation. This instrumentation is used for molecular structure determinations in environmental and biological health effects studies. The instrumentation includes high-field NMR systems (800-MHz, 750-MHz, and two 600-MHz NMR spectrometers) in addition to more conventional NMR systems (two 500-MHz, a 400-MHz, and two 300-MHz NMR spectrometers). Several EPR spectrometers equipped with ENDOR capabilities complement the NMR capabilities. A multiprocessor SGI Origin 2000 computer system provides the data analysis and computing platform for these capabilities. The EMSL virtual NMR capability facilitates access to the facility's capability by offsite users. This capability allows Internet access and combines secure, remote operation of the NMR spectrometers with real-time audio/videoconferencing, computer display sharing, a web-based Electronic Notebook, remotely controlled laboratory cameras, and other unique features. Researchers thus can participate in many aspects of experiments in the EMSL magnetic resonance facility without having to leave their home institution.

Use. The NMR and EPR instrumentation are used in a variety of research programs, with current emphasis on structural biology, microimaging, and materials/catalysis focus areas.

The facility is engaged in molecular structure determination of large molecular assemblies, including proteins and DNA (normal or damaged), as they relate to cellular response and bioremediation effects. An example of such an application is the complex formed in the initial stages of DNA damage recognition. Answers to several questions of interest to researchers are being pursued. How is damage to DNA recognized? What is the structural basis for this damage recognition? The results of such investigations can be coupled to research involving cellular imaging, another area of recent interest. The chief objective of the cellular imaging research is to enable high-resolution visualization of cellular events while providing unique and detailed chemical information. This latter objective lies at the heart of the cellular characterization capabilities being developed at PNNL to enable research related to environmental health issues. In the area of materials/catalysis characterization, the facility takes advantage of the laboratory's solid-state NMR and EPR instrumentation and expertise.

Development of capabilities for high-pressure supercritical fluid work and in situ characterization of heterogeneous and homogeneous catalytic processes is underway in this area.

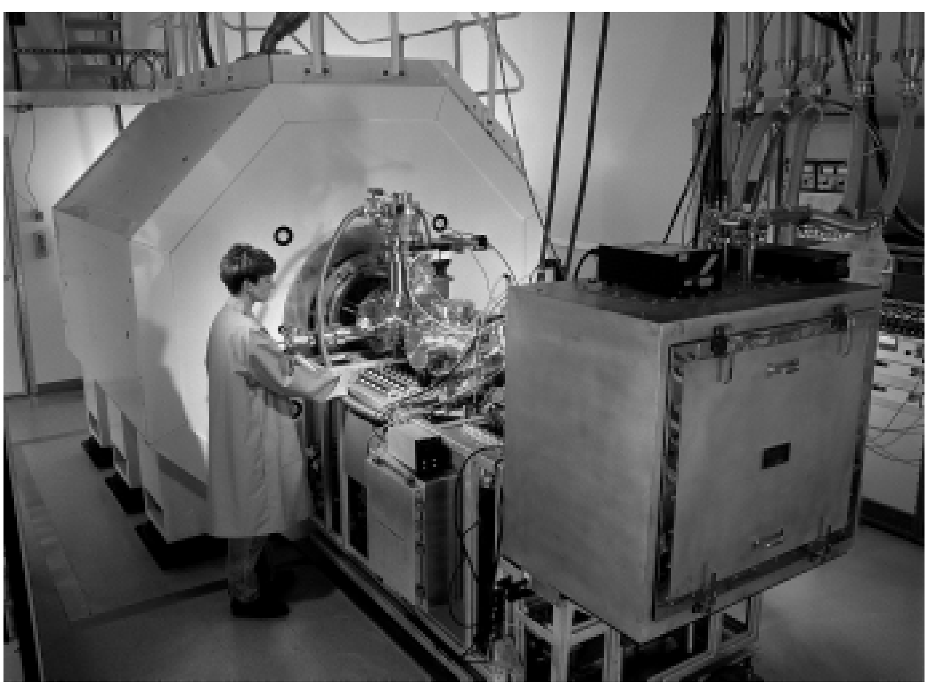
High Field Mass Spectrometry Facility

Contact: David W. Koppenaal

Description. The High Field Mass Spectrometry Facility contains the world's first 11.5-tesla magnetic field Fourier transform ion cyclotron resonance (FTICR) mass spectrometer and state-of-the-art 3.5- and 7-tesla FTICR instruments. This facility specializes in biological and biomedical applications of ultrasensitive and ultrahigh resolution FTICR mass spectrometry and also provides a broad array of other mass spectrometry capabilities to the user community. Current research and unique capabilities focus on mass spectrometry technology improvements aimed at biological applications of these techniques for post-genomic era research.

