Overview

This 2004 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. EMSL is a multidisciplinary national scientific user facility operated by Pacific Northwest National Laboratory (PNNL) for the U.S. Department of Energy's (DOE) Office of Biological and Environmental Research. The resources and opportunities for fundamental research embodied in this facility are the products of DOE's commitment to understanding and resolving environmental and other critical scientific issues. Essential to the success of addressing these issues will be the implementation of the 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. During 2004, two EMSL Grand Challenge projects focused on specific scientific issues in the areas of biogeochemistry and membrane biology were initiated.

EMSL was the vision of Dr. William R. Wiley to establish an innovative multipurpose user facility that provides synergism among the chemical, physical, mathematical, and life sciences. Dr. Wiley, who was PNNL Director from 1984 to 1994, and others at PNNL and DOE believed that molecular-level research was essential for addressing challenges in environmental cleanup, energy efficiency, health, and other areas. From this belief grew the concept for a center for molecular science that would bring together theoreticians with expertise in computer modeling of molecular processes and experimentalists from the chemical, physical, and life sciences.

Construction of EMSL began in July 1994, and the facility was dedicated in Dr. Wiley's honor in October 1996, a few months after his passing. In fulfillment of his vision of a user facility focused on science at the molecular level, EMSL has more than 100 major instrument systems available to the scientific community, and the facility houses more than 300 staff and visiting researchers. The science performed within EMSL has helped establish PNNL as DOE's readily accessible center for research excellence in the chemical, biological, and environmental sciences.

Mission and Future Vision

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 EMSL users a highly efficient and focused resource that enhances their work.

A significant step forward in addressing critical research challenges with a more concerted approach and greater impact has been taken with implementation of the EMSL Grand Challenges. EMSL Grand Challenges differ from typical research projects in that they are multi-institutional (from universities, other laboratories, and industry), multigroup teams that

use numerous facilities within EMSL. Grand Challenges are particularly unique because they address research projects of a scope that cannot be addressed using resources from any single institution.

EMSL's theme of cross-collaboration and interdisciplinary science is reflected in its strategic signature characteristics: 1) integration of theory, modeling, and simulation with experimental approaches to research; 2) use of multidisciplinary teams and collaborative modes of operation to solve major scientific problems; and 3) deployment of teams of scientists and engineers to develop extraordinary tools and methodologies. These characteristics distinguish EMSL from academic research centers and other DOE user facilities, and are essential to the success of the EMSL Grand Challenges. EMSL programs in the areas of advanced computational methods, global proteomics, structural biology, subsurface fate and transport, chemical physics, atmospheric chemistry, nanoscience and nanotechnology, oxide chemistry, and biogeochemistry are all internationally recognized for their excellence. Cutting-edge resources available to EMSL users are grouped into 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, 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 Experimental Scientific Resources, an Associate Director for Scientific Computational and User Resources, and Technical Leads, who are the front-line group managers responsible for the capabilities, staff, and user program within their assigned groups. In addition to the EMSL line managers, 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.

The primary role of the Director is to provide scientific and business leadership for EMSL. The Director also oversees the activities of the Associate Directors and works with the EMSL management team and the external committees to conceive and implement the EMSL vision and mission, and to develop strategic plans for achieving the vision and mission while supporting the Grand Challenges. The EMSL Director also is ultimately responsible for all aspects of the environmental, safety, and health program within EMSL as well as stewardship of the user program.

As shown in Figure 1, EMSL resources are grouped into Scientific Experimental Resources and Scientific Computational and User Resources. In addition to the groups that provide staff and support to the six user facilities, EMSL has an Instrument Development Laboratory, a Computing and Networking Services group, and a User Services and Outreach group.

