Overview

This W.R. Wiley Environmental Molecular Sciences Laboratory (EMSL) 2005 Annual Report describes the research and accomplishments of staff and users of the EMSL in Richland, Washington. Essential to the success of resolving environmental and other critical scientific issues important to the U.S. Department of Energy (DOE) is the implementation of EMSL Grand Challenges, which are research projects that address complex, large-scale scientific and engineering problems using multi-institutional teams with high-performance scientific resources.

Mission

The management of EMSL, together with DOE, its Pacific Northwest Site Office, and Pacific Northwest National Laboratory (PNNL) management, has developed the following mission statement for EMSL.

> *EMSL, a national scientific user facility at Pacific Northwest National Laboratory, 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.*

EMSL strives for simultaneous excellence in 1) high-impact science and marquee capabilities, 2) outstanding management and operations, and 3) exceptional user outreach and services, and uses these tenets to deliver its mission and implement its strategy. The central focus of EMSL's strategy is delivery on the mission of the scientific user facility. In addition to its mission, EMSL has a vision and strategy that show where the user facility intends to be in the next 10 years and the progress that will be made during the next 5 years, respectively.

EMSL Resources and Facilities

EMSL is a national scientific user facility available to researchers worldwide from academia, industry, and national laboratories. Its users pursue the understanding of molecular systems essential to scientific breakthroughs and discoveries for a broad set of DOE missions in energy, environment, climate, and national security. Staff at EMSL develop and maintain extensive advanced research and development capabilities that are used to generate new scientific knowledge. EMSL delivers substantial value to its users by understanding their needs, creating responsive new ideas and capabilities, and delivering exceptional results—all achieved through the expertise of facility staff, demonstrated excellence in management and laboratory operations, and high-value partnerships with its users.

The DOE Office of Biological and Environmental Research provides the operating budget for EMSL, while the research conducted within the facility is beneficial to the DOE Office of Science and many other funding agencies, including other programmatic offices within DOE, the National Institutes of Health, the National Science Foundation, and the U.S. Department of Defense.

Since beginning operations in October 1997, EMSL has provided advanced and one-of-a-kind experimental and computational resources to scientists engaged in fundamental research in the physical, chemical, and biological processes that underpin environmental remediation and other important scientific issues facing DOE and the nation. In addition to physical resources, EMSL provides unprecedented technical support and expertise, allowing its users a highly efficient and focused resource that enhances their work.

Cutting-edge resources available to EMSL users are available in the following six facilities:

- *Chemistry and Physics of Complex Systems Facility* for understanding and mitigating the environmental impacts of energy use and contaminant release, and fostering fundamental research in the natural sciences to provide the basis for new and improved energy technologies.

- *Environmental Spectroscopy and Biogeochemistry Facility* for studying complex chemical phenomena and mechanisms on mineral and microbe surfaces and on heterogeneous environmental materials.

- *High-Field Magnetic Resonance Facility* for determining and imaging molecular structures that impact environmental remediation and biological health effects.

- *High-Performance Mass Spectrometry Facility* for analyzing the response of biomolecules to environmental stimuli.

- *Interfacial and Nanoscale Science Facility* for studying chemical transformations at surfaces and for fabricating and characterizing materials with nanoscale features.

- *Molecular Science Computing Facility* for theory, modeling, and simulation of complex phenomena in chemistry, biology, climate science, and subsurface fate and transport.

Additionally, the following three organizations within EMSL provide services that enable effective computer, instrument, and user support:

- *Computing and Networking Service*s for operation and maintenance of EMSL's computing infrastructure.

- *Instrument Development Laboratory* for design, development, and deployment of advanced, state-of-the-art instruments, and custom-application software.

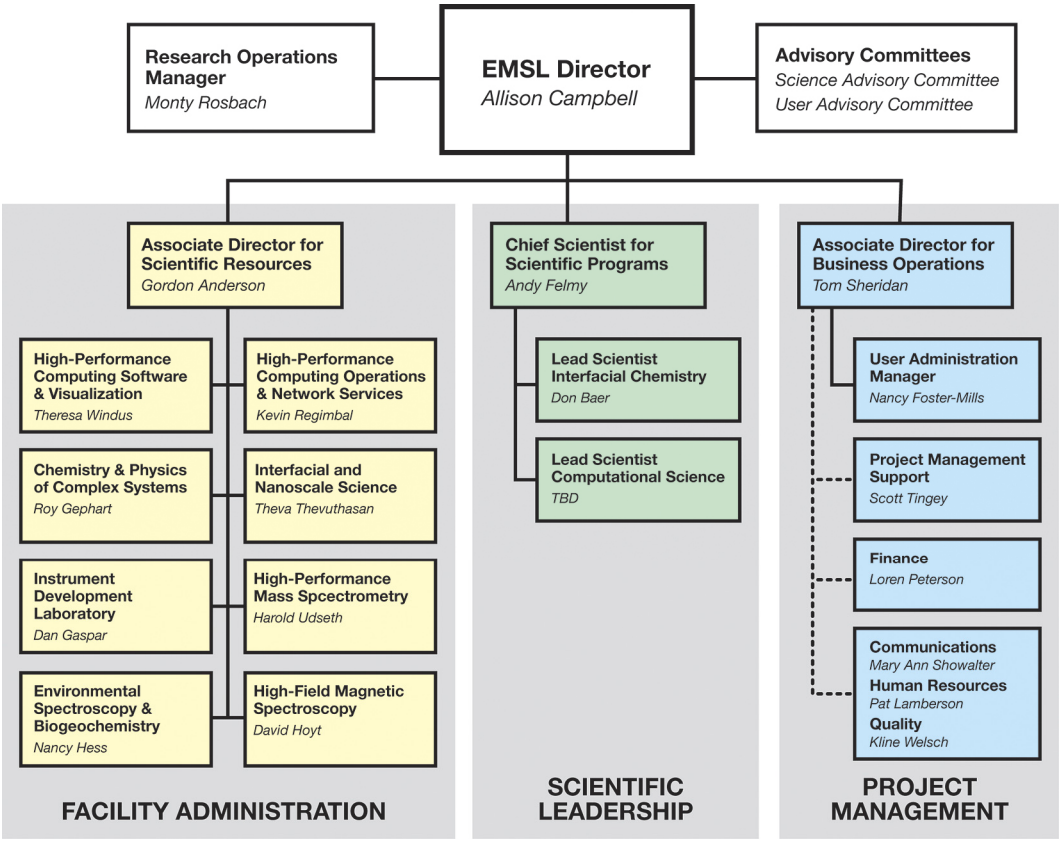
- *User Services and Outreach* to facilitate and promote the effective use of EMSL resources by staff and users.

Organization

EMSL is managed by a Director, an Associate Director for Scientific Resources, an Associate Director for Business Operations, a Research Operations Manager, a Chief Scientist, and the Scientific Facility Leads who are the front-line project managers responsible for user projects within their facilities. In addition, two advisory committees, the

User Advisory Committee (UAC) and the Science Advisory Committee (SAC), provide advice on short-term, user-related issues and longer-term scientific direction.

As shown below, the EMSL project is organized into Scientific Resources, Scientific Programs, and Business Operations groups.



User Advisory Committee

The UAC is an independent body charged with providing objective, timely advice to EMSL leadership. Responsibilities of the committee include:

- Advising on how to facilitate the effective use of EMSL. This responsibility includes advocating user interests and making recommendations for integration of the various demands on EMSL equipment and staff resources to optimize usage and impact on all users.
- Advising on priorities and strategies to effectively address the mission of EMSL. This responsibility includes exploring new paradigms for instrument use and user activity associated with EMSL's broad-based and often unique instrumentation resources.

In addition, the UAC advocates and promotes effective communication between EMSL leadership and the user community to facilitate maximum scientific impact by EMSL users.

In 2005, the UAC was composed of the following individuals:

- Leonard D. Spicer, Committee Chair, Duke University, Durham, North Carolina

- Neal R. Armstrong, University of Arizona, Tucson, Arizona
- J. Thomas Dickinson, Washington State University, Pullman, Washington
- G. Barney Ellison, University of Colorado, Boulder, Colorado
- Joseph W. Nibler, Oregon State University, Corvallis, Oregon
- B. Montgomery Pettitt, University of Houston, Houston, Texas
- Phil J. Reid, University of Washington, Seattle, Washington
- Karin D. Rodland, Pacific Northwest National Laboratory, Richland, Washington
- Z. Jimmy Yu, Motorola, Tempe, Arizona.

Science Advisory Committee

The independent SAC provides objective advice on long-term scientific direction to the EMSL Director on topics including EMSL's focus on national priorities and scientific challenges; the strategy for accomplishing EMSL's vision; potential opportunities for transferring science to applications; and stewardship of the facility, its capabilities, and the expertise of its staff. Composed of scientists from across the United States, the committee is built around the major capability areas at EMSL. In 2005, the SAC was composed of the following individuals:

Biological Sciences

- Ruedi Aebersold, Institute for Systems Biology, Seattle, Washington
- Mina J. Bissell, Lawrence Berkeley National Laboratory, Berkeley, California
- Marvin Cassman, University of California, San Francisco, San Francisco, California
- David J. Galas, Keck Graduate Institute, Claremont, California
- Leonard D. Spicer, Duke University, Durham, North Carolina.

Environmental Sciences

- Gudmundur S. "Bo" Bodvarsson, Lawrence Berkeley National Laboratory, Berkeley, California
- Gordon E. Brown, Jr., Stanford Synchrotron Radiation Laboratory, Stanford, California
- Barbara J. Finlayson-Pitts, University of California, Irvine, California
- Mary P. Neu, Los Alamos National Laboratory, Los Alamos, New Mexico
- James M. Tiedje, University of Michigan, Ann Arbor, Michigan.

Molecular Science

- Mark A. Barteau, University of Delaware, Newark, Delaware
- Charles T. Campbell, University of Washington, Seattle, Washington

- George W. Flynn, Columbia University, New York,, and member of the Basic Energy Sciences Advisory Committee.

Theoretical Science

- Bruce E. Bursten, Committee Chair, The Ohio State University, Columbus, Ohio
- Peter J. Rossky, University of Texas at Austin, Austin, Texas
- Mary F. Wheeler, University of Texas at Austin, Austin, Texas.