Use. Capabilities under development aim at improving the ability to manipulate and characterize extremely small biological samples and extending to the realm of single cells using capillary electrophoresis combined with mass spectrometry. Of particular note are capabilities for rapid and precise characterization of proteomes, which are the broad protein complements expressed by cells at a given time or in response to an environmental perturbation. This avenue of research is initially being applied to microbial systems, such as Deinococcus radiodurans, and eukaryotic systems such as yeast. Studies aim to determine and understand how the proteome responds to environmental stresses so as to improve risk assessment and to provide a scientific basis for mitigation of possible adverse health effects.

By applying perturbations (e.g., radiation damage) to microorganisms or cell populations, the systems-level responses of the proteome can be studied in a holistic fashion. Capabilities for producing isotopically distinctive versions of proteomes have been developed and are used to provide "internal standards" for entire proteomes. These methodologies allow precise measurement of the results of perturbations for large numbers of proteins in a single analysis.



11.5-Tesla FTICR Instrument in the High Field Mass Spectrometry Facility

Molecular Science Computing Facility

Contact: David A. Dixon

Description. The Molecular Science Computing Facility (MSCF) contains a high-performance, massively parallel, 512-processor IBM RISC System/6000 Scalable POWERparallel (IBM SP) computer system. The system currently has 262 gigabytes of memory, ~5 terabytes of disk space, and 250 gigaflops of peak performance; a 96-processor IBM SP parallel computer system (with symmetric multiprocessor nodes—16 four-way nodes and 4 eight-way nodes) with an aggregate peak performance of 71 gigaflops; and a 20-terabyte EMASS hierarchical storage management system with EMSL Scientific Data Management software. A high-performance Silicon Graphics Onyx graphics and visualization system and an integrated digital video and audio editing system support the MSCF Graphics and Visualization Laboratory (GVL). The GVL also has the first version of IBM's Scalable Graphics Engine, which connects directly to the switches of the massively parallel computers to provide extremely high data and image analysis throughput.

A new generation of software, the Molecular Science Software Suite (MS^3) has been developed in the EMSL to take full advantage of the advanced computing systems installed in the MSCF. MS^3 is a comprehensive, integrated set of tools that enables chemists to easily couple the power of advanced computational chemistry techniques with existing and rapidly evolving high-performance, massively parallel computing systems. MS3 consists of three major components: 1) Northwest Computational Chemistry Software (NWChem), 2) Extensible Computational Chemistry Environment (Ecce), and 3) Parallel Software Development Tools (ParSoft). More detailed information about MS^3 and each of its

512-Processor IBM SP Computer System in the EMSL Molecular Science Computing Facility

components can be accessed via the Capabilities link from the EMSL web site. In 1999, MS[3] received an *R&D 100 Award* as one of the year's top 100 technologically significant new products.

Use. The MSCF supports a wide range of environmental molecular science, from calculations on small molecules at high accuracy to reliable calculations on large molecules including the behavior of actinide-containing compounds and catalysts to simulations of large biomolecules at both the ab initio and molecular dynamics levels. Applications so far include predicting the behavior of the uranyl ion in a broad range of environments; designing novel separation systems for radionuclides; developing highly accurate methods for predicting molecular thermodynamics and kinetics such as reactions of importance in combustion processes; predicting reactions of chlorohydrocarbons in solution; designing catalytic systems based on zeolites; predicting the behavior of silica glasses for waste storage; and modeling the initial nucleation steps in the formation of atmospheric aerosols. In addition, the computing capabilities of the MSCF have been used to study a number of biological systems including charge distributions in lipopolysaccharides, and the behavior of proteins such as acetylcholinesterase, HIV-1 integase, and green fluorescent protein. Other environmental applications include studying the fate and transport of pollutants in the Hanford vadose zone, predicting precipitation levels in the Pacific Northwest based on regional climate models, and developing an atmospheric chemistry code that includes heterogeneous chemistry, transport processes, and gas phase chemistry.

