Overview

This 2006 EMSL Annual Report describes the research and accomplishments of staff and users of the William R. Wiley Environmental Molecular Sciences Laboratory (EMSL), located in Richland, Washington.

Mission

> *EMSL, a national scientific user facility at Pacific Northwest National Laboratory (PNNL), 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. EMSL 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 operating budget for EMSL is provided by DOE Office of Biological and Environmental Research (BER), while the research conducted within the facility is beneficial to the DOE Office of Science and many funding agencies, including other offices within DOE, the National Institutes of Health, the National Science Foundation, and the 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:

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

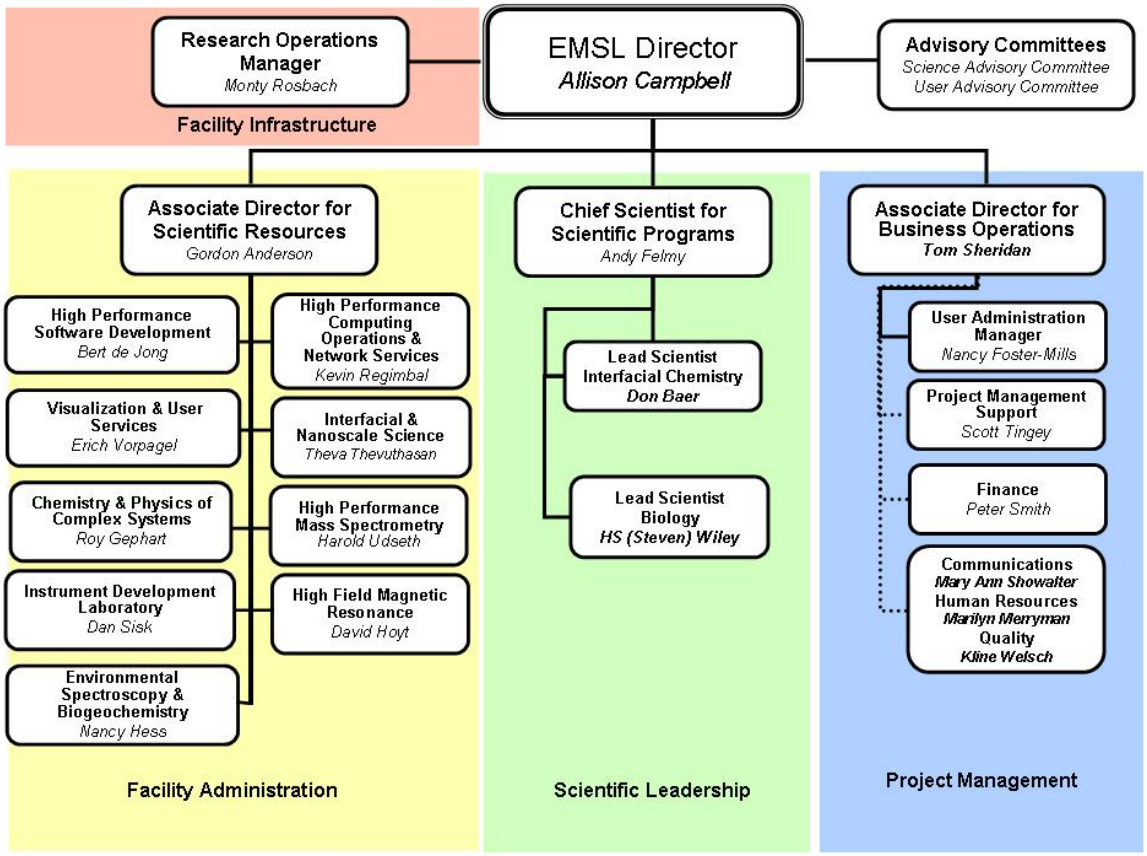
- *High-Performance Computing and Networking Service*s for operation and maintenance of EMSL's computing infrastructure.

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

Organization

The EMSL project 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 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. EMSL's SAC was refreshed during Fiscal Year 2006, and the UAC is targeted to become a self-electing committee in Fiscal Year 2007.

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 of experts from academia, industry, and the national laboratory system that is charged with providing objective, timely advice and recommendations to EMSL leadership. The Committee reports directly to the EMSL Director and serves as the official voice of EMSL's user community in its interactions with EMSL management.

The responsibilities of the User Advisory Committee include the following:

- Provide a clear channel for the exchange of information and advice between EMSL users and management.
- Provide a formal vehicle for EMSL users to transmit concerns and recommendations to the EMSL Director.
- Design and oversee the EMSL User Meetings.
- Provide advice and recommendations to the EMSL Director on how to facilitate the effective use of EMSL.
- Nominate active users for future membership to the committee.

In Fiscal Year 2006, the UAC charter was revised to call for a self-electing committee. Preparations were made for nomination and election processes that would take place for a refreshed UAC in Fiscal Year 2007.

Science Advisory Committee

The independent SAC provides objective advice on long-term science direction to the EMSL Director related to topics such as:

- EMSL's focus on national priorities and science challenges
- strategy for accomplishing EMSL's vision
- potential opportunities for transferring science to applications
- stewardship.

The SAC is comprised of distinguished scientists from academia, national laboratories, and research institutions across the United States who provide expertise in EMSL's major capability areas of biology, environmental science, molecular science, and theory. The committee reports to the Director, Pacific Northwest National Laboratory. Responsibilities and activities of the Science Advisory Committee include:

- providing advice on scientific direction for the EMSL user program
- recommending appropriate balance of instrument time for Grand Challenges, general users, and capability development activities

- assisting EMSL with formulating policies related to facility scientific output, scientific impact of the EMSL user program, user access, and other issues, as needed
- performing periodic reviews of scientific impact from the various elements of the EMSL user program.

In Fiscal Year 2006, the SAC membership was refreshed. The committee meets annually at EMSL and the 16 members serve staggered 4-year terms. The current members of the SAC are as follows:

- Len Spicer, Duke University (Chair)
- Mark A. Barteau, University of Delaware
- Gudmundur S. "Bo" Bodvarsson, Lawrence Berkeley National Laboratory
- Gordon E. Brown, Jr., Stanford Synchrotron Radiation Laboratory
- Charles T. Campbell, University of Washington
- Marvin Cassman, University of California
- Gregory Choppin, Florida State University
- Barbara J. Finlayson-Pitts, University of California
- George W. Flynn, Columbia University
- David J. Galas, Keck Graduate Institute
- Sam Kaplan, University of Texas-Houston Medical Center
- Mary P. Neu, Los Alamos National Laboratory
- Julia Rice, IBM Almaden Research Center
- Peter J. Rossky, University of Texas at Austin
- James M. Tiedje, University of Michigan
- Mary F. Wheeler, University of Texas at Austin.