Proposals and User Access Modes

Potential users may submit proposals to conduct research at EMSL in response to calls. Different approaches are available to optimize scientific impact and facilitate evolution of EMSL facilities and science to address cutting-edge science questions.

Calls for Proposals

Proposals may be submitted in response to specific calls for proposals or at any time during the year. Resource allocation depends on the nature of the proposal.

- **Response to Science Theme Calls.** Users are encouraged to submit proposals that fit into major areas of current and growing user activity associated with scientific challenges that address topics of societal importance. To highlight these areas, theme-based calls for proposals are planned to occur at least once a year. The duration of work proposed in response to a science theme can be renewed for up to 3 years. Some EMSL resources may be especially dedicated to science theme proposals.
- **Response to Specific Facility Calls.** The Molecular Science Computing Facility (MSCF) and High-Field Magnetic Resonance Facility (HFMRF) have calls based on the specific natures of those facilities. The MSCF calls occur approximately once a year with allocations lasting up to 3 years, while the HFMRF calls occur twice a year with time allocated on a 6-month basis.
- **Request to join an EMSL Scientific Grand Challenge.** In the past year, EMSL launched two Scientific Grand Challenges that will bring together some of the world's best minds to study questions in membrane biology and biogeochemistry. Collectively, these PNNL-supported Scientific Grand Challenges bring together scientists from more than 20 universities and research institutions worldwide. Results from these Scientific Grand Challenges could show us how to use microbes and biological processes to address currently intractable issues in environmental remediation. Progress in these areas can help DOE resolve the significant problems associated with environmental contamination that currently exist at many of its sites, thereby saving DOE and the nation hundreds of millions of dollars and reducing risk to humans and the environment.

Types of Proposals

- **General.** General-use proposals may be submitted to EMSL throughout the year and are evaluated by EMSL prior to commencement of work. Proposals may be submitted by individuals or groups who need access to EMSL to carry out their research, using existing equipment in the facility. The scope of this type of proposal can vary from a

proposal to conduct a single experiment to a proposal for a more comprehensive research program. Individual and group proposals, including collaborative proposals with EMSL staff, are encouraged.

- **Partner.** Partners are individuals or groups who not only carry out research at EMSL, but also enhance the capabilities within the facility. Typically, they develop facility instrumentation, bringing with them outside financial and/or intellectual capital. These contributions are made available to general users as well. In recognition of their investment of resources or intellectual capital, and in order to facilitate and encourage their involvement, partners may be allocated limited access to one or more facilities over a period of several years, with the possibility of renewal. New partner proposals can be submitted in response to science theme or other calls and are subject to the same peer-review process as general users.

Types of Access

Users can access the capabilities of EMSL in two ways.

- **Standard Access.** Standard access to EMSL facilities can vary from single-visit, single-experiment proposal to a program proposal (valid for multiple visits and substantial access to a range of equipment extended over multiple years). Before work can start on a proposed project, the proposal must pass peer review. This is the most common mode of access to EMSL Capabilities.
- **Rapid Access.** In limited cases, users may need rapid access to EMSL capabilities (e.g., for thesis work, project progress reports, and paper publication or proposal preparation). A rapid access proposal can request up to one month of EMSL use. Under the rapid-access mechanism, the proposed work on can be started subject to instrument and resource availability and approval of the Science Facility Lead. However, a peer review of the proposed work will be conducted as work is initiated. After a maximum of one month, the work must either have been approved and become a Standard Access project or ended. Proposed research that has identified safety concerns is not eligible for and will not be consisered under this Rapid Access mechanism. Use agreements with users must be completed before access to EMSL capabilities will be scheduled.

Proprietary Status

- **Non-Proprietary Researc**h. Research and equipment usage conducted at EMSL for which results and information are fully disclosed and disseminated are considered non-proprietary. Authors of non-proprietary proposals may retain rights to intellectual property resulting from the use of EMSL, but the government is granted a non-exclusive license to use the intellectual property.
- **Proprietary Research.** EMSL facilities can be used for proprietary research under standard or rapid access use. DOE requires that researchers who perform such work must pay full-cost recovery of the facilities used, which includes, but is not limited to, labor, equipment usage, consumables, materials, and EMSL staff travel.

EMSL Science Themes

In 2005, EMSL began developing and refining science themes that will help define and develop key collections of user projects. The initial four science themes, which will become more formalized in 2006, are 1) Biological Interactions and Interfaces, 2) Geochemistry/ Biogeochemistry and Subsurface Science, 3) Atmospheric Aerosol Chemistry, and 4) Science of Interfacial Phenomena.

Biological Interactions and Interfaces

Recent advances in whole-genome sequencing for a variety of organisms and structure/ function relationships of proteins have contributed to a rapid transition of the biological research paradigm towards understanding biology from a global perspective. As a result, biology is evolving into a quantitative, ultimately predictive science in which the ability to collect and productively use large amounts of biological data is crucial. This requires global measurement of proteins because of their primary role in nearly all cellular processes. Under this science theme, EMSL will seek users whose research focuses on determining protein or metallo-protein abundance, activity, composition, and structure. Preference will be given to users who address post-translational modifications of protein structure and function, multi-protein complexes or complex mixtures of proteins, or who probe important properties of biological interfaces, including cell/environment interactions.

Geochemistry/Biogeochemistry and Subsurface Science

One of the most challenging and pressing issues confronting DOE and the nation is the safe, cost-effective management of environmental pollutants and the remediation of hazardous waste sites. DOE is responsible for managing 40 million cubic meters of contaminated soils and 1.7 trillion gallons of contaminated groundwater. Under this science theme, EMSL will seek users who seek to unravel reaction mechanisms at both the mineral/water and microbe/mineral interfaces. Preference will be given to users who will either elucidate specific interfacial molecular mechanisms or focus on identifying the molecular form of contaminants or radionuclides in and on the surfaces of natural materials.

Atmospheric Aerosol Chemistry

Atmospheric aerosols play an important role in global climate change, and variations of aerosols are recognized as significant forcing factors that alter the planetary radiation balance onto and away from Earth. There is a need to understand the molecular mechanisms of nucleation, growth, and aging effects of atmospheric aerosols. Organic matter, in particular, is one of the major and least studied fractions of ambient aerosols, even though it accounts for 20 to 50 percent of their total mass, and the amount of organic aerosol present in the atmosphere can be overwhelmingly high on the regional and local scales. Under this science theme, EMSL is seeking users who are attempting to obtain molecular understanding of atmospheric aerosol chemistry. Specifically, research will focus on characterizing and understanding the chemical properties of organic aerosols and/or linking experiments to the development of theoretical models of aerosol nucleation and growth. Topics of particular interest include processes involved in aerosol formation and how the composition and

chemistry of aerosols change over time (aging studies) when exposed to atmospheric radiation, free radicals, and other atmospheric components.

Science of Interfacial Phenomena

Under this science theme, EMSL will seek users who contribute to the atomic- and molecular-level understanding and control of the dynamic, reactive, and transport properties of interfaces having possible environmental and energy implications. Material systems with interfaces designed and optimized, or tailored, with specific properties will be essential to technologies needed to maintain a secure environment and obtain a stable energy future. Technical areas that will rely on improved understanding and control of molecular-level structural, dynamic, and transport properties of interfaces include hydrogen production and storage; solid-oxide fuel cell research and development; materials for next-generation nuclear reactors; radiation detectors and chemical sensors; a new generation of selective, efficient and stable catalysts; and solid-state lighting.

EMSL Scientific Grand Challenges

EMSL is challenging the traditional approach to research with two Scientific Grand Challenges, which are complex, large-scale scientific and engineering problems with broad scientific and environmental or economic impacts whose solution can be advanced by applying high-performance scientific techniques and resources. EMSL Scientific Grand Challenges differ from typical research projects in that they are performed by multi-institution (universities, other federal laboratories, and industry), outcome-driven multidisciplinary teams that use the cutting-edge resources available in EMSL.

During the past year, two EMSL Scientific Grand Challenges were launched to study issues in membrane biology and biogeochemistry. Progress in these areas can help DOE resolve the enormous problems associated with environmental contamination across the DOE complex, thus saving DOE and the nation hundreds of millions of dollars and reducing risk to humans and the environment. As stated previously, the EMSL Scientific Grand Challenges have brought together some of the world's best minds and have engaged scientists from more than 20 universities and research institutions worldwide.

EMSL's Membrane Biology Scientific Grand Challenge addresses questions related to structure and dynamics of key membrane proteins and how certain processes are affected by the environment, while the Biogeochemistry Scientific Grand Challenge focuses on the fundamental question of electron transfer across membrane/mineral interfaces.

Membrane Biology Grand Challenge: Systems Analysis of Cyanobacterial Physiology in Membrane Biology

The EMSL Scientific Grand Challenge in membrane biology is using a systems biology approach to understand the network of genes and proteins governing the structure and function of membranes and the components responsible for photosynthesis and nitrogen fixation in cyanobacteria (blue-green algae). Cyanobacteria are oxygenic photosynthetic

organisms that make major contributions to global biological carbon sequestration and are the only known bacteria that exhibit a circadian rhythm.

The target organism for the Membrane Biology Scientific Grand Challenge is *Cyanothece 51142*, a marine cyanobacterium that has the amazing ability to perform two biochemically incompatible activities, photosynthetic oxygen evolution and nitrogen fixation, in the same cell. It uses an inherent diurnal rhythm of photosynthesis during the day and nitrogen fixation at night to accomplish these activities.

The goal of this Scientific Grand Challenge is to determine the underlying network that coordinates the interactions of environmental signals with the cellular machineries and, in particular, the membrane systems. The results will provide the first comprehensive systems-level understanding of how environmental conditions influence key carbon-sequestration, nitrogen-fixation, and hydrogen-generation processes at the gene/protein/organism level.

The integration of molecular measurements and environmental controls will allow a predictive understanding of these key biological processes to be developed. This issue addresses critical DOE science interests, and uses novel model microorganisms to apply high-throughput biology technologies and computational modeling approaches.

Collaborators in this Scientific Grand Challenge include biologists, computer scientists, physicists, and chemists from PNNL, Purdue University, St. Louis University, the Donald Danforth Center for Plant Science, and the Shanghai Institute for Biological Sciences.

