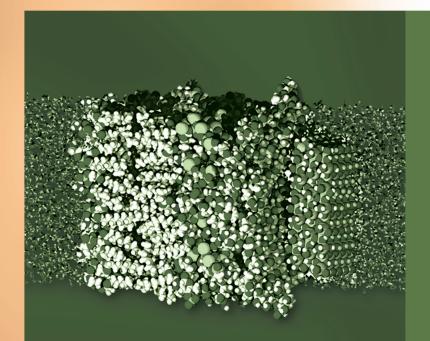


EMSL Strategic Plan 2006



Science and Marquee Capabilities

Management and Operations

User Outreach and Services

Implementing Our Vision



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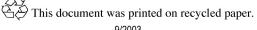
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Front cover, bottom: Electrostatic potential isocontours of the rough LPS membrane of pseudomonas aeruginosa. The interaction of organics, metals, minerals, and microbes form a complex web that must be understood in order to design DOE environmental management strategies. This research fills a huge gap in our knowledge of the interaction of microbes with the subsurface.



PNNL-15578

EMSL Strategic Plan 2006

Dr. Allison A. Campbell EMSL Director December 2005

Prepared for the U.S. Department of Energy under Contract DE-AC06-76RL01830

Pacific Northwest National Laboratory Richland, Washington 99352

EMSL Director Dr. Allison A. Campbell

EMSL Director's Message

Since opening our doors in 1997, the William R. Wiley Environmental Molecular Sciences Laboratory (EMSL)—located on the campus of the Pacific Northwest National Laboratory in Richland, Washington—has made extraordinary progress toward our vision to be the sought-after national scientific user facility for molecular science-based research. Our scientific staff and users are recognized nationally and internationally for their significant contributions to challenging scientific problems. We have explored new scientific frontiers by organizing a vibrant and diverse user community in support of our mission as a national scientific user facility that 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. Users from around the world—from academia to industry and national laboratories to international research organizations—use the resources of EMSL because of the quality of science that EMSL enables.

Our strategy builds upon our proven ability to engage the intellectual, experimental, and computational capabilities across EMSL. We will continue to attract world-class scientists from across the scientific community, becoming the focal point for environmental molecular sciences. We will focus on the nation's most important and challenging scientific problems through a set of scientific themes that optimize the impact of EMSL assets. We will push EMSL's cutting-edge capabilities to new frontiers and create a transparent and supportive user environment to meet the challenges of multidisciplinary research. Our strength in integrating the chemical, physical, and biological sciences will provide a new generation of scientists with the methods, tools, and experience to respond to tremendous opportunities in the environmental molecular sciences.

We will emphasize our management philosophy of simultaneous excellence the delivery of high-impact science and marquee capabilities, enabled by improvements in management and operations, and accompanied by a strong outreach and partnership with our user community. We have developed a strong culture of continuous improvement and self-assessment with a renewed emphasis on making our research more productive and impactful.

The ultimate proof of our value lies in the tangible results we deliver. We have worked very hard to establish a national scientific user facility that provides a collection of minds, methods, and capabilities to the scientific community, and we invite our staff and users to become part of the next wave of scientific discovery taking place in EMSL.

Allison A. Campbell

Director

W.R. Wiley Environmental Molecular Sciences Laboratory Pacific Northwest National Laboratory

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Appendix A - EMSL Science Themes



Acronyms

BER	Office of Biological and Environmental Research (DOE)
DOE	U.S. Department of Energy
EMSL	William R. Wiley Environmental Molecular Sciences Laboratory
EPRS	EMSL Proposal Review System
ERS	EMSL Resource System
IPAMS	Integrated Planning and Assessment Management System
PNNL	Pacific Northwest National Laboratory
PNSO	Pacific Northwest Site Office (DOE)
SAC	Science Advisory Committee
SBMS	Standards-Based Management System
SFL	Scientific Facility Leads
UAC	User Advisory Committee

1.0 PURPOSE AND FRAMEWORK

This strategic plan documents the 5-year strategy for meeting the U.S. Department of Energy (DOE) Office of Biological and Environmental Research's (BER's) goals for the William R. Wiley Environmental Molecular Sciences Laboratory (EMSL) as a premier national scientific user facility.

1.1 The Value of the Strategic Plan

This strategic plan describes the elements of EMSL's 5-year strategy to provide outstanding value to our user community and to meet evolving BER goals. While this is a 5-year plan, it reflects our understanding of the long-term stewardship we must work toward to meet the needs of DOE and the nation for the next several decades. This is a particularly exciting time for science because the scientific challenges of the 21st century require an integrated approach and problem-solving environment for scientific discovery—a challenge to which EMSL is extraordinarily well suited. We are determined to seize this opportunity, and through this strategic plan we have built the framework to successfully meet these challenges.