Proposals and User Access Modes

EMSL users are encouraged to submit proposals in response to periodic or continuous calls for proposals. By responding to different calls for proposals, users have the opportunity to choose from different options regarding the speed of access and the length of time over which a proposal may remain active. Different options for the type of proposal, type of access, and proprietary status are available to optimize scientific impact and facilitate evolution of EMSL capabilities and science to address cutting-edge science questions.

Calls for Proposals

- **Science Theme Call.** 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. EMSL's four science themes are: Atmospheric Aerosol Chemistry, Biological Interactions and Interfaces, Geochemistry / Biogeochemistry and Subsurface Science, and Science of Interfacial Phenomena. To highlight these areas, theme-based calls for proposals occur at least once a year. Science Theme proposals are valid for one year and can be extended twice for a total period of three years. Some EMSL resources may be especially dedicated to science theme proposals. EMSL's first Science Theme call for proposals was sent out in April 2006.

- **Grand Challenge Computational Call.** EMSL's Molecular Science Computing Facility (MSCF) sends out a call for Computational Grand Challenges once a year, providing that computer time is available. The call includes research applications in biology, chemistry, climate, and subsurface science and is open to all research entities regardless of research funding source. Computer time for Computational Grand Challenges is allocated for up to three years, with the computer allocation appropriate for the scope of research to be performed.

- **Capabilities-based Call.** The EMSL Capabilities-based call for proposals is focused on new and extended use of EMSL capabilities. Proposals that use EMSL's unique and new or developing capabilities, that apply EMSL capabilities in specific developing areas, or that propose environmentally or other important work that may not fit within the EMSL four science themes will be encouraged. The EMSL Capabilities-based call replaced the previous semi-annual High-Field Nuclear Magnetic Resonance Facility call. Proposals in response to this call are valid for one year and can be extended only once for a total open period of two years.

- **Open Call.** EMSL users can continue to submit general-use proposals at any time. This type of proposal may not be extended and will be valid for only one year. A new proposal is required each year.

Types of Proposals

- **General.** Use of existing EMSL resources typically falls into this General use category. General use proposals may be submitted to EMSL at any given time throughout the

year. General Use proposals are evaluated by peer review prior to work. Proposals may be from individuals or groups who need access to the facility to carry out their research, using existing equipment in the EMSL. The scope of a General Use proposal can vary from a single experiment proposal to full project proposal (valid for multiple visits and substantial access to a range of equipment extended over multiple years). Individual and group proposals, including collaborative proposals with EMSL staff, are encouraged.

- **Partner.** Partner proposals are individuals or groups who not only carry out research at EMSL but have developed an agreement to also enhance the capabilities. Typically they develop the facility instrumentation in some way, bringing outside financial and/or intellectual capital into the evolution of EMSL. These contributions must be made available to the general users and so benefit them as well as the facility. In recognition of their investment of either resources or intellectual capital and in order to facilitate and encourage their involvement, Partner proposals may allocate participants with limited access to one or more facilities over a period of several years, with the possibility of renewal. Partner user activities are negotiated among the teams involved. New Partner proposals can be submitted in response to Science Theme or other calls, but requires information and discussions beyond the two page proposal work description required for a general type of proposal. Partner proposals are subject to the same peer review process as general proposals. Teams planning a partner proposal should have discussions with EMSL team leads before this type of proposal is submitted.

Types of Access

EMSL users can access the capabilities of the user facility in two ways.

- **Standard Access.** Standard access to EMSL facilities can vary from a single visit, single experiment proposal to a full project proposal (valid for multiple visits and substantial access to a range of equipment extended over multiple years). Prior to any work, a proposal must pass peer review. This is the most common mode of access to EMSL capabilities.

- **Rapid Access.** In limited cases, users may need access to EMSL capabilities where rapid turnaround of data is required (e.g. thesis work, project progress, and paper publication or proposal preparation). If approved, a rapid access proposal will be valid for no more than one month of EMSL use. These proposals must clearly justify why Rapid Access is needed. Work on proposals can be started subject to instrument and resource availability and subject to approval of the Scientific Facility Lead. Proposals will undergo internal peer review that will be conducted as work is initiated. However, all other reviews, including ES&H and the business office, must be complete before usage can begin. If users need rapid access for research that they may want to continue, they may also submit (possibly at the same time) a standard access proposal.

Proprietary Status

- **Non-Proprietary Research.** Research and equipment usage conducted at EMSL where the 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 nonexclusive license to use the intellectual property.

- **Proprietary Research.** EMSL facilities can be used for proprietary research. DOE requires that such work pay full-cost recovery of the facilities used which includes, but is not limited to, labor, equipment usage, consumables, materials, and EMSL staff travel.

Science Themes

EMSL established key science themes that focus the strengths of the facility and its user program on increased scientific impact. Science themes guide user outreach efforts, help prioritize investments in equipment and staff, and guide review of user proposals. The objective of science themes is to define and develop key collections of user projects that, taken together, can significantly and positively impact an important area of environmental molecular science.

EMSL's four science themes are:

- **Atmospheric Aerosol Chemistry.** Expanding a global- to molecular-scale understanding of aerosol processes and their impacts.

- **Biological Interactions and Interfaces.** Developing a molecular-scale understanding of cells and biomolecules to provide a scientific solutions approach to biological systems.

- **Geochemistry/Biogeochemistry and Subsurface Science.** Expanding a molecular-level understanding of subsurface fate and transport and biogeochemical cycling.

- **Science of Interfacial Phenomena.** Tailoring interfacial structures for dynamics, reactivity, and transport.

In April 2006, the first-ever EMSL Science Theme Call for Proposals was sent out to users. The inaugural call was a success, with 98 proposals received: 8 for Atmospheric Aerosol Chemistry, 13 for Biological Interactions and Interfaces, 21 for Geochemistry/Biogeochemistry and Subsurface Science, and 56 in Science of Interfacial Phenomena. Based on instrument availability and scientific merit, 90 of the proposals were selected and the principal investigators notified in July 2006. The next Science Theme Call for Proposals will be sent out in February 2007.

EMSL Scientific Grand Challenges

EMSL has been challenging the traditional approach to research with two Scientific Grand Challenges—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 EMSL's cutting-edge resources.

Progress in EMSL's two Scientific Grand Challenges can help DOE resolve the enormous problems associated with environmental contamination across the complex, saving DOE and the country hundreds of millions of dollars and reducing risk to humans and the environment. The Scientific Grand Challenges have brought together some of the world's best minds and engage scientists from more than 20 universities and research institutions worldwide.