In 2005, several accomplishments were made under this Scientific Grand Challenge, including:

- Completion of genome sequencing of *Cyanothece ATCC 51142* at 12 times the coverage, and is in the final stages of polishing and annotation. An annotation website has been established for the team.

- Development of a genetic exchange system for *Cyanothece*.

- Characterization of the structure and association of the various membranes in another cyanobacterium, *Synechocystis 6803*, using imaging electron microscopy techniques. The physical discontinuity of thylakoid membranes from the plasma membrane has been illustrated, and a publication on this work was submitted to *Protoplasma*.

- Completion of the design and procurement of a versatile photobioreactor system.

- Generation and analysis of several hundred *Cyanothece* samples, covering 7- to 14-day cultivation periods with multiple time-point resolution, for proteomic, metabolomic, and metallomic characterization.

- Acquisition and submittal of separated fractions of outer, plasma, and thylakoid membranes for proteomic analysis in order to identify proteins unique to each membrane.

- Design and printing of a microarray for *Cyanothece*, containing 11,000 probes for dual coverage of the entire organism's genome.

- Determination of the molecular structures of several *Cyanothece* proteins using crystallographic techniques.

- Establishment of several new EMSL capabilities to assist research, including a linear ion trap and Orbitrap mass spectrometers for proteomic and metabolomic analysis.

Biogeochemistry Scientific Grand Challenge: Electron Transfer from Multi-Heme Cytochromes to Mineral Surfaces

The Biogeochemistry Scientific Grand Challenge is investigating how microorganisms exchange energy and electron flux with mineral matter in soils, sediments, and subsurface materials. This exchange occurs between outer membrane-associated, multi-heme cytochromes of bacteria and mineral surfaces across a complex interface that is a minute, but chemically active, domain whose molecular workings have perplexed scientists for decades. This Scientific Grand Challenge is providing an unprecedented, detailed view of how organisms engage with mineral surfaces to exchange energy and electron density required for life function.

The Biogeochemistry Scientific Grand Challenge is using EMSL's advanced instruments and high-performance computing capabilities as well as the capabilities in other DOE user facilities to understand both the biological and physical architecture of this remarkably complex domain and the microbe-mediated chemical reactions that occur within it. The research will allow scientists to develop an understanding of this most basic earth-life interaction, which is fundamental to the migration of environmental contaminants, to water quality, and to soil fertility and trace metal availability. This understanding has the potential to further advance the understanding of bacteria-driven geochemical processes that regulate water chemistry and contaminant migration in subsurface and sediment/water systems.

The team involved in this Scientific Grand Challenge is made up of more than 25 scientists from PNNL and other science institutions in the United States, the United Kingdom, and Canada.

In 2005, the approach of the EMSL Biogeochemistry Scientific Grand Challenge, which integrates surface geochemistry, molecular microbiology, and computational modeling, has led to discoveries related to the central hypothesis: The outer membrane cytochromes MtrC/OmcA are responsible for direct electron transfer to Fe(III) oxide. By combining mutagenesis studies that produced and studied organisms without specific cytochromes with experiments that purified and characterized the reactivity in solution of the cytochromes (and combinations of cytochromes) to various aqueous species and with atomic force microscopy and electron microscopy studies of cytochrome localization on the outer surface of the microorganism, it appears that a protein complex anchored to the outer cell membrane containing two distinct cytochromes (MtrC and OmcA) is responsible for electron transfer to solid-phase electron acceptors. From these studies, it has been determined that these two cytochromes exhibit different internal redox properties that

spatially and chemically couple in ways that remain under investigation. Computational studies have determined that the electron transfer from the complex is much slower to solid-phase electron acceptors because of orientation and approach distance effects at the solid-water-organism interface. The combination of experiments has shown that the whole cell behavior is a complex function of cytochrome localization, concentration, and adaptive cellular response to the mineral surface and its topography and energetics.

The biochemical redox machinery of metal-reducing bacteria, the first tier of earth-life interaction, is remarkably fascinating and complex. Understanding the molecular and physiologic basis for metal reduction and its coupling with the mineral world provides concepts for a number of important processes, including 1) a sustainable environment (biogeochemical element cycles, water and soil quality), 2) sequestration and immobilization of harmful metals and radionuclides, 3) biochemical energy storage and redox gating for technological applications, 4) bioenergy sources, and 5) metal ore genesis. Finally, understanding the unique interfacial processes involved in the interaction of microbes with minerals may have tremendous technological benefits with a better understanding of the physiologic strategy for optimizing heme orientation and exposure at the interface, adaptive engagement and response of the outer membrane to mineral topography and energy fields, and electron transfer reactions involving long-range tunneling and folded, adaptive molecules.

EMSL Collaborative Access Teams

In 2005, EMSL initiated a pilot program for Collaborative Access Teams (CATs). The purposes of CATs are to enable and conduct high-impact science using multiple capabilities in EMSL and provide a mechanism for maintaining EMSL's position at the forefront of science. CATs are composed of teams of scientists who use EMSL facilities and capabilities to conduct funded programmatic research around focused science themes. These teams provide a means to attract and increase the number of high-impact users in a focused research environment and build new capabilities for use by both CAT and general users. Membership in a CAT is open to members of the scientific community who, in the opinion of the CAT lead, would contribute significantly to the scientific goals of the CAT. Four CATs existed in 2005 in the areas of structural genomics, catalysis, atmospheric chemistry, and analytical mass spectrometry.

EMSL management is evaluating the success of the CAT program to determine whether they will continue with this effort in future years.

Structural Genomics. The Structural Genomics CAT is led by PNNL researcher MA Kennedy. The goal of structural genomics is to make the three-dimensional, atomic resolution structures of most proteins easily available from their corresponding DNA sequences. The primary goal of the Structural Genomics CAT is increasing throughput of these structures, maximizing efficiency of existing resources, and developing technology to increase throughput and efficiency.

The Northeast Structural Genomics Consortium (www.nesg.org), which is supported by the National Institutes of Health Protein Structure Initiative II, makes extensive use of HFMRF

to acquire nuclear magnetic resonance (NMR) spectometry data for protein structure determination. During the last 6 years, data collected at HFMRF have been used for the determination of dozens of protein structures. In 2005, approximately 50 weeks of instrument time was devoted to NMR data collection for structural genomics.

NMR structures and one x-ray structure of eight structural genomics target proteins were determined with data collected using resources in HFMRF and deposited in the Protein Data Bank (www.rcsb.org) in 2005. For more information, see the "Structural Genomics Collaborative Access Team" highlight in the HFMRF User Highlights section.

Catalysis. The Catalysis CAT, led by PNNL researcher CHF Peden, uses the unique experimental and computational resources at EMSL to conduct basic and applied research in the area of heterogeneous catalysis. Specifically, this CAT works to develop a fundamental understanding of transition metal oxide-catalyzed chemical transformations so that new catalysts could be systematically developed from first-principles. Research efforts are targeted to critically relate the surface chemistry, surface morphology, atom connectivity, and pore dimensions for controlling catalytic activity and selectivity of target acid-base and redox reactions.

When this CAT proposal was submitted, a specific focus was to develop a fundamental understanding of catalyzed chemical transformations so that new catalysts could be systematically developed from first principles. The research efforts endeavor to critically relate surface chemistry, surface morphology, atom connectivity, and pore dimensions as controlling properties for catalytic activity and selectivity of acid-base and redox reactions. Several approaches are being used to achieve this goal: 1) molecular-level simulations of heterogeneous catalysts, synthesis and characterization of heterogeneous catalysts using methods that provide nanoscale precision in the type, number, and distribution of active sites; detailed kinetics measurements on model and realistic catalytic systems; and development and testing of new experimental approaches for addressing complex catalysis issues.

More than 10 papers were published as a part of this CAT and associated proposals in 2005. More than half of these publications involved multiple facilities. Among the publications in top-10 journals, the joint publication in Science by C Campbell from the University of Washington and CHF Peden from PNNL is notable. High-profile users included Professors C Campbell from University of Washington and W Goodman from Texas A&M University, both of whom both visited EMSL as a part of this CAT. Professor Goodman spent his sabbatical at EMSL with his postdoctoral research associate, P Han. During their stay, they investigated a model bimetallic catalyst made by depositing palladium atoms on a crystalline gold support using the variable-temperature ultrahigh vacuum scanning tunneling microscope. Another notable outcome associated with this CAT is related to the development of a magic-angle turning solid-state NMR probe capability with discrete sample rotation to in situ catalyst studies.

Atmospheric Chemistry. The Atmospheric Chemistry CAT was established to lead the EMSL research thrust addressing "atmospheric chemistry for the future." The focus articulates a strong vision of challenges in the atmospheric chemistry field, defines major collaborative projects in that field to address the scientific challenges, and develops and

deploys measurement equipment. The CAT was initiated in 2005, and research related to modeling data analysis for the evolution of meteorology and ozone over the Great Lakes region in 1999 and 2001 used EMSL's supercomputing capabilities to support the CAT.

Analytical Mass Spectrometry. The Analytical Mass Spectrometry CAT, led by PNNL researcher J Laskin, was formed for researchers to achieve a fundamental understanding of the reaction kinetics and dynamics of activating and dissociating complex molecular ions. These processes are the scientific foundation for tandem mass spectroscopy (MS/MS), one of the most important analytical methods developed in the last century. The collisional activation and dissociation of protonated model peptides, a particularly important class of complex molecules whose characterization by MS/MS is central to the emerging field of proteomics, were investigated, resulting in 10 publications. In 2005, research efforts to support this CAT involved studying the energetics and mechanisms of fragmentation of post-translationally modified peptides, the soft landing of peptide ions on surfaces, the energetics of dissociation of peptide radical cations, the gas-phase ion chemistry of 4Fe-4S complexes, and surface-induced dissociation of polyatomic ions. Capability development under this CAT involved the design and construction of a novel ion deposition chamber for studying soft landing of biomolecules on a variety of surfaces. This technique allowed researchers to carry out the first atomic force microscopy imaging studies ever conducted of surfaces modified by soft landing.

EMSL Highlights

EMSL Science Highlights

In 2005, staff and users from the six EMSL research facilities performed leading-edge research in a variety of scientific disciplines. Below are brief research summaries for each research facility, with more in-depth detail provided in subsequent sections of this annual report.