Nanostructural Materials Facility

Contact: J. William Rogers

Description. The Nanostructural Materials Facility is made up of equipment and capabilities that can be focused on the design, synthesis, and characterization of a wide variety of materials with nanodimensional sizes for basic studies and industrial application. Synthesis and processing capabilities include the production and characterization of atomic and molecular clusters (five cluster-generating instruments with laser, photoelectron, and mass spectrometry), production and characterization of particles and colloids (including XRD, field flow fractionation, surface force apparatus), production and characterization of high-quality thin films (including MBE, CVD with SPM, XRD, and LEED), and microfabrication and testing. In addition, a set of bulk-processing (furnaces) and near-surface analysis methods are available (SEM, TEM, Mossbauer, FTIR, RAMAN).

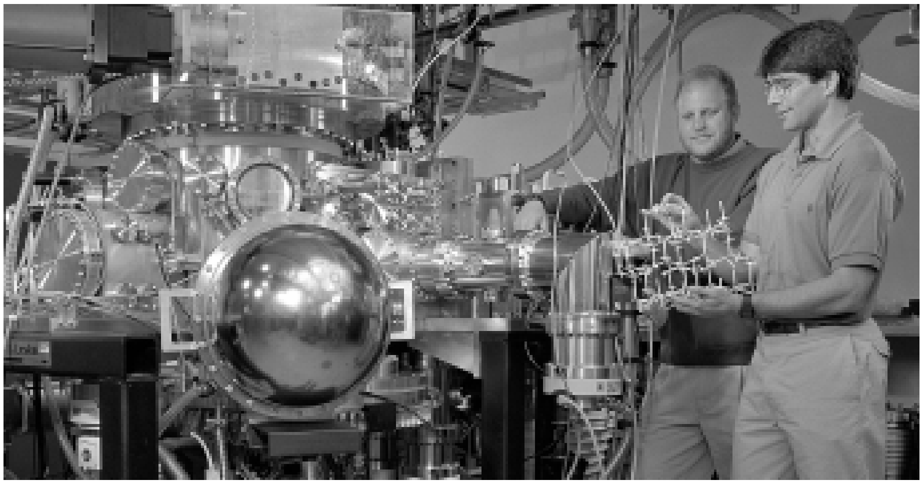
Use. The Nanostructural Materials Facility is directly involved in a wide range of research that ranges from fundamental studies of the unique properties of molecular clusters to the creation of new types of materials for removing contaminants from the environment. Unique well-defined oxide surfaces created by MBE and CVD are being used to gain new levels of information about environmental and biological interactions at surfaces. Microfabrication capabilities are being used to develop new microanalytical capabilities with nuclear waste and biological applications. Staff members are applying other advanced characterization methods to studies as varied as exploring environmental damage to fruit, looking at corrosion of ancient bronzes, and examining nuclear waste form stability.

Interfacial Structures and Compositions Facility

Contact: J. William Rogers

Description. The Interfacial Structures and Compositions Facility includes an extensive range of state-of-the-art equipment used for determining the atomic and molecular structure, defect structure, and compositional and structural variations along and through solid/solid, gas/solid, gas/liquid, and liquid/liquid interfaces. Methods that can probe the atomic or molecular species at interfaces (optical and electron energy loss), map surface topology, structure, and composition (scanning probe microscopy, electron microscopy, and high spatial resolution surface analysis instruments), surface composition (laser, ion, and electron spectroscopies), as well as thin layer composition and depth profiles (energetic ion analysis and sputter profiling) are included. Many of these instruments can be used with a "common" specimen holder that allows specimens to be moved among many systems for synthesis, processing, or analysis without exposure to air.

Use. This set of capabilities is used extensively for a wide range of studies in materials, chemical, processing, and environmental sciences. This facility is extensively used for the study of oxides and minerals as relevant to catalysis, contaminant transport in the environment, and development of biocompatible and other new materials systems. Special portable experimental stations allow state-of-the-art analysis



Molecular Beam Surface Scattering System in the EMSL Reactions at Interfaces Facility

capabilities to be used in combination with synthesis or environmental exposure capabilities to create unique experimental arrangements. These capabilities have been used to examine plasma modified surfaces, stress corrosion cracking, the reactivity of defects on oxide surfaces, and microbe reduction of iron oxides.