Biogeochemistry Scientific Grand Challenge

A Scientific Grand Challenge in biogeochemistry, led by PNNL scientists John Zachara and Jim Fredrickson, is studying how organisms exchange energy and electron flux with mineral matter in soils, sediments, and subsurface materials. This exchange occurs across a mineral-microbe interface that is a minute, but chemically active domain whose molecular workings have perplexed scientists for decades. The Biogeochemistry Scientific Grand Challenge uses EMSL's advanced instrumental capabilities and high-performance computing capabilities to understand the biologic and physical architecture of this remarkably complex domain and the microbe-mediated chemical reactions that occur within it. The research allows scientists to understand this most basic earth-life interaction that is fundamental to the migration of environmental contaminants, to water quality, and to soil fertility and trace metal availability. Publications involving the Biogeochemistry Scientific Grand Challenge in Fiscal Year 2006 include the following:

- A manuscript detailing research performed under the Biogeochemistry Scientific Grand Challenge was published in the July 2006 issue of *Journal of Bacteriology*. The article describes work in which a protein complex implicated in the reduction of manganese and iron was purified and its subunits were identified. To clarify the roles of cytochromes OmcA and MtrC in the bacterium *Shewanella oneidensis* MR-1, the researchers—EMSL scientists, EMSL scientific consultants, and staff and users from PNNL—cloned, expressed, and purified the cytochromes, permitting for the first time direct measurements of their metal-reducing activity and functional association. The results of this study will help provide an important understanding of how metal reductase activities can function in the reductive immobilization of toxic metals at contaminated sites. Future experiments will measure the possible association and function of a reconstituted OmcA-MtrC complex against solid metals to determine whether binding and metal reduction involve a direct association with individual proteins.

- EMSL researchers, along with scientists from PNNL, Argonne National Laboratory, and the University of Wisconsin, Milwaukee, are studying the biomolecular mechanisms of the *S. oneidensis* and uranium interaction. Under anaerobic conditions, microbes like *S. oneidensis* can donate electrons to, or reduce, metals. Changing a metal's chemistry in this way affects its solubility. For example, *S. oneidensis* reduces very soluble hexavalent uranium, U(VI), to less soluble uranium oxide, UO_2, limiting its movement in groundwater. To study electron transfer at the microbe-mineral interface and how extracellular UO_2 is formed, the researchers used a novel combination of high-resolution electron microscopy analyses at EMSL and synchrotron-based X-ray fluorescence microscopy at Argonne's Advanced Photon Source. The team is the first to confirm that *c*-type cytochromes, which are proteins on the bacterial outer membrane, are essential for U(VI) reduction and UO_2 particle formation. Further, the cytochromes and biogenically reduced UO_2 particles are co-localized in the extracellular polymeric substance (EPS), a protective matrix on the outside of some bacteria. The association of cytochromes and UO_2 in the EPS may shed some light on the long-term fate of biogenically reduced UO_2 in the environment. The EPS may affect the fate of UO_2 by influencing its susceptibility to oxidation or its transport in soils and sediments. Results of this research were reported in the *Public Library of Science Biology*.

Membrane Biology Scientific Grand Challenge

Dr. Himadri Pakrasi from Washington University in St. Louis is leading a Scientific Grand Challenge in membrane biology that uses a systems approach to understand the network of genes and proteins that govern the structure and function of membranes and their components responsible for photosynthesis and nitrogen fixation in cyanobacteria (blue-green algae). A systems approach integrates all temporal information into a predictive, dynamic model to understand the function of a cell and the cellular membranes. These microorganisms make significant contributions to harvesting solar energy, planetary carbon sequestration, metal acquisition, and hydrogen production in marine and freshwater ecosystems. Cyanobacteria are also model microorganisms for studying the fixation of carbon dioxide through photosynthesis at the biomolecular level. The results of this Scientific Grand Challenge are providing the first comprehensive systems-level understanding of how environmental conditions influence key carbon fixation processes at the gene-protein-organism level. This topic was selected because it addresses critical DOE science needs, provides model microorganisms to apply high throughput biology and computational modeling, and because it takes advantage of EMSL's experimental and computational capabilities. Publications involving the Membrane Biology Scientific Grand Challenge in Fiscal Year 2006 include the following:

- In the June 2006 issue of *Proceedings of the National Academy of Sciences of the United States of America*, Nicole Koropatkin, Himadri Pakrasi, and Thomas Smith of EMSL's Membrane Biology Scientific Grand Challenge team describe the first structure determined for a nitrate receptor, that of NrtA in a species of cyanobacteria. Nitrate is the most important nutrient for photosynthesis and growth, and cyanobacteria are capable of both nitrogen fixation and photosynthesis. NrtA represents a previously uncharacterized class of transport proteins. The closest homologue of NrtA is CmpA, a bicarbonate-binding protein found in several species of cyanobacteria. The similarity of NrtA to other nitrate

and bicarbonate receptors sheds light on the possible differences between nitrate and bicarbonate binding and reveals a previously unknown link between nitrate and bicarbonate uptake in cyanobacteria. Knowledge gained by studying photosynthesis and nitrogen fixation can be applied to issues of environmental sustainability, such as improvements in solar energy conversion and carbon sequestration.

EMSL Highlights

EMSL Science Highlights

In Fiscal Year 2006, staff and users from the six research facilities at EMSL performed leading-edge research in a variety of scientific disciplines. Below are brief research summaries for each research facility, with more in-depth highlights of research provided in subsequent sections of this annual report.

Air Campaign Studies Role of Hydrocarbons and Aerosols in Industrial Setting. Three portable mass spectrometers that are part of the Chemistry and Physics of Complex Systems Facility's suite of state-of-the-art research instruments played an important role in a study of hydrocarbons and aerosols in the atmosphere during a field campaign in Houston. The September 2006 campaign involved EMSL researchers and users as well as scientists from PNNL, who joined forces with colleagues from around the world to examine the distribution of ozone-damaging gas and particles in an industrialized environment within the greater Houston area. Measurements were taken using the mass spectrometry combination from three locations associated with elevated ozone levels: (1) in the southeast portion of the city near the largest complex of petrochemical and oil refineries in the world; (2) in southwest Houston, where nitrogen emissions from automobiles are prevalent; and (3) north of Houston, near natural sources of hydrocarbons. The combined use of the mass spectrometers—a Quadrupole Aerosol Mass Spectrometer, a Time-of-Flight Aerosol Mass Spectrometer, and a Proton Transfer Reaction-Mass Spectrometer—resulted in a unique data set that will help the researchers answer questions related to hydrocarbon/aerosol interactions. This recent study followed a campaign conducted in 2000 to provide an understanding of how ozone levels in Houston far exceeded those found elsewhere in the United States, and how they amassed in such a short time. Results from the 2006 study will help researchers now determine the effectiveness of emissions controls, implemented following the 2000 study, in reducing high ozone episodes.

Three portable mass spectrometers and EMSL research experts were instrumental in a September 2006 atmospheric field campaign in industrialized Houston.