Researchers investigate role of mineral dust particles in climate forcing and atmospheric chemistry. EMSL researcher A Laskin and his collaborators from EMSL and the University of Iowa used EMSL resources, such as computer-controlled scanning electron microscopy with energy-dispersive x-ray analysis, environmental scanning electron microscopy, and inductively coupled plasma mass spectrometry to study the heterogeneous chemistry of mineral dust with nitric acid (HNO_3) to identify and characterize particles with the greatest reactivity and determine changes to physiochemical properties. The data obtained from this study suggested that a portion of each of four mineral dust aerosol samples from specific source regions may exhibit substantial reactivity with gas-phase HNO_3, leading to formation of hygroscopic $Ca(NO_3)_2$-containing particles. Once $Ca(NO_3)_2$ particles are formed in the atmosphere, they remain in the aqueous phase and never dry out, even over desert areas. These liquid particles may change the optical properties of mineral dust, serve as effective cloud condensation nuclei, and modify clouds as well. In addition, these modified particles may open up the possibility of new multiphase reaction chemistry. It follows that a significant fraction of the dust from these specific locations will change their physical and chemical properties when transported over polluted areas. These changes may have an important impact on climate forcing and atmospheric chemistry.

Sensor development activities help detect groundwater contamination. PNNL researcher and EMSL user A Del Negro and his collaborators from PNNL, the University of Cincinnati, and the University of Wyoming are studying technetium and its common isotopes, and the ability of these elements to migrate quickly and harmfully into soil. Through this research, a sensor is being designed that has the capability for onsite monitoring, either by immersion in subsurface water for continuous monitoring or for immediate analysis of collected samples. The device combines electrochemistry, spectroscopy, and selective partitioning capabilities, the combination of which substantially improves selectivity. This research and sensor development has led to the discovery of the first luminescence from trans-dioxo-technetium(V) complexes and is allowing the researchers to develop a theoretical model that can be used to predict the optical behavior of technetium complexes in general.

EMSL capabilities used to explore effects of low-energy electron exposure to DNA. A tautomer is one of two or more structural *isomers*—a compound having the same molecular formula but different structures—that exist in equilibrium and are readily converted from one isomeric form to another. Rare tautomers of nucleic acid bases are involved in mispairing of nucleic acid bases in DNA and, thus, in the development of point mutations. PNNL scientist and EMSL user M Gutowski, in collaboration with researchers from the University of Gdansk and Adam Mickiewicz University, both in Poland, are using EMSL capabilities to focus on chemical transformations of nucleic acid bases induced by low-energy electrons. The resulting anionic tautomers might contribute to the chemistry of RNA and DNA exposed to low-energy electrons in condensed-phase environments.

Spintronics research investigates magnetic properties in quest for quantum computers. Continued progress in spintronics—an area of research that will support development of quantum computers—requires the discovery of ferromagnetic semiconductors in which magnetically aligned dopant spins couple to the band structure of the host lattice, resulting in spin polarization of free carriers. PNNL researcher and EMSL user TC Kaspar, along with collaborators from EMSL, the University of Washington, the IBM Almaden Research Center, the Stanford Synchrotron Radiation Laboratory, and Yale University, has synthesized crystalline films and determined the properties of a number of magnetically doped transition metal oxides to probe the structure-magnetic/electronic function relationships in this deceptively complex class of materials. One of the prototypical systems under study around the world is doped TiO_2 anatase. These collaborators have shown, through painstaking growth and characterization, that magnetic ordering in these materials is driven by structural defects and is not an intrinsic property.

New pulse technique allows first-ever study of titanium materials by NMR spectroscopy. Characterization of the titanate phases of synroc and titanosilicate glasses is an important step to understanding the materials chosen to immobilize high-level waste streams generated by nuclear fuel reprocessing. However, the spectroscopy of titanium is complicated by several issues, such as titanium's low gyromagnetic ratio and the fact that the material is a quadrupolar nuclide with two active isotopes having NMR frequencies nearly coincident. PNNL researcher and EMSL user AS Lipton, along with collaborators from the Royal Veterinary and Agricultural University and the University of Cambridge in the United Kingdom, has developed a novel pulse program equipped with frequency-selective excitation that allows normal titanium samples, including materials simulated to study radioactive waste

vitrification, to be studied for the first time by NMR spectrometry. Study of these materials in their natural abundance is crucial for structural studies on glasses used for immobilizing radioactive waste.

EMSL mass spectrometry capabilities instrumental in studying causative agent of plague. With the potential re-emergence of pandemic diseases, such as avian influenza, the most effective means of protecting the nation's citizens will be to gain a better understanding of how infecting organisms cause diseases. *Yersinia pestis* is the causative agent of the "Black Death" or bubonic plague, and work performed at EMSL with this bacterium is an important step to understanding which proteins are used by the microbe to infect other cells. EMSL researcher KK Hixson and her collaborators from Lawrence Livermore National Laboratory and PNNL have grown *Y. pestis* in four conditions that mimic growth of the bacterium and are using EMSL state-of-the-art mass spectrometry capabilities to study the components of the bacterium and formation mechanisms.

EMSL Staff Highlights

In 2005, EMSL staff received continued recognition for progress in development of state-of-the-art capabilities and expertise, and for their professional contributions.

EMSL Director receives American Chemical Society Regional Industrial Innovation Award. Dr. AA Campbell, EMSL Director, was selected by the American Chemical Society and received the 2005 Regional Industrial Innovation Award for her work in bioceramic coatings. Under her guidance, researchers at PNNL have developed a biomimetic process that addresses the poor interfacial bonding between a metal implant and bone tissue in artificial joint implants, such as those used for hip and knee replacements.

MSCF makes a splash in first issue of new computational chemistry journal. The very first issue of the new *Journal of Chemical Theory and Computation* (January/February 2005) included three articles that contained acknowledgments of research use of the MSCF at EMSL. These publications resulted from work performed in conjunction with three MSCF Computational Grand Challenges focused on understanding 1) the synthesis and reactivity of nanoparticles for use in microfabrication and other processes (Barnard et al. 2005); 2) the rational design of catalysts (Harder et al. 2005), where one significant research effort in support of this Computational Grand Challenge is the development of new computational chemistry methods to address large systems; and 3) the properties of aluminum in nanoclusters (Schultz and Truhlar 2005). The complete citations for these articles follow:

- Barnard AS, P Zapol, and LA Curtiss. 2005. "Modeling the Morphology and Phase Stability of TiO_2 Nanocrystals in Water." *Journal of Chemical Theory and Computation* 1(1):107-116.

- Harder E, B Kim, RA Friesner, and BJ Berne. 2005. "Efficient Simulation Method for Polarizable Protein Force Fields: Application to the Simulation of BPTI in Liquid Water." *Journal of Chemical Theory and Computation* 1(1):169-180.

- Schultz NE and DG Truhlar. 2005. "New Effective Core Method (Effective Core Potential and Valence Basis Set) for Al Clusters and Nanoparticles and Heteronuclear Al-Containing Molecules." *Journal of Chemical Theory and Computation* 1(1):41-53.

PNNL team captures StorCloud challenge, finishes second in Bandwidth challenge. Image-analysis algorithms designed for optimal segmentation, feature extraction, and object recognition in three-dimensional data were developed for use with data captured by NMR and confocal microscopes at EMSL. For the Supercomputing 2005 (SC05) conference in Seattle, these algorithms were adapted to perform image recognition in video streams by treating the video stream as a three-dimensional volume.

Video streams captured on the SC05 exhibitor floor were stored in a Hewlett-Packard-provided Scalable File Share (SFS) storage solution, which is based on Hewlett-Packard's open source Lustre file system. With contributions from Cisco Systems, Inc., and Federal Network Services, a two-layer network over four bonded 10-Gigabit links to PNNL was used to mount the 32-node SFS filesystem on a 128-node Itanium 2 cluster. For PNNL's entry into the SC05 Bandwidth and StorCloud challenges, the Itanium cluster was used to deconstruct the video streams into the individual frames. After calculating RBG (i.e., red, blue, green) histograms and three Shannon entropy values, a summary of each frame was written back to the SFS file system.

PNNL took first place in the StorCloud challenge and finished second in the Bandwidth Challenge. The effort was led by EMSL researcher TS Carlson and featured EMSL High-Performance Computing and Networking Services members R Mooney, EJ Felix, and KP Schmidt, as well as numerous scientists from across PNNL.

Associate Director featured as Great Laboratory Manager. GA Anderson, EMSL Associate Director for Scientific Resources, was featured as a "Great Laboratory Manager" in the February 2005 issue of Reed Business Information's *Laboratory Equipment*. In the issue, he is honored for his leadership of a team that manages data produced by in-house and visiting researchers using 15 state-of-the-art instruments in EMSL's High-Performance Mass Spectrometry Facility (HPMSF).

GA Anderson

Biogeochemistry Scientific Grand Challenge members engage at working meeting. The first working meeting of the Biogeochemistry Scientific Grand Challenge was held at EMSL in June 2005 to engage all investigators on the latest technical progress, as well as enhance the overall coordination, information exchange, and synthesis needed to achieve the outcomes of the Scientific Grand Challenge.

Initiated in December 2004, the Biogeochemistry Scientific Grand Challenge is a three-year integrated investigation to understand the mechanisms by which bacteria interact with and transfer electrons to the mineral surfaces on which they live. This understanding has implications for environmental remediation and energy production as well as the development of engineered devices. The coordinators are PNNL senior chief scientists JM Zachara and JK Fredrickson. EMSL staff and resident users involved include MK Bowman, TC Droubay, DJ Gaspar, MA Kennedy, SN Kerisit, BH Lower, HP Lu, S Ni,

D Pan, KM Rosso, and S Yanina. Other PNNL staff involved included AS Beliaev, YA Gorby, M Romine, L Shi, and TP Straatsma.

Approximately 35 researchers from 12 institutions attended more than 20 presentations about technical progress, near-term research plans, and how research addresses the Scientific Grand Challenge's hypothesis that outer membrane cytochrome(s) MtrC/OmcA are responsible for direct electron transfer to Fe(III) oxide.

The meeting provided the investigators an opportunity to ask questions and discuss issues related to individual research elements within the initiative and to coordinate research efforts, sharing of materials, and collaborative experiments. The results of the meeting will help the coordinators continue developing the initiative roadmap.