Reactions at Interfaces Facility

Contacts: John M. Zachara, Steven D. Colson, J. William Rogers

Description. In the Reactions at Interfaces Facility, environmentally relevant materials and interfaces can be produced and characterized, and their surface chemistry and that of natural materials can be studied under controlled conditions using a broad suite of analytical techniques. The capabilities of this facility typically are used to determine contaminant reaction mechanisms on model or natural surfaces, or as mediated by intra- or extra-cellular microbiologic processes. These capabilities are often used in conjunction with those in the Interfacial Structures and Compositions Facility.

Research in surface chemistry and kinetics is conducted on well-characterized surfaces and interfaces created by controlled deposition and molecular beam epitaxy techniques. Specialized equipment for creating environmentally relevant materials is available in this facility. Supersonic molecular beams and surface analytical techniques, including energy-loss, surface scattering, and laser spectroscopy, are used. Equipment available for this kind of research includes high-vacuum chambers, a surface photochemical system, a low-energy ion beam line, and both low-temperature (20K) and room-temperature scanning tunneling microscopes for imaging molecules on surfaces. Areas of emphasis are dissociative chemisorption processes, reactive scattering, and the trapping and solvation of ions and molecules on ice surfaces. All of these processes are important in environmental chemistry, geochemistry, and aerosol formation.

Energetic reactions occurring in solids and at interfaces are probed under ultrahigh-vacuum conditions using electron-beam and photon sources and a suite of analytical techniques including photoemission, resonance-enhanced multiphoton ionization spectroscopy, mass spectrometry, and infrared absorption spectroscopy. The objective of this research is to develop a detailed molecular-level understanding of the electronic structure and photochemistry of interfaces and adsorbed species, high-energy electron- and photon-stimulated reactions, and the quantum state distributions in reaction products. Applications include the catalytic degradation of hydrocarbon contaminants, the development of analytical techniques for hazardous waste samples and contaminated soils, and understanding high-energy processes that occur in the outer solar system.

Capabilities exist to study the mechanisms of surface chemical reactions of organic and inorganic contaminants on synthetic mineral material (e.g., Al(III), Fe(III), and Mn(IV)-oxides and layer silicates) and on inorganic and organic materials taken from soil, sediment, or subsurface materials. Both in situ and ex situ techniques are available. Equipment for this research includes a full complement of instrumentation for conducting laser spectroscopy (fluorescence, Raman, photoacoustic), FTIR and far-IR spectrometry, conversion electron Mossbauer spectroscopy, and EPR spectroscopy. A variety of unique sample cells are available for spectroscopic studies of different environmental media and for stop-flow kinetic studies. Environmental chambers are available for controlled-atmosphere studies of mineral, microorganism, or soil suspensions. Equipment interfaces exist that allow spectroscopic studies within the chambers. A scanning probe microscopy center with emphasis on water-wet samples and flow-through reaction studies under controlled atmosphere is present to image surface structure and mineral/microbe associations. Various chemical microscopy techniques including IR, fluorescence, and Raman are available for spatially resolved applications.

Also present is a modern analytical laboratory containing instrumentation (e.g., ICP-MS, AA, LC/GC-MS, IC-MS, and capillary electrophoresis) for analysis of a broad array of organic and inorganic solutes that may be experimental targets or byproducts of complex surface or microbial reactions. Nearby is housed a physical chemistry laboratory where a pressure jump apparatus is available for surface kinetic studies and microcalorimetry instrumentation exists for thermodynamic studies of surface reactions.

Use. Much of the chemistry underlying environmental issues occurs on particle or microbial surfaces and at the interfaces with gas, water, or other solids. Interfacial reactions in soil and groundwater control the rate of contaminant migration, while this same reaction type is fundamental to catalytic processes needed in green technologies. Capabilities available in the Reactions at Interfaces Facility support research in areas such as environmental geochemistry and biogeochemistry, bioremediation, catalysis and corrosion, atmospheric aerosol chemistry, development of diagnostic and analytical techniques, and chemistry induced by plasmas and by electron and photon excitation, and its application to waste destruction and conversion. All of these research areas are crucial to DOE's missions and national environmental health issues.

Gas- and Liquid-Phase Monitoring and Detection Facility

Contact: Steven D. Colson, J. William Rogers

Description. Capabilities in the Gas- and Liquid-Phase Monitoring and Detection Facility support research involving optical spectroscopy for gas-phase detection, microsensors, and microfluidics.