Flow and Transport Capabilities Support Effort to Strengthen Permeable Reactive Barrier. A permeable reactive barrier installed in the late 1990s at the Hanford Site has been used to prevent chromate—used by early DOE agencies to prevent fuel element corrosion in nuclear reactors—from reaching the nearby Columbia River. However, the toxic material

has been detected in several groundwater monitoring wells at the site, indicating premature loss of reductive capacity of the barrier. To inhibit chromate migration, the EMSL Environmental Spectroscopy and Biogeochemistry Facility's subsurface flow and transport capabilities were used to conduct column and flow cell experiments to assess the viability of adding zero valent iron enhanced with polymer solutions to portions of the barrier that have lost reductive capacity. The experiments effectively yielded the necessary polymer, polymer concentration, and injection parameters to considerably improve the effectiveness and longevity of the barrier. These results are now being used by Fluor Hanford—the prime Hanford Site contractor for environmental cleanup—for the design of a pilot test for the insertion of the zero valent iron and polymer solution to the barrier in Fiscal Year 2007.

Using One of the Highest Available Fields to Characterize Hanford's Most Abundant Radionuclide. Strontium is the most abundant radionuclide found in tank waste at the Hanford Site in Richland, Washington. Using the marquee 900-MHz NMR spectrometer at EMSL's High-Field Magnetic Resonance Facility—one of the highest NMR fields available—and pulse sequence methods developed at EMSL, users from Pennsylvania State University and the University of Illinois, along with researchers from EMSL, are characterizing strontium binding in various synthetic clay soils. The molecular-level structure of strontium binding sites has rarely been explored in clay minerals by direct spectroscopic means and is not well understood, yet strontium binding directly affects the transport, sequestration, and remediation of the radionuclide released from high-level waste storage tanks. This research, outlined in the February 2006 issue of *Solid State Nuclear Magnetic Resonance* and the April 13, 2006, issue of *Journal of Physical Chemistry B,* has implications for understanding how strontium contaminants can be contained in clay soils.

EMSL's 900-MHz NMR spectrometer is helping users characterize strontium binding in various synthetic soils.

Researchers Make Strides Toward Neurodegenerative Disease Studies. EMSL users from PNNL, in collaboration with scientists from UCLA's David Geffen School of Medicine, are researching the precise connection between oxidative stress—cell damage caused during metabolism when the oxygen in the body assumes ever more chemically reactive forms—and neurodegenerative diseases such as Parkinson's, Alzheimer's, and Lou Gehrig's. Through use of the EMSL High-Performance Mass Spectrometry Facility's state-of-the-art mass spectrometry capabilities that allow protein identification and separation with unprecedented precision, researchers were able to conduct this important study from the largest and most detailed proteomic analysis of a mammalian brain generated to date—nearly 8,000 different, detectable proteins in the brain of a mouse. Results of the study suggested that many neurodegenerative diseases leave the biomarker, nitrotyrosine, which could be used to predict the earliest stage of brain impairment and perhaps lead to detection of

disease states before symptoms occur. The researchers will continue their study using tissues with neurodegenerative diseases. This research was described in detail in *Biochemistry*, while details of characterization of the mouse brain proteome were detailed in *Journal of Proteome Research*.

New Model System Offers Fundamental Insight into Catalyst Structure and Behavior. A new model system of tungsten nano-structures offers chemists a view into the structure and reaction mechanisms of metal oxides. Developed by users of EMSL's Interfacial and Nanoscale Science Facility from PNNL, the University of Texas-Austin, and Washington State University, formation of the model system was reported in the June 23, 2006, online issue of *Angewandte Chemie, International Edition*. The discovery may offer a platform for fundamental reactivity studies of metal oxides used as catalysts in converting hydrocarbons into fuels and value-added chemicals. The model system—where all the molecular clusters are the same size, are evenly dispersed, and are oriented in one of two directions on a single layer of titanium oxide crystals—holds promise as a platform for studying the behavior of early transition metal oxides.

Modeling of Water Cluster Results in a Sustained Peak Flop Efficiency of 63 Percent. High-level correlation modeling of water clusters has provided researchers with the most accurate interaction energies ever calculated, which will be used to gain insight into water's unique properties. These calculations also demonstrate the unique capabilities of NWChem and EMSL's supercomputer, located at the Molecular Science Computing Facility. Researchers from EMSL and PNNL used the highly scalable and parallel NWChem software to calculate accurate energetic information of a cluster of eight water molecules. The coupled cluster singles doubles with perturbative triples, or CCSD(T), calculation and an aug-cc-pVQZ basis set (1376 basis functions, 32 correlated orbitals) required 1840 processors, almost the entire machine, and 37 hours to complete. This huge NWChem CCSD(T) sustained an average of more than 63 percent of peak flops efficiency (6.99 teraflops) during the calculation, demonstrating the unique capabilities of the NWChem software and the supercomputer architecture and meeting a stretch goal of DOE's Office of Advanced Scientific Computing Resources outlined in PNNL's contract.

EMSL Staff Highlights

In 2006, EMSL staff received continued recognition for progress in development of state-of-the-art capabilities and expertise, and for their professional contributions.

EMSL Staff Member Receives a 2005 Presidential Early Career Award for Scientists and Engineers. In July 2006, Yanwen Zhang, an EMSL materials physicist in the Interfacial and Nanoscale Science Facility, was notified that she had been chosen to receive a 2005 Presidential Early Career Award for Scientists and Engineers (PECASE), the highest honor bestowed by the U.S. government on outstanding scientists and engineers who are beginning their independent careers. Zhang and 55 other recipients were honored by President Bush and received their awards from John Marburger, director of the White House Office of Science and Technology Policy. The award recognizes scientists and engineers who show exceptional potential for leadership in scholarship, service, and education.

EMSL staff member Yanwen Zhang shakes hands with Secretary of Energy Samuel Bodman during a ceremony to receive the prestigious PECASE Award.

To be eligible for the presidential award, Zhang first had to be selected by DOE for its Early Career Scientist and Engineer Award. As a Presidential Early Career Award recipient, Zhang receives a commitment from DOE's Office of Science to continue funding the research for which the award was given for 5 years.

Zhang's research focuses on interactions of energetic ions with solid materials and how those interactions can be applied to the analysis and study of those materials. Zhang developed a novel way of measuring the energy loss of atomic particles as they pass through materials. Accurate measurements of such energy loss were a long-standing problem until Zhang successfully used high-resolution, time-of-flight spectroscopy to determine energy loss over a continuous range of energies.