EMSL User Highlights

The following is a sampling of the many user highlights that occurred in 2005 as a result of research conducted at EMSL.

EMSL user honored as 2005 Guggenheim Fellow. L-S Wang, Washington State University-Tri-Cities, was honored as a 2005 Guggenheim Fellow by the Guggenheim Foundation. Fellows are appointed on the basis of distinguished achievement in the past and for exceptional promise for future accomplishments. Wang was selected for his work in atomic clusters and multiplying charged anions. He also received the 2005 College of Sciences Distinguished Faculty Award from Washington State University for his research at PNNL, leadership in the field of nanoclusters, and pioneering research in the study of multiply charged anions.

L-S Wang

EMSL user elected to International Academy of Quantum Molecular Science. M Dupuis, an EMSL user and PNNL Laboratory Fellow, was elected to the International Academy of Quantum Molecular Science at its 42nd annual meeting held in Menton, France, in July 2005. Dupuis is part of several EMSL Computational Grand Challenge projects that are running calculations on EMSL's supercomputer.

M Dupuis

The Academy was created in Menton in 1967. Originally, it was limited to 25 regular members under the age of 65, with no limit on senior members. However, the Academy has expanded to 35 regular members under the age of 65 and currently includes 88 members worldwide. Members are selected among scientists from all countries who have distinguished themselves in the broad field of the application of quantum mechanics to the study of molecules and macromolecules. The main goal of the Academy is to provide a forum for international contact and collaboration and a periodical evaluation of the main developments, advances, and promising directions of research in the broad field of its interest.

EMSL postdoctoral fellow selected for 2004 MT Thomas Award. AA Shvartsburg was selected as the 2004 recipient of the MT Thomas Award for Outstanding Postdoctoral Achievement. This award recognizes Shvartsburg's accomplishments in the development of ion mobility-based methods and instrumentation, including both ion mobility spectrometry and field asymmetric waveform, which involved comprehensive theoretical modeling and computational simulations. He has applied his insight into ion mobility fundamentals towards the invention and practical implementation of new high-performance analytical technologies and platforms at PNNL. These novel approaches, which use extremely fast gas-phase separations, provide the physical basis for accelerating biological analyses by orders of magnitude, thus enabling numerous frontline applications in high-throughput proteomics and metabolomics.

2004 MT Thomas Award recipient, AA Shvartsburg (third from left). Also pictured (from left) are RJ Smith, MT Thomas, and AA Campbell, EMSL Director.

Five EMSL users named American Association for the Advancement of Science Fellows. Five EMSL users from PNNL were elected Fellows of the American Association for the Advancement of Science. GJ Exarhos was recognized for his "innovative research on charge transport processes in dielectric films and the use of light-scattering methods to probe structure/property relationships." LL Lasure was honored for her "sustained and effective leadership in industrial microbiology, particularly the innovative use of fungal enzymes in product development." BD Kay was elected for his "innovative use of molecular beams to elucidate chemical kinetics and dynamics at environmentally relevant aqueous and oxide interfaces." S Singhal was recognized for his "outstanding leadership in developing and promoting solid oxide fuel cells for clean and efficient power generation." Finally, S Wiley was elected a Fellow for his "significant contributions in the newly emerging area of systems biology and important achievements in the quantitative analysis of the Epidermal Growth Factor receptor system."

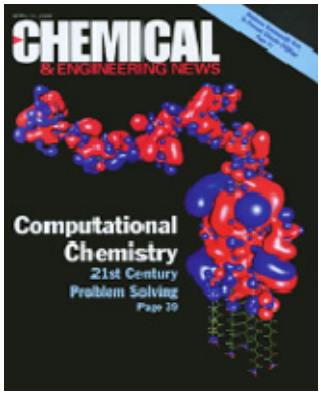
EMSL user receives Best Poster Award at Migration '05. In September 2005, EMSL user Z Wang attended the 10th International Conference on Chemistry and Migration Behavior of Actinides and Fission Products in the Geosphere at Avignon, France. His poster presentation "A Spectroscopic and Microscopic Study of Uranium Speciation in the Infiltration Pond Sediments at Hanford, USA" (co-authors: JM Zachara, SK Shelly, JP McKinley, SC Smith, O Qafuko, and SM Heald) was co-recipient of the best poster award out of 275 poster presentations.

EMSL crystalline ice research one of top physics stories of 2005. *The Bulletin of Physics News* reported that the American Institute of Physics selected the article entitled "Hydrophobic Water Monolayer in Crystalline Ice Growth on Pt(111)" as one of the top physics stories of 2005. GA Kimmel, NG Petrik, Z Dohnalek, and BD Kay, EMSL users from PNNL, were the first to observe that three-dimensional crystalline ice completely covers the hydrophobic monolayer only when there is an amount of overlying water equivalent to about 40 or 50 layers.

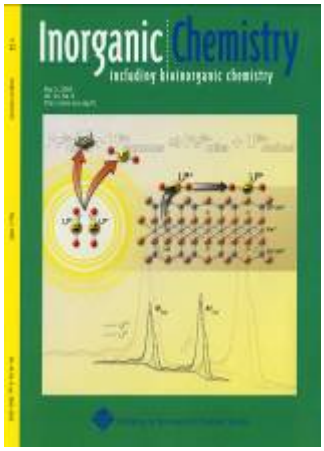
Journal Covers

During 2005, research by EMSL users and staff was highlighted on nine scientific journal covers. The following describe the research that led to these covers.

Research highlighted on the cover of the *Journal of Physical Chemistry B.* The team of PNNL researchers and EMSL users, HP Lu, D Hu, and D Pan, combined atomic force and confocal Raman microscopy techniques to follow interfacial electron transfer in a dye-sensitized semiconductor system. The new results are a significant step forward in characterizing site-specific inhomogeneous interfacial charge transfer dynamics—a process important to several fields such as chemistry, physics, and biology. The research was featured on the cover of the September 1, 2005, issue of *Journal of Physical Chemistry B.* Citation: Duohai P, D Hu, and HP Lu. 2005. "Probing Inhomogeneous Vibrational Reorganization Energy Barriers of Interfacial Electron Transfer." *Journal of Physical Chemistry B* 109(34):16390-6395.



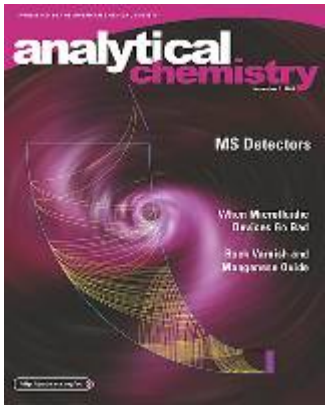
EMSL user featured in *Chemical and Engineering News.* L-S Wang, Washington State University-Tri-Cities, Richland, Washington, was featured in the October 24, 2005, issue of *Chemical and Engineering News* for reporting the first experimental evidence for d-orbital aromaticity. This research was originally featured in the October 17, 2005, issue of *Angewandte Chemie International Edition.* Citation: Huang X, HJ Zhai, B Kiran, and LS Wang. 2005. "Observation of d-Orbital Aromaticity." *Angewandte Chemie-International Edition* 44 (44):7251-7254.



Research highlighted on the cover of *Inorganic Chemistry*. PNNL researcher E Ilton and his collaborators used high-resolution x-ray photoelectron spectroscopy to demonstrate that reduction of aqueous U^{6+} at ferrous mica surfaces at 25ºC preserves U^{5+} as the dominant sorbed species over a broad range of solution compositions. Polymerization of sorbed U^{5+} with sorbed U^{6+} and U^{4+} is identified as a possible mechanism for how mineral surfaces circumvent the rapid disproportionation of aqueous U^{5+}. The general nature of this mechanism suggests that U^{5+} could play an important, but previously unidentified, role in the low-temperature chemistry of uranium in reducing heterogeneous aqueous systems. This research was originally featured in the May 2, 2005, issue *of Inorganic Chemistry*. Citation: Ilton ES, A Haiduc, CL Cahill, and AR Felmy. 2005. "Mica Surfaces Stabilize Pentavalent Uranium." *Inorganic Chemistry* 44(9):2986-2988.

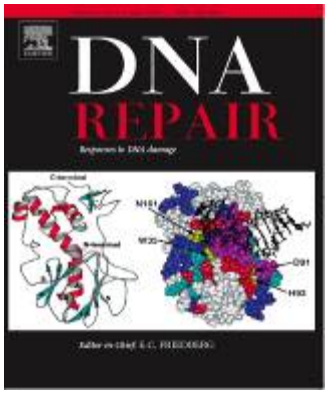
Research highlighted on the cover of the *Journal of Physical Chemistry*. PNNL researcher L Dang studied sodium and iodide ions at the liquid/vapor interface of methanol and water using a polarizable classical molecular dynamics technique he developed. The probability of finding iodide anions at the water/air interface is significantly greater than at the methanol/air interface. Such simulations elucidate the role solvent effects play on ions at liquid/air interfaces and contribute to the understanding of aerosols and droplet formation in the atmosphere. The research was featured on the cover of the October 21, 2004, issue of *The Journal of Physical Chemistry A*. Citation: Dang LX. 2004. "Ions at the Liquid/Vapor Interface of Methanol." *Journal of Physical Chemistry A* 108(42):9014-17.

Imaging system success story featured on the cover of *Scientific Computing & Instrumentation*. How a team of PNNL and Utah State University scientists and programmers overcame problems with a unique microscope developed for obtaining live images and cells and proteins was the topic of a cover story in the October 2005 issue of *Scientific Computing & Instrumentation*. The story, "Pixel Perfect – A Real-Time Image Processing System for Biology," describes how a multispectral confocal microscope developed at PNNL works and how the instrument's image registration problems were solved. The team consisted of EMSL researchers DF Hopkins and BL LaMarche; PNNL researchers MB Sowa and KA Perrine; and S Budge, Utah State University. PNNL chief scientist S Wiley developed the microscope, and the work was sponsored by PNNL's Biomolecular Systems Initiative. Citation: Perrine KA, DF Hopkins, BL Lamarche, and MB Sowa. 2005. "Pixel Perfect: A Real-Time Image Processing System for Biology." *Scientific Computing & Instrumentation* 16-20.