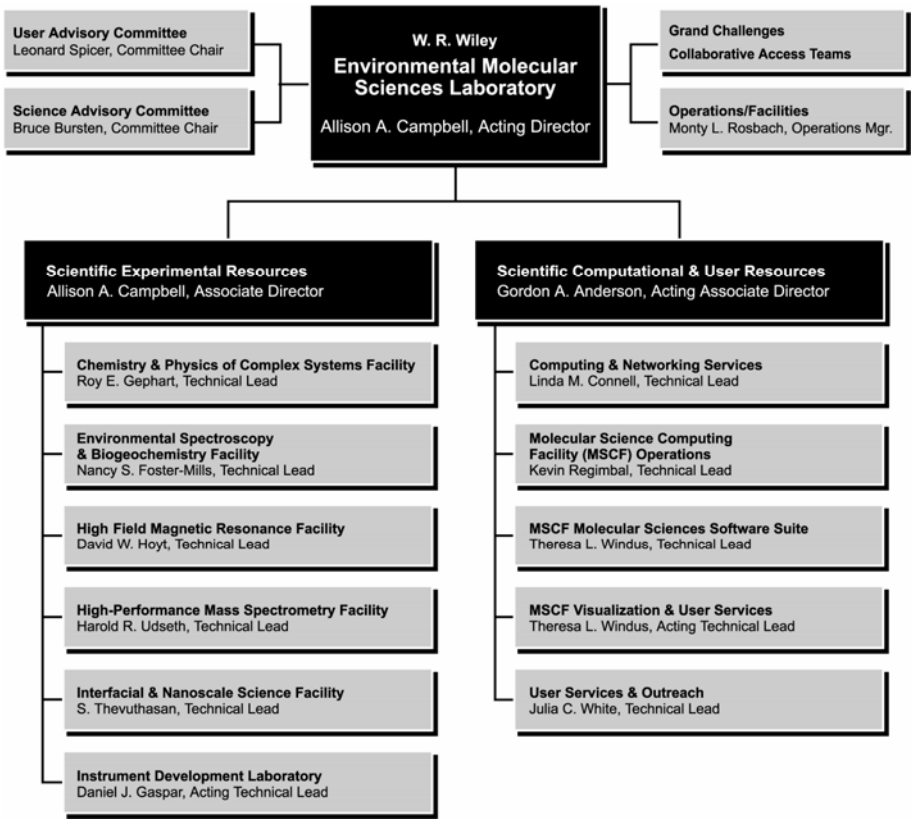

Figure 1. EMSL organization chart

User Advisory Committee

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

- Advise how to facilitate the effective use of EMSL. This responsibility includes advocating for 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.
- Advise on priorities and strategies to effectively address the multiple missions 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 achieving maximum scientific impact by EMSL users.

Currently, the UAC is 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 science 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 country, the committee is built around the major capability areas at EMSL. The current members of the SAC are:

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, New York, and member of the Basic Energy Sciences Advisory Committee (BESAC)

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

Scientific Approach

In 2004, EMSL launched two Grand Challenges and further established Collaborative Access Teams (CATs) in a continued paradigm shift in our approach to meet high-impact scientific challenges.

Grand Challenges

Grand Challenges investigate complex, large-scale scientific and engineering problems with broad scientific and environmental or economic impacts whose solutions can be advanced by applying advanced, high-performance scientific techniques and resources. EMSL Grand Challenge projects differ from typical projects in that they involve multi-institutional (from universities, other laboratories, and industry), multigroup teams that use multiple facilities within EMSL.

EMSL is *the* uniquely qualified scientific user facility that can serve as the resource and collaboration center to address scientific investigations of such a massive scope.

The scope of these Grand Challenges and future scientific challenges requires multidisciplinary teaming. The breadth of such undertakings will be of a magnitude that cannot be addressed at any other single, existing facility. These challenges will generally have a set of well-defined science or capability-development goals and a specified duration, and will require significant management and coordination to meet their aggressive goals. The Grand Challenges are expected to attract and involve users who are among the world's best scientists in the challenge area.

In 2004, EMSL launched two scientific Grand Challenges that bring together some of the world's best minds to study questions in the areas of biogeochemistry and membrane biology. The primary purpose of these Grand Challenges is to address important scientific questions through a focused collaborative approach that uses the capabilities of EMSL. This approach increases the scientific impact and robustness both of EMSL as a user facility and of the scientific programs at PNNL. These Grand Challenges are consistent with DOE mission areas, are focused on critical milestones in the advancement and use of science, are user-driven, and fully encompass the unique capabilities, resources, and technical expertise available in EMSL.

Collectively, these PNNL-supported Grand Challenges bring together scientists from more than 20 universities and research institutions worldwide. Results from these 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 enormous problems associated with environmental contamination across the complex, saving the DOE and the nation hundreds of millions of dollars and reducing risk to humans and the environment.

Biogeochemistry

PNNL scientists, Drs. John Zachara and Jim Fredrickson, are leading a Grand Challenge in biogeochemistry that is focused on how organisms exchange energy and electron flux with

mineral matter in soils, sediments, and subsurface materials. These exchanges occur across a mineral-microbe interface that is a minute, but chemically active, domain whose molecular workings have perplexed scientists for decades. The biogeochemistry Grand Challenge will use advanced instrumental capabilities and the high-performance computing capabilities of EMSL to understand the biologic and physical architecture of this remarkably complex domain and the microbe-mediated chemical reactions that occur within it. The research will enable 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.