With more than 100 publications and several long-term international research collaborations, Zhang is recognized for her contributions in ion-solid interactions, irradiation effects, and ion-beam techniques. She also is active in several professional societies, has received many international scientific and academic awards, and is involved in educational activities and community service. She routinely hosts visiting scientists at EMSL's ion-beam user facility; lectures on topics related to ion-beam physics; mentors postdoctoral fellows, graduate students, summer undergraduates, and high school interns; serves on Ph.D. committees;

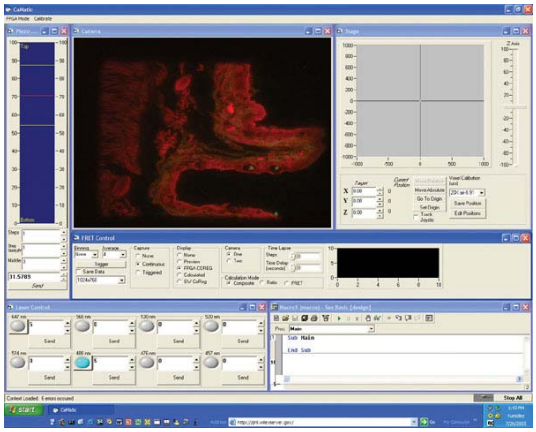
assists local middle schools with Chinese translations; and serves as a judge for local science fairs.

Zhang holds two doctorate degrees—one in engineering physics from Lund University in Sweden and another in science from Beijing Normal University in China.

EMSL Director's Research Earns Two Prestigious Awards. EMSL Director Allison Campbell received a 2006 Federal Laboratory Consortium Excellence in Technology Transfer Award and a 2006 R&D 100 Award for a novel water-based process for depositing bioactive calcium-phosphate coatings containing therapeutic agents on orthopedic implants and medical devices. The surface-induced mineralization process provides patients with a two-fold benefit: implants that are bacteria resistant and are easily assimilated into the body. The process involves unique calcium-phosphate coatings containing an antimicrobial agent that was proven in tests to kill infection-causing bacteria or greatly inhibit bacteria growth in the body, helping prevent dangerous and costly post-surgical infections. The water-based deposition process, coupled with the bioactive therapeutic agent, also provides an advanced method for applying pure calcium-phosphate coatings to artificial joints, allowing enhanced bone bonding.

EMSL Director Allison Campbell (back, center) shared R&D 100 Award honors with team members (from left) Barbara Tarasevich, Peter Rieke, and Shari Li.

Instrument Development Laboratory Staff Develop Remote Control Software for State-of-the-Art Confocal Microscope. EMSL Instrument Development Laboratory staff Derek Hopkins and Brian LaMarche, intern Anoop Mayampurath, and research staff from PNNL developed software to control a state-of-the-art confocal microscope in real time from a remote location. In a recent demonstration, live cell images were acquired and streamed across a 1-gigabit Ethernet connection at 15 and 30 frames per second. This capability will ultimately enable external researchers to use unique instruments found only at PNNL, as well as provide unique opportunities for real-time collaboration.



Confocal microscope software developed by EMSL Instrument Development Laboratory staff along with researchers from PNNL.

This development expands the potential reach of the EMSL user program by providing a framework for remote access of state-of-the-art instrumentation. The demonstration displayed the potential of remote control software tools to expand availability by enabling researchers around the world to remotely access instrumentation, limited only by the available bandwidth.

Current studies on cell physiology and reaction to stimuli usually are performed using cells cultured on two-dimensional surfaces. This geometry greatly simplifies the methodology used to observe and propagate cells; however, it places great constraints on how one can investigate intercellular communication and stress responses. The high-speed confocal microscope is a tool necessary to analyze cell signaling in a three-dimensional environment. It provides users the ability to look at cellular signaling, protein interactions, and cellular localization/translocation of signaling molecules, in real time and in living cells. These capabilities are being applied to research in cell, cancer, and radiation biology.

The microscope control software was based on the flexible Surf-O-Matic architecture developed initially at EMSL for surface science research. The application has controls for setting the laser wavelength and amplitude, three-axis stage positioning, and image capture settings, and allows the user to write Visual Basic-like scripts to automate all aspects of the application. This provides the unique capability to run highly configurable experiments unattended for long periods of time. The imaging portion of the software interfaces two Coreco PC-DIG capture cards capable of frame rates up to 30 frames per second. At full frame resolution, the software captures 15 frames per second—or 14.4-million pixels per second. Each frame captured is approximately 1.3 MB in size. Coupled with automated experiments running days on end while generating images at 15 fps, this system is capable of generating large amounts of data in a short time span. The software is also unique because it corrects for physical defects in the images (e.g. lens distortion) by using a distinctive image registration technique that allows a pixel-perfect match in real time.

EMSL Researcher Honored for Safety Role. Jim Follansbee, a staff member in EMSL's Instrument Development Laboratory, was honored by PNNL as the first-ever Cognizant Space Manager of the Year. Follansbee has been responsible for several laboratory areas in EMSL since the user facility opened in 1997. During this time, he has maintained an accident-free environment within these spaces—which are used frequently by PNNL staff, visiting users, and local students. He was honored on September 12, 2006, at a luncheon and awards ceremony.

Instrument Development Laboratory staff member Jim Follansbee (right) accepts the first-ever PNNL Cognizant Space Manager of the Year Award from Mike Schlender, Deputy Laboratory Director for Operations.

EMSL User Highlights

The following is a sampling of the many user highlights that occurred in Fiscal Year 2006 as a result of research conducted at EMSL.

Finlayson-Pitts Elected to Two Prestigious Academies. Within a week's time, Barbara Finlayson-Pitts was elected Fellow of the American Academy of Arts and Sciences and the National Academy of Sciences. Finlayson-Pitts is involved in the study of chemical reactions in the lower atmosphere to better understand air pollution in urban and remote areas and has studied the effects of sea salt on urban smog formation and on remote atmospheres, as well as how chemical reactions on the surfaces of buildings and roads affect urban air quality and models of air pollution.

Barbara Finlayson-Pitts

Bruce Kay

Kay Honored by American Association for the Advancement of Science. Bruce Kay was inducted as a Fellow in the American Association for the Advancement of Science, which cited his "meritorious efforts to advance science or its applications."

Julia Laskin

Laskin Appointed to American Society for Mass Spectrometry Board of Directors. Julia Laskin has been appointed to the American Society for Mass Spectrometry Board of Directors. Laskin will act as treasurer of the Board. In this role, she will make recommendations to the Board relevant to preserving the economic health of the Society and will present a financial report at each annual meeting.

Kerisit Receives 2005 M.T. Thomas Award. Sebastien Kerisit was selected as the 2005 recipient of the M.T. Thomas Award for Outstanding Postdoctoral Achievement in recognition of such accomplishments as seminal and novel theoretical advancements in understanding electron transfer reactions at environmental interfaces and the impact on the field of geochemistry. Use of his unique combination of molecular dynamics simulations, electronic structure calculations, and kinetic Monte Carlo simulations constitutes the first attempt to computationally model the bioreduction of iron at mineral surfaces at the atomic level. Kerisit has used these techniques to contribute significantly to the EMSL Biogeochemistry Scientific Grand Challenge, where he has computed rates of electron transfer in iron oxide lattices and from heme groups in outer-membrane cytochromes to various hematite (α-Fe_2O_3) surfaces. His work has been published in the

Sebastien Kerisit received the 2005 M.T. Thomas Award for Outstanding Postdoctoral Achievement.