Mass spectrometer expertise highlighted on the cover of *Analytical Chemistry.* PNNL researcher DW Koppenaal and his collaborators provide expert commentary on the variety of types of mass spectrometer detectors and the consideration and needs related to various research areas. The commentary was featured on the cover of the November 1, 2005, issue of *Analytical Chemistry*. Citation: Koppenaal DW, CJ Barinaga, MB Denton, RP Sperline, GM Hieftje, GD Schilling, FJ Andrade, and JH Barnes IV. 2005. "MS Detectors." *Analytical Chemistry* 77(21):418A-427A.

Research highlighted on the cover of the *Physical Chemistry Chemical Physics.* PNNL researcher MS Gutowski and Polish scientists RA Bachorz and J Rak from the University of Gdansk and Adam Mickiewicz University, respectively, performed highly accurate computer calculations on rare isomeric forms of the nucleic acid base uracil stabilized by an extra electron. Extra electrons can be formed by low doses of radiation and cause mispairing of nucleic acid bases in DNA that can lead to mutations. The research was featured on the cover of the May 21, 2005, issue of *Physical Chemistry Chemical Physics*. Citation: Bachorz RA, J Rak, and MS Gutowski. 2005. "Stabilization of Very Rare Tautomers of Uracil by an Excess Electron." *Physical Chemistry Chemical Physics* 7(10):2116-2125.



Research highlighted on the cover of *DNA Repair.* The team of PNNL researchers and EMSL users GW Buchko, K McAteer, SS Wallace, and MA Kennedy used NMR spectroscopy, including data from the 900-MHz spectrometer, to measure the conformational mobility of a DNA repair protein in solution and bound to DNA. The observed changes in mobility upon binding provided new insights into how this class of DNA molecules repair proteins functions. The research was featured on the cover of the March 2, 2005, issue of *DNA Repair*. Citation: Buchko GW, K McAteer, SS Wallace, and MA Kennedy. 2005. "Solution-State NMR Investigation of DNA Binding Interactions in *Escherichia coli* Formamidopyrimidine-DNA Glycosylase (Fpg): A Dynamic Description of the DNA/Protein Interface." *DNA Repair* 4(3):327-339.

Research highlighted on the cover of *Journal of Molecular Biology.* The team, including PNNL researchers and EMSL users TA Ramelot, JR Cort, and MA Kennedy, used NMR spectroscopy to solve the solution structure of an important Iron-Sulfur Cluster Assembly Protein (IscU). The new results are a significant advance in understanding the function of this highly conserved protein, which is critical for metabolic health and is important in medicine, biology, and chemistry. The research was featured on the cover of the November 19, 2004, issue of *Journal of Molecular Biology*. Citation: Ramelot TA, JR Cort, S Goldsmith-Fischman, GJ Kornhaber, R Xiao, R Shastry, T Acton, B Honig, G Montelione, and MA Kennedy. 2004. "Solution NMR Structure of the Iron-Sulfur Cluster Assembly Protein U (IscU) with Zinc Bound at the Active Site." *Journal of Molecular Biology* 344(2):567-583.

Patents

EMSL staff and their collaborators received four patents in 2005.

1. **U.S. Patent 6,808,694**. "NO_x Reduction Methods and Apparatuses" was issued on October 26, 2004, to RG Tonkyn and GD Maupin, SE Barlow, and ML Balmer.

2. **U.S. Patent 6,869,588**. "Stimulus Sensitive Gel with Radioisotope and Methods of Making" was issued on March 22, 2005, to RE Weller, MA Lind, DR Fisher, A Gutowska, and AA Campbell.

3. **U.S. Patent 6,873,415**. "Photoacoustic Spectroscopy Sample Array Vessel and Photoacoustic Spectroscopy Method for Using the Same" was issued on March 29, 2005, to J Amonette, ST Autrey, NS Foster-Mills, and D Green.

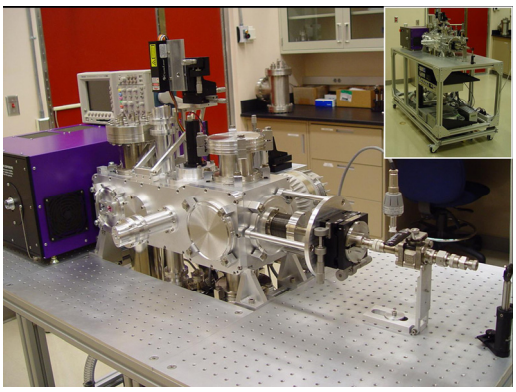
4. **U.S. Patent 6,911,649**. "Particle Generator" was issued on June 28, 2005, to WP Hess, AG Joly, KM Beck, DP Gerrity, PV Sushko, and AL Shluger.

Capability Developments

In 2005, several instruments were developed for use at EMSL to support user research.

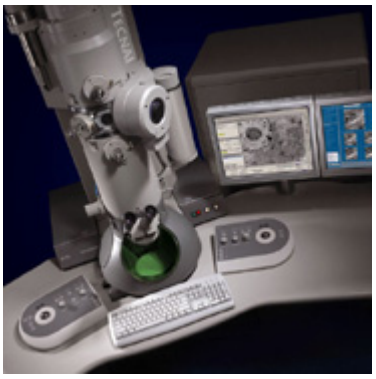
- Single-particle mass spectroscopy (SPLAT II)
- CryoTEM with tomography
- Scanning probe microscope for protein imaging and force measurements
- LTQ mass spectrometer
- 12-tesla magnet coupled with Fourier-transform ion cyclotron resonance (FTICR) mass spectrometer.
- Stopped-flow absorbance spectrometer system.

SPLAT II. Construction of SPLAT II was completed in 2005. In its basic form, the instrument can measure the size and chemical composition of individual aerosol particles down to 50 nm with extremely high sensitivity and unprecedented precision. The mass spectral signatures are generated in two steps: 1) a pulsed CO_2 heats the particle and evaporates the semi-volatile fraction, and 2) a time-delayed excimer laser pulse ionizes the resultant plume.

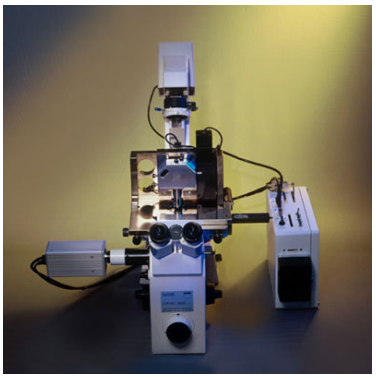


Combining SPLAT II with differential mobility analyzers and the EMSL aerosol flow reactor enables unparalleled detailed studies of chemical and microphysical transformations of individual size-selected aerosol particles in real time. It allows monitoring of simultaneous changes in size with sub-monolayer precision, shape, density, fractal dimension, and mass spectral signature of each individual particle.

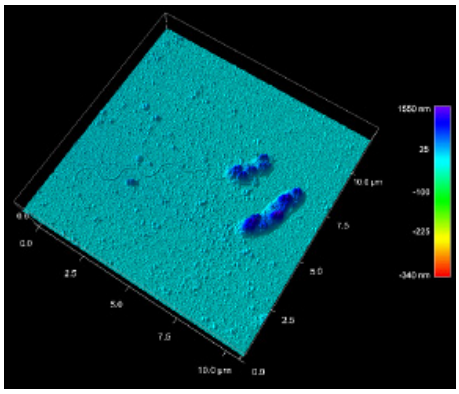
CryoTEM. This new EMSL capability adds major transmission electron microscopy (TEM) capabilities for life sciences: three- dimensional reconstruction by TEM tomography will literally bring a new dimension into all structural analyses. This state-of-the-art technology is based on acquirement of tilt series of a specimen and its software reconstruction and rendering. The TEM cryostage will allow visualization of cells and macromolecules in their native hydrated state by physical fixation within ultra-thin, vitrified ice layer. Gaining these capabilities lead to a whole new area of structural biology investigations at PNNL that has been so far limited to the conventional TEM imaging. This new instrument provides a vital tool for morphological and functional studies in the area of cell biology and proteomics.



Scanning Probe Microscope for Protein Imaging and Force Measurements. An Asylum Research MFP-3D Atomic Force Microscope situated on top of a Nikon 300TE inverted optical microscope has been purchased and installed. This new capability is essential to the Biogeochemistry Grand Challenge. It will be used for protein imaging and force measurements, and it will help researchers to meet the special requirements of life sciences microscopy (e.g., studies of delicate biological samples under physiological conditions) and provide detailed observations of molecular structures with unprecedented resolution and without the need for rigorous sample preparation and labeling. The system can be used for studying cellular membrane structures, drug-receptor and virus-cell binding, and single-molecule recognition of molecular complexes (e.g., antibody-antigen,



ligand-receptor, DNA-protein, DNA-DNA, protein-protein interactions). Presently, the system is being used by researchers on the EMSL Biogeochemistry Scientific Grand Challenge to examine if the bacterium *Shewanella oneidensis* can generate energy for growth by using cell-surface proteins, called cytochromes, to transfer electrons generated inside the cell directly to Fe(III)-bearing minerals located outside the cell. This research is important in determining the effects that bacterial Fe(III) reduction has on the geochemistry of modern environments and how this can impact the bioremediation of subsurface environments contaminated with organic or metal contaminants.



Three-dimensional image of *Shewanella* bacteria on hematite imaged with atomic force microscopy.

LTQ Mass Spectrometer. The state-of-the-art mass spectrometry capabilities within this facility focus on proteomics—the study of proteins—with a highly developed ability to analyze microbial systems and a developing ability to analyze cells from higher-order systems and tissues. The facility's mission is to advance fundamental knowledge of the biological processes important to DOE's environmental missions and national research priorities in health effects and homeland security. The facility contains unique capabilities ranging from high-performance FTICR mass spectrometers to specially designed liquid chromatographic separations systems and a laboratory information management system designed and written by PNNL staff. In addition, the facility contains a complement of unique and state-of-the-art laboratory instruments that include ion trap, time-of–flight, and quadrupole-time-of-flight mass spectrometers. These unique capabilities are fully integrated to provide unparalleled quantitative proteomics analyses capabilities.