Membrane Biology

Dr. Himadri Pakrasi from Washington University in St. Louis, Missouri, is leading a Grand Challenge in membrane biology that will use a systems approach to understand the network of genes and proteins that govern the structure and function of membranes and the components of membranes 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 Grand Challenge will provide the first comprehensive systems-level understanding of how environmental conditions influence key carbon fixation processes at the gene-protein-organism level. This focus was selected because it addresses critical DOE science needs, provides model microorganisms to apply high-throughput biology and computational modeling, and takes advantage of EMSL's experimental and computational capabilities.

Collaborative Access Teams

CATs enable and conduct high-impact science that use 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, can contribute significantly to the scientific goals of the CAT. Currently, four CATs exist in the areas of structural genomics, catalysis, atmospheric chemistry, and analytical mass spectrometry.

Structural Genomics. The Structural Genomics CAT, composed of more than 35 scientists from 16 different institutions, performs research focused in structural genomics and related research areas with a primary goal of increasing throughput, maximizing efficiency of existing resources, and developing technology to increase throughput and efficiency.

Catalysis. The Catalysis CAT brings an integrated experimental and theoretical approach to a molecular-level understanding of oxide-catalyzed chemical transformations. Investigators on this team will take advantage of the unique experimental and computational resources at EMSL to conduct basic and applied research in the area of heterogeneous catalysis.

Atmospheric Chemistry. The Atmospheric Chemistry CAT was established to lead the EMSL research thrust that is addressing "atmospheric chemistry for the future." This CAT seeks to articulate a strong vision of challenges in the atmospheric chemistry field, define major collaborative projects in that field to address the scientific challenges, and develop and deploy measurement equipment.

Analytical Mass Spectrometry. The Analytical Mass Spectrometry CAT will continue the DOE's distinguished reputation for developing novel mass spectrometry instrumentation and deploying the technology to determine key thermodynamic and kinetic parameters for complex ions. The general objective of this CAT is to achieve a fundamental understanding of the reaction kinetics and dynamics of activating and dissociating complex molecular ions.

Highlights

As we look forward, we are committed to increasing the impact of our user program by performing compelling Grand Challenge science in pursuit of DOE missions using extraordinary facilities, scientific tools, and technical expertise. In 2004, EMSL staff saw continued recognition for progress in development of state-of-the-art capabilities and expertise, and for their professional contributions.

J.W. (Bill) Rogers Jr., elected as a **Fellow of the American Association for the Advancement of Science** (AAAS). Former EMSL Director Bill Rogers (Figure 2) was recognized for "distinguished contributions to the field of surface science and its application to the characterization of energetic materials, biomaterials, and technologically important thin films." Election as an AAAS Fellow is determined by peer reviewers, and Fellows are honored for meritorious efforts to advance science or its applications. AAAS began honoring its distinguished members with the title of Fellow in 1874.

Figure 2. Bill Rogers, Director of EMSL from 2002 to 2004, was elected as a Fellow of AAAS in 2004.

In August, Chemistry and Physics of Complex Systems Facility user **Xin Yang** received the **2003 EMSL M.T. Thomas Award** for Outstanding Postdoctoral Achievement (Figure 3). He was selected for his contributions to the development of electrospray-photoelectron spectroscopy techniques and for leading its use in new research directions, including the investigation of complex anion solvations in the gas phase and the electronic structure of the active site of iron-sulfur proteins. His innovative studies on environmentally related solvated anions such as sulfate and nitrate and dicarboxylate dianions, which serve as models for peptide chains, have been published in *Science*, the *Journal of the American Chemical Society*, and the *Journal of Physical Chemistry*. His research has also included the discovery of Coulomb-induced and antiferromagnetic-induced fission in doubly charged cube-like [4Fe-4S] clusters. Such a process has never been observed before and may have important implications in understanding the functionality and transformations of iron-sulfur clusters in biological molecules such as proteins.

Figure 3. (Left to right) Allison Campbell, Director of EMSL, Xin Yang, Lai-Sheng Wang, and MT Thomas.