1.2 Strategic Planning: Integral to Effective Laboratory Management

At EMSL, we continually evaluate the changing needs and opportunities posed by our stakeholders (i.e., DOE, users, advisory committees), work closely

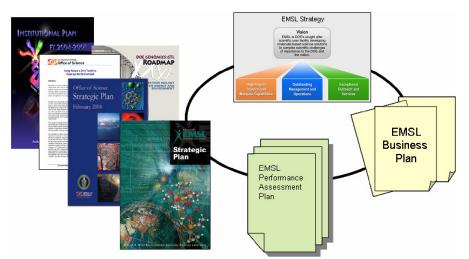


Figure 1-1. Strategic planning and validation process.

with them to understand and respond to those changes, and align our strategy in response to those needs and opportunities (Figure 1-1). The DOE Office of Science's Strategic Plan and mission strategies give us the context for our highest-level goals and scientific objectives. Through our strategic planning process, we solidify the objectives, measures, and targets that will guide our work during the next several years. Our strategic plan provides the context and our business plan provides the internal business plans and allocation of resources.

2.0 STRATEGIC PLAN

2.1 EMSL's Mission, Vision, and Strategy

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 our mission and implement our strategy.

The central focus of EMSL's strategy is delivery on the mission of the scientific user facility. EMSL's vision and strategy, respectively, show where we intend to be in the next 10 years and what progress we will make during the next 5 years.

2.1.1 Mission

The management of EMSL together with DOE, the Pacific Northwest Site Office (PNSO), and Pacific Northwest National Laboratory (PNNL) management, have developed a shared mission statement for EMSL.

EMSL, a national scientific user facility at Pacific Northwest National Laboratory, provides integrated experimental and computational resources for discovery and technological innovation in the environmental molecular sciences to support the needs of DOE and the nation.

EMSL is a national scientific user facility available to researchers worldwide from academia, industry, and the national laboratory system. Users of EMSL pursue the understanding of molecular systems essential to scientific breakthrough and discovery for a broad set of DOE missions in energy, environment, climate, and national security. We develop and maintain significant research and development capabilities to generate new scientific knowledge. We deliver substantial value to our users by fully understanding their needs, creating responsive new ideas and capabilities, and delivering exceptional results—all achieved through our expert staff, demonstrated excellence in management and laboratory operations, and high-value partnerships with our users. The operating budget for EMSL is provided by DOE BER, while the research conducted within the facility benefits 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.

2.1.2 Vision

EMSL is the sought-after scientific user facility developing molecular science-based solutions to complex scientific challenges of importance to the DOE and the nation. We will deliver accelerated, leadership-class scientific accomplishments through stateof-the-art signature capabilities; expert scientists and staff; and multidisciplinary collaborations with an engaged, proactive user community.

Our vision is to advance the reputation of EMSL to the extent that the most prestigious scientists from around the world seek to be our users. We will measure our progress through increased high-impact publications, distinguished scientists as users, and recognition by the scientific community. We will continue to refine and strengthen our expertise in integrating science across disciplines and capabilities. Our success in this area will be measured by the quality, relevance, and impact of our science and increased roles in supporting our users.

2.1.3 EMSL Strategy

This strategic plan is designed to build on EMSL's strength as a problem-solving environment and preserve and foster our mission and vision. In addition, this plan is a crucial element of the overall PNNL Strategic Plan. Achieving EMSL's vision requires us to deliver to our users high-quality scientific solutions that significantly and positively impact DOE's and the nation's most critical challenges. We value effective and efficient management and operations that support our mission and help ensure the protection of our staff, users, and the environment. By realizing EMSL's vision in a safe and efficient manner, we ensure long-term viability.

We will deliver on EMSL's strategy using Battelle's operating principle of simultaneous excellence in all facets of management. We are committed to making sure that our management attention and discretionary resources are properly balanced across delivering scientific capabilities, conducting work operations with excellence, and addressing the needs of our users.

Our strategy is founded on three fundamental tenets (Figure 2-1) that reflect the value we provide to DOE and provide the basis for our strategic goals.

• **High-impact science and marquee capabilities**. As a national scientific user facility, we focus on enabling scientific discoveries, we develop and

maintain state-of-the art facilities, and our program leadership and scientific accomplishments are widely recognized.

- Outstanding management and operations. EMSL management and operations capabilities are the most effective and efficient in the DOE system at delivering outstanding research and maintaining excellent operational practices.
- Exceptional user outreach and services. EMSL's outreach program attracts users who are proactive and engaged, and our work environment enables our staff and users to work with high efficiency and productivity.

This strategic plan is organized into sections that align with our three primary tenets and is structured according to the following hierarchy: tenets provide the basis for strategic goals; strategic goals are supported by objectives to enable our strategy.