The proteomics capability currently uses multiple ion trap mass spectrometers to build accurate mass and time- (AMT)-tag databases in support of the high-throughput use of the high-performance mass spectrometers. The current generation of linear ion traps offers distinct advantages over the previous generation of ion mass spectrometers. They have more than four times the charge capacity and more than a four times faster scan rate, resulting in over an order of magnitude more data collected per analysis. The end result is that more complete and confident AMT-tag databases can be created in a shorter time. In addition, the proteomics capacity of the facility is fully subscribed and expansion of the business volume is being constrained by lack of capacity. A new linear ion trap mass spectrometer was acquired to increase the high-throughput proteomics capabilities. This instrument adds to the growing capability to acquire MS/MS data more efficiently, providing additional capability for working on new biological systems.

12-Tesla Magnet Coupled with FTICR Mass Spectrometer. A powerful 12-tesla magnet was procured that is enabling unprecedented "top-down" capability for studying proteomics. Manufactured by Magnex Scientific Ltd. for Bruker Daltonics, the superconducting magnet—set up in the HPMSF—allows higher precision and accuracy in mass spectrometry measurements than with previous conventional methods. The top-down analysis provides researchers with an innovative method for helping understand the role, function, structure, and changing nature of cellular proteins within more challenging organisms. Coupled with an FTICR mass spectrometer, this unique tool provides a complementary technique to historically repetitive bottom-up methods, which allows researchers to use mass spectrometry to detect peptides—or pieces of a protein—leading to the positive identification of the presence of particular proteins that compose a cell, resulting in not only a scientific understanding of the protein but potential applications to environmental challenges as well. Very few mass spectrometers of this strength are in existence; the Mayo Clinic installed a 12-tesla FTICR for their proteomics research in 2003.

Stopped-Flow Absorbance Spectrometer System. This new BioLOGIC SFM-400 stopped-flow system was has been installed in EMSL's Environmental Spectroscopy Laboratory. Conventional UV-Vis absorption spectrometers can measure no faster than the second time scale. This stop-flow system allows molecular-level studies of biological and microbial processes that often require characterization of reaction kinetics on faster time scales (ms). The small sample volume needed (i.e., less than 0.03 mL) makes the system ideal for experiments involving biological reactants for which minimum consumption of reagents is desired. This system is used to study protein folding/unfolding and microbial/enzymatic reaction of high-oxidation-state radionuclides, such as uranium (VI) and technetium (VI).

Outreach Activities

EMSL mentors high school students in DOE Science Bowl. T Thevuthasan, Scientific Facility Lead of the EMSL Interfacial and Nanoscale Science Facility, participated in DOE Science Bowl activities involving regional high school students. The DOE Science Bowl took place during February 2005 at Washington State University, Tri-Cities, in Richland, Washington.

EMSL hosts Fabrication and Characterization of Nanomaterials Course. Twelve students from the University of Washington, Oregon Health and Sciences University, Portland State University, and the South Dakota School of Mines and Technology participated in the 2005 Fabrication and Characterization of Nanomaterials course, which was developed through a National Science Foundation grant and held at EMSL. The course was coordinated by F Ohuchi (University of Washington), L-S Wang (Washington State University Tri-Cities), and DR Baer (PNNL), and was led by instructors from the coordinators' institutions as well as Stanford University, University of Idaho, and the University of Alaska. The three-week course involved lectures on specific nanoscience and nanotechnology topics and small project activities in the laboratory, the latter of which provided in-depth training of several EMSL capabilities and involved about 40 percent of the formal class hours. Coordinators view this course as not only a method for sharing the excitement of research at EMSL, but also as a way to grow and train highly qualified future EMSL users.

Students from the Fabrication and Characterization of Nanomaterials Course held at EMSL

EMSL shares optical spectroscopy expertise at Environmental Spectroscopy Symposium. NS Foster-Mills, Environmental Spectroscopy and Biogeochemistry Facility, organized an environmental spectroscopy symposium that focused on presentations related to the application of various optical spectroscopies in environmental research. The symposium was held at the Northwest Regional Meeting of the American Chemical Society in Fairbanks, Alaska, in June 2005.

EMSL staff members participate in PNNL Family Day. On June 18, EMSL opened its doors as part of Family Day, part of PNNL's year-long celebration of its 40th year of operation. Several EMSL staff members participated in the day's events, giving scientific demonstrations, leading tours, and providing information to the hundreds of guests visiting the user facility.

EMSL provides expertise to Eighth International Conference on Laser Ablation. EMSL researcher KM Beck and NB Avery, AG Joly, and WP Hess (all from PNNL) attended the Eighth International Conference on Laser Ablation (COLA 05), which was held September 11-16, 2005, in Banff, Canada. The Conference on Laser Ablation is the leading international conference in the field of laser ablation; it was attended by more than 250 scientists from 25 countries. Avery was the conference organizer, while Hess served as

conference co-chair. All four EMSL/PNNL participants were part of the local coordinating committee. The annual conference explores fundamentals of laser-material interactions and their forefront applications in pulsed laser deposition, nanoscience, analytical methods, materials science, and microprocessing applications.

Hoyt invited to participate in National Science Foundation Panel. EMSL scientist DW Hoyt was invited to serve as a panelist for the National Science Foundation Chemistry Research Instrumentation and Facilities-Multiuser Instrument Acquisition Panel for Fiscal Year 2006. The panel met in Arlington, Virginia, in October 2005.

News Coverage

An article about recent research of artificially petrified wood was featured in the January 28, 2005, news@nature.com article "Furnace Creates Instant Fossils." (http://www.nature.com/news/2005/050124/full/050124-14.html [subscription required]) and the January 25, 2005, *USA Today* article "Topping Mother Nature, Lab Makes Petrified Wood in Days." (http://www.usatoday.com/tech/science/discoveries/2005-01-25-petrified_x.htm). Part of the characterization research was performed using EMSL resources.

A portion of the iron particle research performed at EMSL by researchers from EMSL, PNNL, and the University of Minnesota was featured in the February 10, 2005, *USA Today* article "Nanotech Shows Promise for Cheaper Superfund Cleanup." (http://www.usatoday.com:80/tech/news/nano/2005-02-10-nano-iron-cleanup_x.htm).

PNNL researcher and EMSL user JP Cowin's research on the chemical and physical properties of atmospheric dust and water ice, or "sticky ice," was the subject of a PNNL news release issued March 8, 2005. The research has received considerable coverage in newspapers and publications around the region and nation, including MSNBC's news web site, Discovery.com, *The Oregonian*, and the *Tri-City Herald*. Cowin and his colleagues, including EMSL researcher MJ Iedema, have been using an array of instruments at EMSL to calculate the stickiness of the ice and their formation of planets. Such sticky ice is observed today in comets, planets, and moons in the solar system.

The PNNL press release, "Scientists Team Up for Multiyear Studies of Microbial Mysteries." (http://www.pnl.gov/news/2005/05-37.stm), highlighted the launch of the EMSL Scientific Grand Challenges, focusing on the work that has begun on both the Biogeochemistry Scientific Grand Challenge and the Membrane Biology Scientific Grand Challenge.

The PNNL press release, "Genomic Sequences Processed in Minutes, Rather Than Weeks." (http://www.pnl.gov/news/2005/05-45.stm), featured ScalaBLAST, a sophisticated sequence alignment tool that can divide the work of analyzing biological data into manageable fragments so that large datasets can run on many processors simultaneously.

EMSL User Survey

Each year in February and August, EMSL solicits user feedback via an online survey. In 2005, 283 survey responses were received from users who provided information in the following areas:

- capabilities used
- nature of the EMSL use (remote and onsite)
- manner in which the EMSL environment facilitated scientific accomplishments
- availability of existing EMSL facilities and equipment
- general EMSL performance satisfaction
- satisfaction with support provided by EMSL staff
- possible additional capabilities that EMSL should possess
- appropriateness of safety and training procedures
- benefits resulting from the use of EMSL
- suggestions for better meeting the needs of users
- interest in services that could make use more productive
- User Housing Facility (accommodations on the PNNL campus to house users)
- the ease of using the EMSL User Proposal System
- suggested changes for improvements.

Responses to the 2005 survey are summarized below.

Nature of EMSL Use (onsite and remote)

Of the respondents, 70 percent visited EMSL as part of their proposed research, while 30 percent indicated that their use of the facility did not require an onsite visit: 92 percent of the respondents were from U.S. institutions and the remaining 8 percent were from non-U.S. institutions. Following is a breakdown of users by the institutional categories surveyed.

- U.S. academia – 60 percent
- PNNL staff member – 27 percent
- Other – 2 percent
- DOE laboratories other than PNNL – 6 percent
- Private industry – 2 percent
- U.S. government agencies – 1 percent
- Foreign national laboratories – 1 percent.

Respondents also selected one or more descriptions of the nature of their use of EMSL.

- Collaborative interaction with EMSL staff – 45 percent
- Technical assistance from EMSL staff – 42 percent
- Short-term use of equipment not otherwise available to them – 26 percent
- Part of team using an EMSL capability – 33 percent
- Month or longer use of state-of-the-art capabilities not otherwise available to them – 30 percent
- Month or longer use of unique capabilities – 24 percent
- Use of a single capability – 11 percent
- Individual researcher using an EMSL capability – 18 percent
- Use of unique materials provided by EMSL – 5 percent.

Manner in which EMSL Environment Facilitated Scientific Accomplishments

In rating the manner in which the EMSL environment facilitated scientific accomplishment, 95 percent of the respondents were satisfied or very satisfied. Users acknowledged the scientific expertise, outstanding support from staff, quality of the instruments, and collaborative environment as key factors in their satisfaction.

Availability of Existing EMSL Facilities and Equipment

Respondents to the survey were 97 percent satisfied or very satisfied with the availability of existing EMSL facilities and equipment, although noting that access to some instruments was difficult and the maintenance of other instruments at a modern level insufficient.

General EMSL Performance Satisfaction

When asked how satisfied users were with EMSL performance (e.g., were facilities and equipment maintained close to specifications?), 94 percent of the respondents replied that they were satisfied or very satisfied, many specifically noting excellent staff assistance.

Satisfaction with Support Provided by EMSL Staff

Of the respondents, 95 percent reported being satisfied or very satisfied with the support provided by EMSL staff, and noted that responses were prompt and staff were extremely supportive and knowledgeable.