Harold Udseth, Technical Lead for the High-Performance Mass Spectrometry Facility, was among the recipients of a **2004 Federal Laboratory Consortium (FLC) Award of Excellence in Technology Transfer** for the use of the electrodynamic ion funnel with mass spectrometry (Figure 4). The electrodynamic ion funnel provides a huge gain in sensitivity for many forms of mass spectrometry. The funnel's

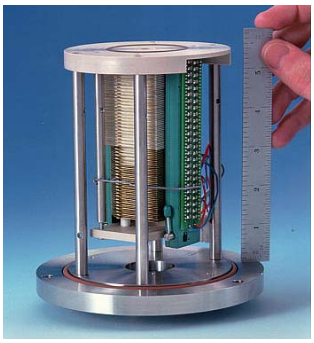

Figure 4. Electrodynamic Ion Funnel.

capability for focusing significantly more ions into the mass spectrometer for analysis will result in lower detection limits, improved data collection, new applications, and greater understanding of the substances analyzed. Realization of the potential of the ion funnel will benefit a host of important commercial activities, including drug discovery and biotechnology development, where sensitivity plays a key role. Each year, the FLC presents no more than 30 Awards for Excellence in Technology Transfer to federal laboratory employees who have done outstanding work in transferring U.S. government-sponsored technologies to the public and private sectors.

David Hoyt, Technical Lead for the High Field Magnetic Resonance Facility, was invited to participate in proposal reviews for the Chemistry Research Instrumentation and Facility Program of the **National Science Foundation** in Arlington, Virginia.

EMSL User Highlights

As a scientific user facility, it is gratifying for EMSL to hear news of outstanding recognition of its users when EMSL resources have contributed to their success. Events and awards of this nature speak to the quality of the science conducted using EMSL resources and reflect the caliber of the scientists who come to EMSL as users and collaborators.

EMSL users **Robert Wind** and **Bruce Garrett** were elected as **Fellows of AAAS**. Wind was recognized for "contributions to the field of multinuclear magnetic resonance spectroscopy and imaging and its applications to solid-state and biomedical research." Garrett was recognized for "distinguished contributions to the development of rate theories for polyatomic reactions in the gas-phase and to the study of the kinetics of important environmental processes."

Environmental Spectroscopy and Biogeochemistry Facility user and scientific consultant **Kevin Rosso** (PNNL) was the 2004 winner of **The Mineralogical Society of America Award** (Figure 5). This award is one of the most prestigious awards in the entire field of geosciences and recognizes outstanding published contributions to the science of mineralogy by individuals early in their professional careers. This award results from Rosso's contributions to the development of a fundamental understanding of the reactivity of mineral surfaces. Rosso's work has introduced a new theoretical model for calculating the kinetics of electron transfer reactions involving metal ions in aqueous solution, and his contributions have led to the definition of the proximity effect on semiconducting mineral surfaces.

Figure 5. Len Peters (left), Laboratory Director for PNNL, congratulates Kevin Rosso (right) for his Mineralogical Society of America Award.

Scott Chambers was the 2004 recipient of the **E.W. Mueller Award** for outstanding research in surface science. He was recognized for advancing the science of molecular beam epitaxy and applying it to fundamental investigations of the structural, electronic, and magnetic properties of metal oxide films, surfaces, and interfaces. A user of the Interfacial

and Nanoscale Science Facility, he has been associated with EMSL from the facility's inception, and he developed the state-of-the-art oxide molecular beam epitaxy facility at EMSL.

Interfacial and Nanoscale Science Facility user, **Zsuzsanna Balogh**, was named **Outstanding Graduate Student in the Department of Geology at Washington State University**. She used the electron microscopy suite for her research in the effects of rooted plants on chemical weathering of minerals.

Lai-Sheng Wang, Washington State University, Richland, Washington, was featured in the May 28 special, edition of *Science*, "Many Origins, One Destination." The feature edition highlighted six foreign-born scientists' interest in studying and working in the United States and their impact on U.S. academic science. Wang performs his research using the Chemistry and Physics of Complex Systems Facility.

Tiffany Kaspar, a graduate student from the University of Washington, won the **Leo M. Falicov Student Award** for her work enabled by the Interfacial and Nanoscale Science Facility. In collaboration with Scott Chambers at the EMSL oxide molecular beam epitaxial laboratory, she developed new dilute magnetic semiconductor materials. The award, which was established by the American Vacuum Society, recognizes outstanding research performed by a graduate student in areas of interest to Magnetic Interfaces and Nanostructures Division.

Publications

In calendar year 2004, 322 publications – 266 EMSL collaborative publications and 56 user-only publications – describing research performed using EMSL capabilities appeared in the literature. Research by EMSL users was featured both on the covers of several scientific journals and in published articles.