Journal of Chemical Physics and *Geochimica et Cosmochemica Acta.*

Kimmel Featured in *Chemical and Engineering News*. Greg Kimmel was featured in the September 26, 2006, issue of *Chemical and Engineering News*. Kimmel was one of 200 scientists from around the world who attended a Nuclear Energy Workshop held by the U.S. Department of Energy to identify key areas of science in which fundamental research has the potential to make a significant impact on the future of nuclear power.

Greg Kimmel

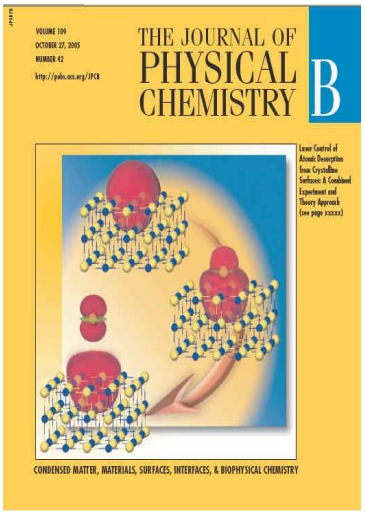
Lin Receives Several Publishing Honors. Publications detailing research of carbon nanotube—materials 10,000 times smaller than a human hair that have potential application for the next generation of biosensors and for high-efficiency fuel cells—performed using the capabilities of EMSL's Interfacial and Nanoscale Science Facility have earned Yuehe Lin several prestigious citation honors. Among them, a paper by Lin and PNNL postdoctoral fellow Guodong Liu, "Carbon Nantotube-Templated Assembly of Protein," was featured on the April 2006 cover of the *Journal of Nanoscience and Nanotechnology*. A paper published in 2003 by Lin and his collaborators in *Advanced Materials* is featured on the Institute for Scientific Information's Essential Science Indicators as one of the highly cited papers in the field of materials science. Finally, a paper by Lin and his collaborators published in the *Journal of the American Chemical Society* was the most cited paper of nearly 10,000 papers published in that journal from January 2003 to December 2005, based on ISI's citation data.

Yuehe Lin

Bowman Serves on Thesis Defense Committee. Mike Bowman traveled to Washington State University, Pullman Washington, to serve on a Thesis Defense Committee. He participated in the doctoral thesis defense of Dr. Jonathan Cape. Dr. Cape's thesis topic was "The Mechanism of Quinol Oxidation in the Cytochrome bc complex." This doctoral defense included work performed as a user in the EMSL High-Field Magnetic Resonance Facility.

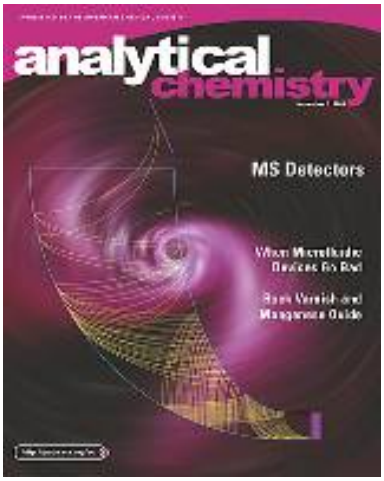
Journal Covers

During Fiscal Year 2006, research by EMSL users and staff was highlighted on six scientific journal covers. The following describe the research that led to these covers.



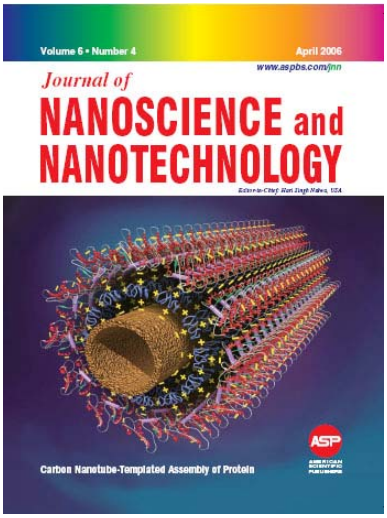
Wayne Hess, Alan Joly, Ken Beck, and Matthias Henyk, along with their collaborators at University College London, have focused on hyperthermal desorption of halogen atoms and show that yield, electronic state, and velocity distributions of desorbed atoms can be selected using tunable laser excitation. Results show that desorption of these materials leads to controlled modification of their surface geometric and electronic structures. This research was featured on the cover of the October 27, 2005, *Journal of Physical Chemistry B*.

Hess WP, AG Joly, KM Beck, M Henyk, PV Sushko, PE Trevisanutto, and AL Shluger. 2005. "Laser Control of Desorption through Selective Surface Excitation." *Journal of Physical Chemistry B* 109:19563–19578.



Dave Koppenaal and his collaborators provided 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*.

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.

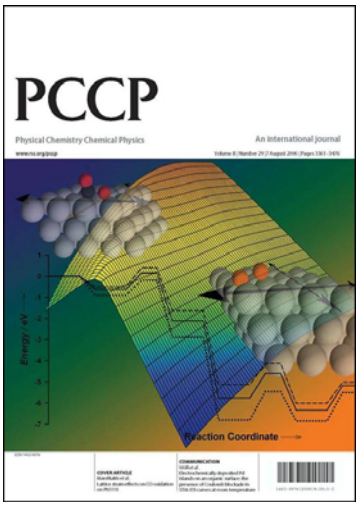


Guodong Liu and Yuehe Lin describe a novel general strategy for fabricating protein–polyion multilayers by electrostatic layer-by-layer self-assembly on carbon nanotube templates. Such a noncovalent functionalization method is important for preserving the activity of biomolecular, the mechanical, and electrical properties of carbon nanotubes. The research was featured on the April 2006 cover of the *Journal of Nanoscience and Nanotechnology*.

Liu G, and Y Lin. 2006. "Carbon Nanotube-Templated Assembly of Protein." *Journal of Nanosscience and Nanotechnology* 6(4):948–953.

LS Wang, EMSL user from PNNL, and collaborators from the University of Nebraska have uncovered a class of gold atom clusters that are the first known metallic hollow equivalents of the famous hollow carbon fullerenes known as buckyballs. This research has so far led to stories in several journals and websites, including *Chemical & Engineering News*; the *Seattle Post-Intelligencer*; *Chemistry World*, which is published by the Royal Society of Chemistry in the United Kingdom; and *Nanotechwire*. This work was also featured on the cover of the May 30, 2006, issue of the *Proceedings of the National Academy of Science*.

Bulusu S, X Li, LS Wang, and XC Zeng. 2006. "Evidence of Hollow Golden Cages." Proceedings of the National Academy of Science 103(22):8326–8330.



Lars Grabow, Ye Xu, and Manos Mavrikakis, University of Wisconsin-Madison, conducted research that discovered that surface strain plays a major role in determining the rate limiting step and catalytic activity of platinum for CO oxidation. This research was featured on the cover of the August 7, 2006, issue of *Physical Chemistry Chemical Physics (PCCP)*.