Possible Additional Capabilities that EMSL Should Possess

Although overall the respondents were pleased with the instruments in EMSL, 28 percent suggested possible additional capabilities, such as:

- long path cells
- a compiler on mMPP2 that will compile WRF-Chem
- a faster computer to replace MPP2

- a confocal microscope
- a high-energy (100 keV) electron source
- a high-speed, magic-angle spinning probe (e.g., 35 kHz with tuning down to at least CI35 for the 750-MHz NMR
- stopped-flow spectrometry
- an infrared refractometer
- a transient absorption spectrometer
- an updated microbeam facility
- additional capabilities for dynamic calculations in NWChem
- a next-generation Auger spectrometer
- a next-generation x-ray photoelectron spectrometer
- a next-generation TEM with a focused ion beam
- characterization of thin magnetic films
- Class-100 clean-room fabrication facilities
- a next-generation time-of-flight secondary ion mass spectrometer
- an environmental TEM cell
- high-speed rotors for solid-state NMR
- a small-sample x-ray diffraction with anoxic sample capability
- stable isotope mass spectrometry
- x-ray absorption fine structure spectroscopy
- a Brunauer-Emmett-Teller analyzer
- more liquid chromatograph-FTICR spectrometers to increase proteomics throughput
- matrix-assisted laser desorption/ionization time-of-flight spectrometry
- liquid surface tension and interfacial tension measurement capabilities.

Appropriateness of Safety and Training Procedures

When users were asked if they found the training and safety procedures to be easy, quick, and appropriate, 89 percent responded positively—a decrease from 95 percent in 2004. Users commented that they found the process to be cumbersome, time consuming, and not particularly useful.

Benefits Resulting from Use of the EMSL

Benefits resulting or soon to result from EMSL use included the following:

- Created new fundamental knowledge such as basic research – 64 percent

- Disseminated new knowledge via publication in peer-reviewed open literature – 57 percent
- Disseminated new knowledge via presentations at professional society meetings – 48 percent
- Trained students – 33 percent
- Facilitated collaborative interactions – 42 percent
- Dissemination of new knowledge via other presentations/media – 23 percent
- Discovered other new knowledge such as applied research – 29 percent
- Established a new network of collaboration – 20 percent
- Furthered DOE missions – 29 percent
- Obtained new research funding – 16 percent
- Developed a new or improved product, process, or technology – 19 percent
- Acquired a patent – 1 percent.

Suggestions for Better Meeting the Needs of Users

When asked how EMSL could better meet their needs, users requested more EMSL staff time for collaboration and support, travel grants, and desk space. Users also suggested that the process for gaining access to the facility (e.g., time taken to review proposals, time required for training) should be streamlined and accelerated.

Ease of Use of the EMSL Proposal System

Finally, 93 percent of respondents found the EMSL User Proposal System easy to use, a decrease from 98 percent in 2004. Users suggested that EMSL develop a capability that would allow users to review their proposals after submission and to check what publications are associated with their proposals. Users also suggested that clear descriptions of equipment be available, especially when multiple instruments exist.

User Services and Outreach

The User Services and Outreach (USO) group promotes the awareness, reputation, and use of EMSL, leading to increased use and impact to science, and facilitates and documents this use for the national user facility and its sponsors. Outreach activities, which are undertaken to increase local, regional, and national awareness of the capabilities and accomplishments at EMSL, include:

- organizing the EMSL User Meeting and workshops
- providing tours of EMSL
- promoting the facility through local and offsite events
- collaborating with the EMSL Communications Manager (CM) to create print media, such as brochures, newsletters, posters, fliers, photos, and to develop and maintain electronic media and websites.

The USO group oversees the systems that enable users to effectively submit proposals for research and EMSL staff to track the users' proposals. The USO group also provides reports to PNNL, DOE, federal, and state regulators to document the success of EMSL as a national user facility. Activities include:

- providing training for the EMSL User System (EUS)
- producing the EMSL annual and bi-monthly reports.

Activities in 2005 included participation in various local and regional meetings, the continued production of outreach-related materials, and ongoing efforts in the areas of user services and the facilitation of access to the facility by users.

Tours. EMSL is one of the main destination points for visitors to PNNL. Each year, nationally elected and appointed government officials, such as cabinet members and members of the U.S. Senate and House of Representatives; local and regional elected officials; senior Battelle and PNNL management; and a broad spectrum of members of the national and international scientific community visit or attend meetings in the facility. As part of EMSL outreach activities, tours of the facility are regularly given. Staff members from the USO group organize, assign, and guide most of these tours. More than 160 tours of EMSL for almost 1200 people were given in 2005.

Access to EMSL. USO staff provide access control and other support services for EMSL. The Front Desk staff members are often the first contacts that users, visitors, and new hires make when entering the facility. These staff members greet visitors, provide information, review requests for access, and process badges and proximity cards. Additional services include distributing various room keys, issuing identification numbers and computer passwords for new accounts, and providing training for users. A USO staff member also works with EMSL management to coordinate office space assignments for staff and visitors. EMSL houses one of two auditoriums on the PNNL campus as well as a number of conference rooms, and USO staff members are the primary points of contact for scheduling these rooms and assisting at events in this facility.

EMSL User and Resource Systems. EMSL has developed electronic tools to automate management of user proposals and track use of EMSL resources.

Released in October 2002, the EMSL Usage System (EUS) tracks the lifecycle of a proposal—from submittal, through review and acceptance, to closure. At various stages in this cycle and at completion, proposal authors are asked for updates of the progress of the research and copies of any publications resulting from the work. Informing the DOE Office of Scientific and Technical Information of these publications is mandated by DOE, and the USO group worked with EMSL groups to develop procedures for meeting these requirements and ensuring compliance, as well as overseeing the incorporation of enhanced features into the software.

The need to manage EMSL's assets and systematically track and report the use of its resources resulted in development of the EMSL Resource System (ERS) to provide data needed to assure maximum efficiency, effectiveness, impact, and continued demand for installed resources. ERS is an online software tool that is used by EMSL staff to schedule,

track, and document the use of major EMSL resources. It provides quarterly and annual resource usage to DOE and other federal agencies. Eliminating the need for paper-log entries of use, ERS provides an at-a-glance view of multiple resources and enables flexibility and instantaneous modification of access schedules. Unexpected changes caused by instrument failure or user requests for alternate access times can be quickly addressed and reflected by scheduling the user on alternate instruments or swapping and matching users with available time slots.

Future Directions

In 2006, the EMSL User Administration Manager and EMSL CM will conduct strategic activities in user outreach and communications in an effort to meet EMSL's mission, goals, and science themes.

User Administration Manager

The User Administration Manager (UAM) is responsible for the administration of the EMSL user program. The UAM is responsible for the operation and maintenance of the management systems used to facilitate access to EMSL. These tools, which include the EUS, the ERS, and the EMSL Proposal Review System (EPRS), have been developed by EMSL staff to manage the user proposals, provide peer reviews of these proposals, and track use of major assets. The UAM is also responsible for the development and management of centralized services to improve the efficiency of providing internal and external user access to the EMSL. The UAM supports the development and management of calls for scientific proposals based of the science signatures of the user facility. The UAM works with the user community, the EMSL UAC, and EMSL senior management to develop procedures and processes to streamline user access and research in EMSL. The operation of EMSL requires reporting to DOE the impact of the user research performed in the facility. The UAM reports the statistics that quantify the impact of our user research and that define the strategic impact of the facility. The UAM will also develop an outreach program.

In 2006, the UAM will focus on the following tasks:

- Update data in the EUS and ERS in a consistent manner.
- Develop EMSL science-theme-based calls for proposals and responsibility for oversight of the peer review processes of these proposals.
- Explore various tactics to achieve a higher response rate for the user survey
- Develop an Outreach Plan to build awareness EMSL research capabilities and expertise. This plan will address ways of:
  - identifying and establishing relationships with potential strategic users
  - accomplishing outreach to regional institutions to increase advocacy for the facility
  - building awareness of EMSL through attendance at national meetings
  - reporting research accomplishments and products to sponsors.
- Implement major capability developments in the EUS/ERS/EPRS

- The EPRS automates, manages, and documents both the external and internal proposal review process as tailored to the needs of each facility. The software manages the proposal review lifecycle, including communications with internal and external reviewers, external access by reviewers where appropriate, documentation of all review results, and reports summarizing current and past review cycles.
- Modify EUS so that Integrated Operations System work locations and hazards for individual user proposal can be identified.
- The ERS will be upgraded to implement user counts based on the new user definition.
- The user survey and logistics will be modified.
- The whole flow of the EUS/EPRS may have to be modified based on new peer-review requirements.

EMSL Communications Manager

The EMSL CM manages and directs the development and implementation of communication activities critical to EMSL's business strategy and scientific user program, particularly in the areas of EMSL science themes, EMSL Scientific Grand Challenges, and refined business practices as they apply to EMSL staff and users. The CM achieves these objectives by employing diverse communications strategies and processes, and through development of multiple strategic products. These accomplishments are conducted through effective partnering and teaming with EMSL staff and users, as well as with peers and staff members in the PNNL Communications and External Relations Directorate, to manage and deliver professional communications expertise and services for EMSL. The CM also provides counsel and information to the EMSL Director and management team and serves as a member of the EMSL management team, addressing a host of directorate issues and priorities.

In 2006, the EMSL CM will focus on the following tasks:

- Develop a plan outlining strategic communications activities to support EMSL's goals, mission, and science themes.
- Continue to improve the EMSL website to provide impactful, timely information to clients, users, and potential users. Particular attention will be focused on the underlying mechanisms that provide the data.
- Continue to support "Action Plan" deliverables (e.g., Strategic Plan, Operations Manual, Staff Handbook).
- Provide DOE and other stakeholders with information and highlights of high-level activities that occur at EMSL.
- Provide booth and symposium presence at American Association for the Advancement of Science National Meeting (February 2006) and American Chemical Society National Meeting (September 2006).
- Continue to improve the bimonthly and annual reporting processes, allowing reuse of content, improved dissemination of information, and significant cost savings related to production.

- Update the internal EMSL website to foster staff/management communication and access to processes and information.
- Further develop targeted overview and facility-specific posters, brochures, and website highlights that link to EMSL science themes and Scientific Grand Challenges and attract distinguished users.
- Further update and improve relevant displays in main EMSL hallway (e.g., posters, brochures) to support the high volume of tours hosted by EMSL.
- Provide support as needed to various PNNL-level requests for EMSL information.

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