Patents

U.S. Patent No. 6,680,477 B2, "High-Spacial Resolution Matrix-Assisted Laser Desorption/Ionization (MALDI)," was issued on January 20, 2004 to K Beck and D Wunschel.

U.S. Patent No. 6,765,476, "Multi-Level RF Identification System," was issued on July 20, 2004 to KD Steele, GA Anderson, and RW Gilbert.

U.S. Patent No. 6,787,760, "Method for Increasing the Dynamic Range of Mass Spectrometers," was issued on September 7, 2004 to M Belov, RD Smith, and HR Udseth.

U.S. Patent No. 6,803,565, "Ionization Source Utilizing a Multi-Capillary Inlet and Method of Operation," was issued on October 12, 2004 to RD Smith, T Kim, and HR Udseth.

Capability Developments

12-Tesla Mass Spectrometer Installation. EMSL installed a powerful new magnet that enables an unprecedented "top-down" capability for the study of proteomics. Manufactured by Magnex Scientific Ltd. for Bruker Daltonics, the 12-tesla superconducting magnet (Figure 7) was installed in EMSL's High-Performance Mass Spectrometry Facility. EMSL and the Mayo Clinic are two of a scant number of entities to possess a mass spectrometer of this strength. Proteomics research has historically focused on "bottom-up" proteomics, which uses mass spectrometry to detect peptides, leading to positive identification of the presence of particular proteins in a cell. While this technique works well for identifying a protein's presence, it cannot detect the actual form of the protein in more complex organisms. The new 12-tesla magnet introduces "top-down" analysis, which helps researchers understand the role, function, structure, and changing nature of complex cellular proteins. The magnet provides a unique mass spectrometry tool that complements the repetitive "bottom-up" method to result in a scientific understanding of proteins as well as potential applications.

Figure 7. Harold Udseth and the new 12-tesla magnet equipped on a Fourier-transform ion cyclotron resonance mass spectrometer.

Subsurface Flow and Transport Experimental Laboratory. The Subsurface Flow and Transport Experimental Laboratory (Figure 8) became operational in 2004 and hosted its first three external users. The laboratory offers several meter-scale flow cells and columns for research in saturated and unsaturated porous media, as well as single and multifluid systems. Some of the flow cells and columns can be used in conjunction with a dual-energy gamma radiation system. These unique experimental systems enable testing of basic theories of flow and transport; studies of coupled processes involved with microbial, reactive chemical, or colloid transport; and experimental simulation of subsurface remediation scenarios. The laboratory also offers a fully automated saturation-pressure apparatus and provides users with full analytical and computational support. Staff, software, and computational facilities are available to design experiments and compare experimental results with numerical predictions.

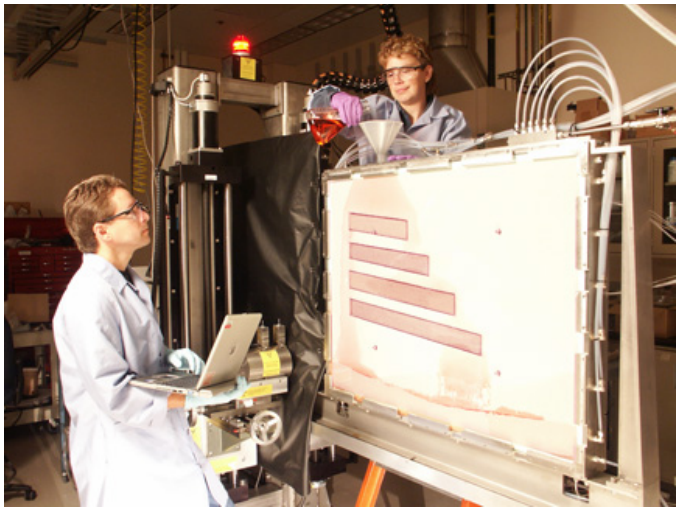

Figure 8. Subsurface Flow and Transport Experimental Laboratory.

Proton transfer and accelerator mass spectrometers. The proton transfer mass spectrometer and the accelerator mass spectrometer developed at EMSL were displayed in the DOE G1 aircraft during the summer 2004 Northeast Aerosol Experiment, a component of the International Consortium for Atmospheric Research on Transport and Transformation. The scientific focus of the G-1 flights included characterizing the contribution of Midwestern sources of aerosols to the aerosol burden in the Western North Atlantic region.