Grabow L, Y Xu, and M Mavrikakis. 2006. "Lattice Strain Effects on CO Oxidation on Pt(111)." *Physical Chemistry Chemical Physics* 8:3369-3374.

Hua-Jin Zhai and Lai-Sheng Wang (Washington State University, Tri-Cities), and Dmitry Zubarev and Alexander Boldyrev (Utah State University) have discovered a new class of endohedreal lead cage compounds that they have named "plumbaspherenes" (see research highlight entitled "Pb_{12}^{2-}: Plumbaspherene"). The existence of these new cage compounds may allow for the insertion of other atoms inside these cages to create new materials with unique properties for a wide range of applications. This research was featured on the cover of the August 31, 2006, issue of the *Journal of Physical Chemistry A*.

Zhai HJ, LS Wang, DY Zubarev, and AI Boldyrev. 2006. "Gold Apes Hydrogen. The Structure and Bonding in the Planar $B_7Au_2^-$ and B_7Au_2 Clusters." *Journal of Physical Chemistry A* 110:1689-1693.

Patents

EMSL staff and their collaborators received three patents in Fiscal Year 2006.

U.S. Patent 6,979,816 for the "Multi-source Ion Funnel" was issued in December 2005 to K Tang, MB Belov, AV Tolmachev, HR Udseth, and RD Smith.

U.S. Patent 6,989,674 for the "Advanced Slow-Magic Angle Spinning Probe for Magnetic Resonance Imaging and Spectroscopy" was issued in January 2006 to RA Wind, JZ Hu, KR Minard, and DN Rommereim.

U.S. Patent 6,999,174 for "Photoacoustic Spectroscopy Sample Array Vessels and Photoacoustic Spectroscopy Methods for Using the Same" was issued in February 2006 to JE Amonette, ST Autrey, and NS Foster-Mills.

Outreach Activities

EMSL Hosts Recapitalization Workshop. On August 1 and 2, 2006, EMSL hosted 104 past and present users from 40 institutions at a recapitalization workshop that centered around EMSL's four science themes. The participants—hailing from academia, industry, and the national laboratory system—worked together in a collaborative mode to identify the technical and scientific challenges they expect to face, including:

Past and current EMSL users from 40 institutions gathered at a recapitalization workshop designed to investigate the future instrumentation needs of EMSL related to work in four science areas.

- Identifying the molecular-level mechanisms by which microbes sense changes in environmental conditions.
- Identifying the mechanisms of nucleation and growth of cloud droplets.
- Unraveling the genesis, properties, and effects of nanominerals and nanostructured materials in the environment.
- Understanding and controlling structure-function relationships of surfaces and interfaces, including those relevant to catalysis and energy production.

The participants, once they identified the key challenges, worked together to identify the instrumentation needed to address the challenges. The results are being rolled up into a facility refreshment plan that will bring state-of-the-art equipment into EMSL during the next five to seven years.

Radiological NMR Spectroscopy Meeting Held in May. On May 1-2, 2006, EMSL brought together 40 users from 11 institutions and 6 countries to discuss the future need for radiological NMR

EMSL hosted 40 users at a radiological NMR spectroscopy workshop in May 2006.

capabilities at EMSL. Many of the participants, representing the computational actinide chemistry community, identified the need to increase capabilities to calculate NMR spectra in agreement with experiment as well as capabilities to perform high-level relativistic calculations for heavy elements. Partially as a result of the workshop, EMSL is planning for construction of a 6700-square-foot annex to house radiological research work in the Fiscal Year 2009 or 2010 timeframe. The radiological annex will contain environmental and molecular sciences research equipment similar to that in the main EMSL facility, but will provide users with unique resources to study samples containing radiological materials.

EMSL Targets User Outreach at Two Large Professional Meetings. EMSL developed a booth presence and provided outreach to attendees at the American Association for the Advancement (AAAS) of Science meeting in St. Louis and the American Chemical Society (ACS) National Meeting in San Francisco in February 2006 and September 2006, respectively. At the AAAS meeting, EMSL led a symposium on its scientific grand challenge approach, and at both meetings booth staff made connections with participants who are potentially future users of EMSL. Investments in such events can help EMSL increase its pool of new users while also raising the visibility of EMSL as a national scientific user facility.

To connect with potential users, EMSL provided a booth presence at the AAAS and ACS meetings in 2006.

EMSL User Survey

The following are the responses to the EMSL April 2006 user survey submitted between April 8, 2006, and July 10, 2006.

- Survey Satisfaction: 92.1%
- Survey Responses: 231
- Surveys Sent: 461
- Survey Response Rate: 50.1%.

1. How satisfied were you with the availability of facilities and equipment?

- 132 Very Satisfied
- 83 Satisfied
- 9 Neither Satisfied nor Dissatisfied
- 3 Dissatisfied
- 3 Not Applicable.

2. How satisfied were you with performance of facilities and equipment (e.g., were they maintained to specifications for your intended use, ready when scheduled, etc.)?

- 130 Very Satisfied
- 85 Satisfied
- 7 Neither Satisfied nor Dissatisfied
- 3 Dissatisfied
- 1 Very Dissatisfied
- 5 Not Applicable.

3. List additional capabilities that you think EMSL should have.

User comments and EMSL responses to this question are grouped by facility and provided at http://www.emsl.pnl.gov/homes/survey.shtml.

4. With the new knowledge gained at EMSL, I expect to (check all that apply):

- 206 - Disseminate new knowledge via publication in peer-reviewed open literature.
- 172 - Disseminate new knowledge via presentations at professional society meetings.
- 16 - Acquire a patent.
- 94 - Further DOE's mission(s).
- 135 - Facilitate collaborative interactions (e.g., stimulated new ideas for future experiment; increased; work; etc.).
- 89 - Train students (undergraduate, graduate or postdoctoral associate).
- 129 - Use data for a future proposal.
- 83 - Establish or grow network and/or further collaboration.

5. How satisfied were you with the assistance provided by EMSL technical staff?

- 145 - Very Satisfied
- 68 - Satisfied
- 10 - Neither Satisfied nor Dissatisfied
- 2 - Dissatisfied
- 5 - Not Applicable.

6. How satisfied were you with the assistance provide by the EMSL administrative staff?

- 121 - Very Satisfied
- 75 - Satisfied
- 11 - Neither Satisfied nor Dissatisfied
- 1 - Very Dissatisfied
- 23 - Not Applicable

7. How appropriate and user friendly were the training and safety procedures?

- 76 - Very Satisfied
- 85 - Satisfied

- 21 - Neither Satisfied nor Dissatisfied
- 3 - Dissatisfied
- 42 - Not Applicable.