EMSL equipment for gas-phase detection includes state-of-the-art, high-resolution spectroscopy equipment (Fourier-transform instruments and tunable diode lasers) operating throughout the infrared region and used in conjunction with long-path sample cells and molecular-beam sources designed to obtain spectra with the highest possible resolution and sensitivity. The emphasis is on basic research of the structures and dynamics of molecular species important in contaminant chemistry, photochemistry, and atmospheric processes and the development of sensitive analytical techniques.

The development and evaluation of chemical microsensors is supported by a wet chemistry laboratory for synthesis and electrochemistry, a laboratory for evaluation of chemical sensor and sensor materials using automated vapor generation and blending systems, and a clean room with selected microfabrication capabilities. A variety of techniques for the application of sensing materials to sensor devices are available and numerous electronic test instruments are available in the sensing laboratories and EMSL's Instrument Development Laboratory. A wide range of surface analysis and characterization instruments in addition to conventional analytical instrumentation in EMSL complement these capabilities. Users may wish to bring new sensing materials to EMSL for application to sensing devices and evaluation, while others may bring complete sensor systems with data collection to couple to our automated vapor generation systems. Research areas include sensor arrays, sensor materials design and synthesis, sensing material/analyte interactions, and chemometric methods.

The microfluidics laboratory provides a capability in flow injection and sequential injection techniques as an automated approach to microscale fluid handling for diverse applications. Several flow injection systems are complemented by absorbance, fluorescence, luminescence, and electrochemical detection methods for downstream or "on-column" detection. A variety of custom flow cells exist for "bead injection" renewable surface techniques for separation and sensing. These capabilities are used to investigate reagent and separation chemistries and to demonstrate prototype microanalytical processes. We offer outstanding opportunities to investigate and apply bead-based chemistries in microanalytical systems. These capabilities complement a range of conventional analytical instrumentation in other EMSL laboratories. Research areas include detection systems for environmental contaminants, radiochemical separations, radionuclide sensors, DNA isolation and detection, biosensors, renewable surface sensors, and biomolecule interaction assays.

Use. Many environmental problems require the ability to detect and monitor trace species in complex sample matrices. Applications include environmental monitoring, assessment of remediation processes, investigating microbial ecology, chemical process control for waste processing, health effects research, and atmospheric chemistry.

Collaboratory

Contact: Raymond A. Bair

The Environmental Molecular Sciences Collaboratory is being developed to make the EMSL facilities and capabilities more available to scientists and engineers located anywhere in the nation or in the world. Collaboratory capabilities include:

- a suite of collaboration tools that can be used on desktop workstations to enable natural and informal interaction among scientists and engineers working at different locations
- an electronic laboratory notebook that enables researchers to share information such as research plans, data, instrument parameters, observations, and analyses
- a new generation of research instruments that permits shared and remote instrument monitoring, control, data acquisition, and analysis
- the EMSL Virtual NMR Facility, which is the first fully integrated production resource using the above capabilities.

For more information, visit the Collaboratory web site at **http://www.emsl.pnl.gov:2080/docs/collab/CollabHome.html**

Accessing the EMSL

As a national scientific user facility, the EMSL supports both general and proprietary research. EMSL research capabilities are available to the general scientific and engineering communities to conduct research in the environmental sciences and other areas relevant to national science and technology issues. Users gain access to the EMSL capabilities by submitting proposals. Proposed research is reviewed for

- scientific merit
- appropriateness for the facilities or capabilities being requested
- relevance to DOE environmental and other missions
- technical competence of the principal investigators.

All DOE user facilities, including the EMSL, require an executed user agreement prior to granting access to the facility. Users also must abide by EMSL Standard Practices and Procedures while using the facility.

General support and appropriate training for the research capabilities required by users will be provided by EMSL staff. Schedules for using facilities and capabilities will be determined by EMSL staff in consultation with users.

General Research

General research includes all research, collaborative and independent, that is nonproprietary. Users engaged in general research will not, in general, be charged for use of the EMSL facilities or equipment. Intellectual property developed in the course of general research will be protected in accordance with DOE policies, which in general assign the intellectual property and any resulting commercial benefits to the discoverer.

Proprietary Research

A limited amount of propriety research may be conducted in the EMSL under a proprietary user agreement. Under the terms of the DOE class waiver, users engaged in proprietary research are obligated to pay the full cost recovery rate for use of the facility. In return, the user has the option to take title to any inventions made during the proprietary research program and to treat as proprietary all technical data generated during the research.

More information about becoming a user can be accessed via the *User Info* and *Proposal Form* links on the EMSL web site at **http://www.emsl.pnl.gov**.

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