Outreach Activities

EMSL2004 – Bridging Technologies in Structural Biology

The High Field Magnetic Resonance Facility (HFMRF) hosted the EMSL2004 technical meeting, "Bridging Technologies in Structural Biology," June 14 to 16, 2004. Over 60 participants attended the meeting. The first day focused on how a wide variety of techniques, including x-ray crystallography, cryo-electron microscopy, small angle neutron scattering, and electron paramagnetic spectroscopy along with NMR, would be needed to tackle Grand Challenges in biology and structural genomics in the future. The meeting also featured users of the EMSL High-Field Magnetic Resonance Facility presenting their research findings.

External invited speakers included:

- Michael Chapman, Florida State University
  Holistic Macromolecular Models–When One Technique is Not Enough
- Thomas Szyperski, State University of New York, Buffalo
  NMR Methods Enabling Rapid Data Collection
- Jinkui Zhao, Oak Ridge National Laboratory
  Small-Angle Neutron Scattering in Structural Biology
- Stanley Opella, University of California, San Diego
  NMR Structure Determination of Mercury Transport Membrane Proteins
- James Penner-Hahn, University of Michigan
  Characterization of "Spectroscopically Challenged" Metals: Zinc in Biological Systems – X-Ray Spectroscopy
- Rachel Klevit, University of Washington
  Assembly of Multicomponent Protein Complexes: NMR Studies of a BRCA1-BARD1 Ubiquitin Ligase Complex
- Huilin Li, Brookhaven National Laboratory
  The Expanding Role of Cryo-Electron Microscopy in Structural and Cell Biology
- Colin Fyfe, University of British Columbia
  High-Field Solid-State NMR Studies of Inorganic Materials at the Pacific Northwest National Laboratory
- Thomas DiChristina, Georgia Institute of Technology
  New Insights into the Molecular Mechanism of Microbial Metal Respiration

Supercomputing "Greenbook" Workshop

EMSL held a workshop on Scientific Computing on December 10 and 11, 2004. The "Greenbook" workshop was initiated as an opportunity to engage computational science leaders from around the country in a focused dialogue to identify the role that the next-generation Molecular Science Computing Facility will have in meeting the needs of the broader scientific community in chemistry, biology, subsurface transport, and regional hydrological climate models. The 50 participants held in-depth conversations on future needs and are using the technical workshop results and previously solicited whitepapers to develop a visionary document that describes the science drivers and the associated

requirements for enhanced high-performance computing resources at EMSL in support of the DOE Office of Biological and Environmental Research.

Surface Analysis '04

EMSL hosted Surface Analysis '04, a joint symposium for the 26th Annual Symposium on Applied Surface Analysis and the 15th Annual Symposium of the American Vacuum Society Pacific Northwest Chapter (PNWAVS), from June 15 to 18, 2004. About 150 registrants attended this topical conference, an annual interdisciplinary meeting held to discuss advances in and applications of surface analysis. The scientific program of the latest meeting covered a wide range of topics: biomaterials and interfaces, nanoscience, catalysis and reactions, advanced methods, oxide thin films, and oxide thin films growth. Some of the leading scientists in these fields presented their recent work at the symposium in a technical program that consisted of 12 invited talks, 36 contributed oral presentations, and 56 poster presentations. A selection of papers from the meeting will be published in a special issue of *Surface and Interface Analysis*. Participants came from the world over, including the United States (135), Canada (4), Republic of Korea (2), Australia (3), France (1), Israel (1), Denmark (1), Great Britan (1), Japan (1), and Puerto Rico (1).

Clay Minerals Society Meeting

EMSL staff member Paul Gassman co-chaired the 2004 Clay Minerals Society 41st Annual Meeting (CMS2004), June 19 to 24, 2004, in Richland Washington, with Jim Amonette of PNNL. CMS2004 was a great success with a total of 185 attendees, 74 of whom registered for the workshop in the EMSL auditorium, and 51 of whom participated in EMSL laboratory tours. A total of 113 papers were presented (86 orally) covering a wide range of fundamental science, practical topics, and the latest advancements in the uses of clay minerals.

American Chemical Society Environmental Spectroscopy Symposium

Nancy Foster-Mills, Technical Lead of the Environmental Spectroscopy and Biogeochemistry Facility, organized a symposium on Environmental Spectroscopy with presentations focused on the application of various optical spectroscopies in environmental research at the Joint Regional Meeting of the Northwest and Rocky Mountain Sections of the American Chemical Society. The meeting was held June 6 to 9, 2004, at Utah State University in Logan, Utah.