8. How satisfied were you with the proposal process (e.g. submission and review)?

- 61 - Very Satisfied
- 81 - Satisfied
- 20 - Neither Satisfied nor Dissatisfied
- 6 - Dissatisfied
- 1 - Very Dissatisfied
- 59 - Not Applicable.

9. How did you learn about the EMSL?

- 32 - Scientific meeting/conference
- 8 - Internet search
- 11 - Journal publication
- 58 - Previous EMSL use
- 82 - Colleague
- 106 - PNNL staff member
- 19 – Other.

10. Is there anything that would have improved your visit to EMSL, your experience using EMSL resources, or you interactions with EMSL Staff?

User comments included:

- I think the attitude in EMSL is one of commitment to improvement. There have been very positive improvements over the last few years and I expect they will keep moving in that direction.
- A great and very useful facility - nothing like it anywhere else.
- This is an easy to use and convenient facility.

- We are long-time collaborators on PNNL projects and we always appreciate the professional level of PNNL/EMSL staff.
- This is the best equipped lab I have ever worked in.
- I have always received EXCELLENT response from both scientific and EMSL staff.
- Staff are extremely knowledgeable and willing to assist in research endeavors.

User Administration

EMSL's User Administration group implements and manages policy and tools for various aspects of the user proposal and access process, as well as reporting statistics that support management and tracking of EMSL's impact. User Administration works with users and EMSL management to address users' issues and concerns in order increase user satisfaction. The group also leads outreach activities, working in conjunction with the EMSL Communications Manager (CM) and Scientific Facility Leads to promote public awareness and recognition of the research and unique integrated experimental and computational resources leading to advocacy for EMSL, as well as increased impact on the nation's largest challenges in the environmental sciences via such avenues as regional and national society meetings, visiting universities, workshops, and courses.

Since 2002, EMSL has developed electronic tools to automate management of user proposals [EMSL Usage System (EUS)], proposal review [EMSL Proposal Review System (EPRS)], and tracking use of EMSL resources [EMSL Resource System (ERS)].

EMSL Usage System

The 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. Highlights of some of the enhancements made to the EUS during Fiscal Year 2006 include:

- the ability to assign hazards to proposals
- revision of user survey logistics, questions, and emails
- electronic automation of the Appendix B of the Non-Proprietary Use Agreement
- installation of a new faster server, and relocation of the application and database.

EMSL Resource System

The ERS is a web-based tool that tracks the use of all significant resources in EMSL. EMSL's need to manage its assets and systematically track and report the use of EMSL resources resulted in development of the ERS to provide data needed to assure maximum efficiency, effectiveness, impact, and continued demand for installed resources. Highlights of improvements made to the ERS in Fiscal Year 2006 include:

- redesign of the system due to new user definition
- creation of a variety of reports for to incorporate strategic metrics
- archival of monthly data

- automatic import of MPP2 users (Gold data).

EMSL Proposal Review System

The EPRS was designed and implemented in Fiscal Year 2006 to automate, manage, and document the proposal review process throughout a proposal's life cycle, including calls for proposals, 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. This system allows:

- a mechanism for communications with reviewers
- a mechanism for external access by reviewers
- the ability for proposal attachments to be reordered and the order of attachments reflected in the peer-review package
- generation of a single PDF of all attachments and the proposal summary so that the reviewer only has to handle one file per proposal
- creation of two reviewer status reports
- creation of reviewer comment reports for proposal authors
- the ability for a reviewer to monitor scores and submit all reviews at once.

Outreach

In addition to the above system enhancements, a variety of management and outreach activities took place in Fiscal Year 2006, including:

- serving as staff liaison to the UAC, including participating in development of the call for nominations and the resulting election website
- serving as staff liaison to the SAC, including coordinating off-cycle visits
- developing the EMSL Outreach Plan
- coordinating the EMSL Science Theme call for proposals
- updating the EMSL external website with new policies
- coordinating EMSL information booths at major scientific society meetings, including the American Chemical Society National Meeting in San Francisco in September 2006 and the American Association for the Advancement of Science Meeting in St. Louis in February 2006

- serving as chair of EMSL's M.T. Thomas Outstanding Post-doctoral Award Committee
- overseeing more than 130 tours of EMSL encompassing nearly 700 people
- revising the user survey (shortening content, reorganizing and rewording to provide clarity and content, refocusing to users within previous six-month period, and adding a reminder email) to serve EMSL users more effectively.

Communications

The EMSL CM manages and directs the development and implementation of communications 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 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.

Future Directions

In Fiscal Year 2007, the EMSL User Administration Manager (UAM) 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

Deliverables of the EMSL UAM in Fiscal Year 2007 include:

- Serve as point of contact for EMSL systems (i.e., EUS, ERS, EMSL EPRS).
- Ensure a transparent proposal process, placing guidance and policy online.
- Enable and broadly distribute calls for proposals, and provide oversight of peer-review and approval processes.
- Increase EMSL name recognition and enhance reputation.
- Diversify portfolio of top universities and minority institutions.
- Increase presence at national professional society meetings.
- Attend/host workshops and symposia, and user meetings.
- Establish a relationship with other user facilities.
- Serve as EMSL's National User Facility Organization (NUFO) representative.
- Serve as liaison for EMSL's User and Science Advisory committees.
- As point of contact for EMSL's user survey, ensure responsiveness and satisfaction of users.
- Develop possible new user-friendly capabilities, such as a user portal, which will allow proposal participants to log in and view a list of their proposals and status, as well as allow them to submit summaries or publications; a staff portal, which will allow coordination among PNNL's electronic systems; and a centralized user administration office.
- Streamline training without affecting user safety.

EMSL Communications Manager

The following actions show the future direction that EMSL's CM support will take in Fiscal Year 2007 and beyond:

- Identify opportunities (press releases, articles) that will raise EMSL visibility nationally and internationally.

- Further develop targeted overview and facility-specific posters, brochures, and website highlights that market EMSL science, facilities, and capabilities.

- Coordinate activities that support EMSL's anniversary as a decade-old user facility.

- Begin a major effort to improve/revamp the EMSL external website, which will provide impactful, timely information to EMSL's client, users, and potential users.

- Work with PNNL's Science and Engineering External Recognition Awards Program and EMSL Scientific Facility Leads to identify staff who can be placed into PNNL awards development pipeline and targeted for external honors.

- Revive the EMSL News as a vehicle for informing past, current, and potential users of science and capabilities of EMSL.

- Provide updates to the EMSL internal website.

- Provide continued booth and symposium presence at major national meetings, and communications support to staff who attend such meetings.

- Provide further updates and improvements to relevant displays in the main EMSL hallway (e.g., posters, brochures) to support the high volume of tours hosted by EMSL. These tours range from high-level political visits to general staff tours. Potential specific posters include an EMSL timeline, overview, map, facility descriptions, mission statement, vision and value statements, supercomputer dynamic content displays, and EMSL Scientific Grand Challenges.

- Provide support as needed to various PNNL-level requests for EMSL information.

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