Washington State University Outreach

Instrument Development Laboratory (IDL) staff members Tom Seim and Eric Choi attended the two-day Washington State University (WSU) Electrical Engineering and Computer Science (EECS) Open House and Advisory Council Meeting. They provided advice for future improvements to and development of the WSU's EECS curriculum, and observed a Programming Language Design class, student teamwork-oriented projects, and a Sumo Robot competition.

In another endeavor, IDL staff members and representatives of the Institute of Electrical and Electronics Engineers (IEEE) student chapter at WSU are teaming with eastern Washington high schools and state of Washington's Mathematics Engineering Science Achievement program to promote science and engineering education through robotics. This outreach effort has not only resulted in successful educational promotion but has also strengthened university, laboratory, and public school communications.

Molecular Science Computing Facility Tutorial

The Molecular Science Computing Facility's Visualization and User Services group held a tutorial entitled "MSCF for Dummies 2004" on March 24. Use of the facility's MPP2 supercomputer was the focus of the tutorial, which was offered in separate sessions for novice and advanced users. The tutorial was streamed live onto the World Wide Web, enabling 75 offsite EMSL users to participate in addition to the 10 onsite participants.

Synthesis and Characterization of Nanomaterials

EMSL's Interfacial and Nanoscale Science Facility hosted a three-week intensive course on the Synthesis and Characterization of Nanomaterials in EMSL from January 5 to 23, 2004. Developed through a National Science Foundation grant, the course is designed to speed undergraduate and graduate students' entry into the field and provide them with direct interaction with laboratory researchers. The course involved lectures and laboratory projects involving synthesis and characterization.

Molecular Modeling Workshop

Environmental Spectroscopy and Bio-geochemistry Facility user and scientific consultant, Kevin Rosso, helped design and instruct a workshop entitled "Molecular Modeling Applied to Environmental Geochemistry" that was held August 15 to 20, 2004. The workshop was sponsored by the American Chemical Society Petroleum Research Fund. Topics included an overview of modeling techniques, molecular dynamics simulation, Monte Carlo simulation, *ab initio* molecular orbital theory, and a variety of calculations. Several new EMSL collaborations and EMSL user proposals have been planned as a direct result.

Summer Educational Outreach

More than 40 students were mentored by EMSL staff during the summer of 2004 through various educational programs, including the DOE Science Undergraduate Laboratory Internship Program, the 2004 Summer Research Institute in Interfacial and Condensed Phase Chemical Physics, the Office of Fellowship Programs, the Young Women in Science Program, the Student Research Apprentice Program, and the Community College Institute of Science and Technology Program.

Student research, presented at summer-end poster session (Figure 8), included ion-beam synthesis of gold nanostructures in oxides, nanofilms and doped ceria electrolytes for solid oxide fuel cell applications, characterization of atmospheric aerosol particles, and purification and characterization of *Shewanella oneidensis* c-cytochromes and proteins. Two local high school students received by outstanding contribution awards by the Pacific Northwest Chapter of the American Vacuum Society.

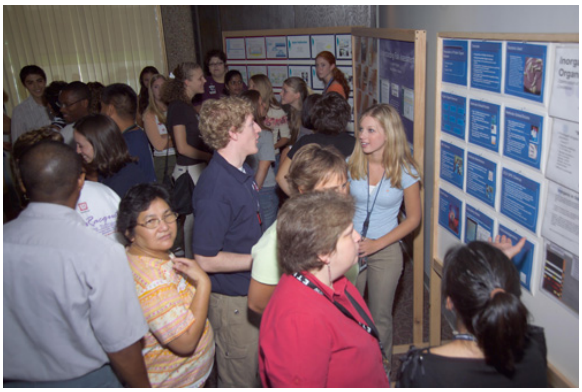

Figure 8. 2004 Summer Fellows Poster Session in August.

EMSL User Survey

Each year in February and August, EMSL solicits user feedback via an online survey. In 2004, 142 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 2004 survey are summarized below.

Nature of EMSL Use (onsite and remote)

Of the respondents, 74% visited EMSL as part of their proposed research, while 26% indicated that their use of the facility did not require an onsite visit: 99% of the respondents were from U.S. institutions and the remaining 1% were from non-U.S. institutions. Following is a breakdown of users by the institutional categories surveyed.

- U.S. academia – 71%
- PNNL staff member – 23%
- Other – 2%
- DOE laboratories other than PNNL – 2%
- Private industry – 1%
- U.S. government agencies – 2%
- Foreign national laboratories – 1%.

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

- Collaborative interaction with EMSL staff – 54%
- Technical assistance from EMSL staff – 46%
- Short-term use of equipment not otherwise available to them – 32%
- Part of team using an EMSL capability – 35%
- Month or longer use of state-of-the-art capabilities not otherwise available to them – 35%
- Month or longer use of unique capabilities – 27%
- Use of a single capability – 8%

- Individual researcher using an EMSL capability – 20%
- Use of unique materials provided by EMSL – 3%.

Manner in which EMSL Environment Facilitated Scientific Accomplishments

In rating the manner in which the EMSL environment facilitated scientific accomplishment, 93% 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 93% satisfied or very satisfied with the availability of existing EMSL facilities and equipment, noting easy accessibility, flexibility in scheduling, variety of instrumentation, and excellent staff assistance. Some users noted downtime of the supercomputer.

General EMSL Performance Satisfaction

When asked how satisfied users were with EMSL performance (e.g., were facilities and equipment maintained close to specifications?), 92% of the respondents replied that they were satisfied or very satisfied. Some respondents commented on difficulties accessing equipment because of high security measures or downtimes, but overall, users indicated that the instruments were expertly maintained and operated.

Satisfaction with Support Provided by EMSL Staff

Of the respondents, 95% 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, 20% suggested possible additional capabilities, such as:

- a triple-resonance, cross-polarization magic angle spinning (MAS), NMR probe for the WB 500-MHz, 5-mm rotors, that spins with stability and can maintain low temperature for durations of days
- 2H static NMR probe for high field work
- 24-hour maintenance and support of the supercomputer
- Accessible user facilities for obtaining Brunauer, Emmett, Teller (BET) surface areas
- Atomic force microscope/scanning tunneling microscope for users
- A high-resolution parallel electron energy loss spectrometer upgrade of the electron microscope facilities
- Capillary eletrophoresis
- Dynamic secondary ion mass spectrometer
- Focused ion beam transmission electron microscope (TEM)
- Field-emission TEM for higher energy resolution spectroscopy

- Web links and suggested literature about the strengths and weakness of mass spectroscopic-based research
- High-speed (i.e., >30 KHz) MAS solids probe for 750- or 800- and 900-MHz NMR spectrometers
- A wet lab in the 331 Building for packing samples to be analyzed in EMSL
- Catalyst chemisorption characterization system for increased availability
- Electron paramagnetic resonance spectrometer linked to an ultrahigh vacuum system
- Liquid helium-cooled manipulator in accelerator laboratory and capability for *in situ* reflectance optical characterization (Raman, Fourier transform infrared resonance, etc.) of samples mounted on manipulator
- Elastic recoil detector
- More compute cycles
- Improvements in NWChem
- Easier installation of Ecce
- More equipment for specialized sample preparation
- More instrumentation and data analysis infrastructure to reduce the sample queue delay
- Walk-on small-molecule mass spectrometer
- Capability to pre-treat samples (e.g., H_2 reduction, or H_2S/H_2 sulfidation) prior to x-ray photoelectron spectroscopy and transmission electron microscopy measurements
- The Bruker IFS 125 HR; the next generation of Bruker instruments for investigation of larger molecules.

Appropriateness of Safety and Training Procedures

When users were asked if they found the training and safety procedures to be easy, quick, and appropriate, 95% responded positively – an increase from 85% in 2003. A few users found the process to be cumbersome and slow.

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 – 67%
- Disseminated new knowledge via publication in peer-reviewed open literature – 59%
- Disseminated new knowledge via presentations at professional society meetings – 47%
- Trained students – 42%
- Facilitated collaborative interactions – 48%
- Dissemination of new knowledge via other presentations/media – 20%
- Discovered other new knowledge such as applied research – 27%
- Established a new network of collaboration – 30%
- Furthered DOE missions – 22%
- Obtained new research funding – 13%
- Developed a new or improved product, process, or technology – 18%
- Acquired a patent – 1%.

Suggestions for Better Meeting the Needs of Users

When asked how EMSL could better meet their needs, users requested more from the EMSL staff for collaboration and support, information on other EMSL users for potential collaboration, more workshops and conferences at the site, and more working time on the supercomputer. Users also suggested that the process for gaining access to the facility and high-security laboratory areas should be streamlined and accelerated.

Ease of Use of the EMSL Proposal System

Finally, 98% of respondents found the EMSL User Proposal System easy to use, a significant increase from 81% in 2003.

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