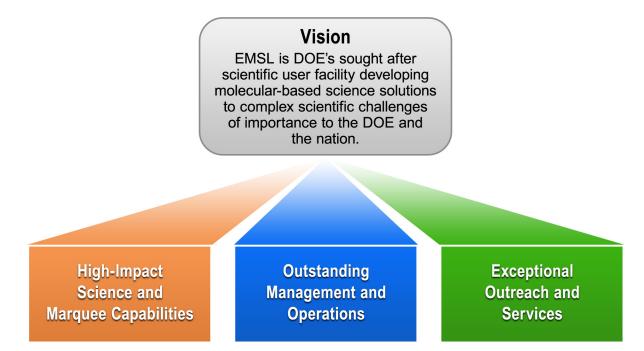


Figure 2-1. Tenets of EMSL's vision.

2.2 High-Impact Science and Marquee Capabilities

EMSL provides our users with new tools and state-of-the-art capabilities that will strengthen the nation's scientific infrastructure, increase the fundamental understanding in the environmental molecular sciences, and produce discoveries that provide the basis for new, mission-relevant applications.

High-impact science is at the core of the EMSL mission and vision. It is essential that scientific leadership at EMSL enables truly high-impact scientific research. Below are the strategic goals we intend to achieve between now and 2010.

High-Impact Science and Marquee Capabilities - Strategic Goals

- Focus research on challenging scientific problems in the environmental molecular sciences in support of the needs of DOE and the nation.
- Maintain EMSL's strategic capabilities at the scientific forefront.

2.2.1 Goal 1

Focus Research on Challenging Scientific Problems in the Environmental Molecular Sciences in Support of the Needs of DOE and the Nation

To achieve this goal, we are targeting EMSL's objectives to on science themes to provide our users with a multidisciplinary, problem-solving environment, and to encourage use of EMSL's capabilities through Scientific Grand Challenges.

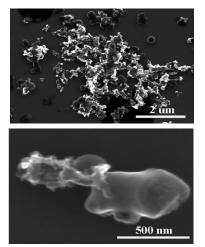
Objectives

Goal 1.1 Focus on Science Themes

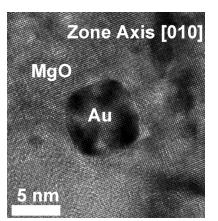
EMSL is establishing key science themes in order to focus the strengths of the facility and its user program for increased scientific impact. Science themes will guide user outreach efforts, help prioritize our investments in equipment and staff, and guide our review of user proposals. The objective 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.

Because EMSL is a DOE national scientific user facility, the selected science themes must meet certain criteria:

- The science themes must have relevance to **DOE and the nation**.
- The science themes should involve excellent and impactful **environmental molecular science**. This does not mean that all projects in the theme portfolio must have both an environmental and molecular component, but the theme as a whole must meet this objective.



One of EMSL's proposed science themes is in the area of atmospheric aerosol chemistry. Aerosols have a major impact on climate change, regional air pollution, and health, making them a national research priority. Here, EMSL researchers and users investigate the impacts of soot taken from the air in Mexico City.



Another EMSL science theme, Science of Interfacial Phenomena, involves the study of catalytic structure-function relationships to allow precise control of catalytic activity and selectivity. Here, EMSL researchers and users are investigating the catalytic role of gold clusters supported on a magnesium-oxide lattice.

- It must be possible to grow a vibrant **national user program** in the science theme. The capabilities and expertise within EMSL must be widely applicable to the theme and a sufficient user base must be available on a national level.
- The science themes should have significant **opportunity** for major scientific progress or capability advances.
- It must be **cost effective**, from a research and management perspective, for EMSL to support the science theme.
- Success in the science themes should have a positive **societal/cultural/** economic impact for the region, nation, or world.

With these criteria in mind, we selected four science themes. They are used to help guide EMSL investments to enable high-priority science. The proposed science themes are as follows (and are discussed in detail in Appendix A):

- **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.
- Atmospheric Aerosol Chemistry. Expanding a global- to molecular-scale understanding of aerosol processes and their impacts (upper left).
- Science of Interfacial Phenomena. Tailoring interfacial structures for dynamics, reactivity, and transport (lower left).

We will continue to refine and vet our science themes with DOE, EMSL's Science Advisory Committee, and our users. Calls for user proposals will be established in 2006 with the goal of attracting a significant additional number of high-impact users to EMSL. EMSL Scientific Facility Leads (SFLs) will work to engage high-impact users around these themes as well as to develop new capabilities that support the scientific directions of the themes.

Goal 1.2 Accomplish high-impact science

For EMSL to achieve its vision of becoming the sought-after scientific user facility, it must establish a leadership position in accomplishing important science that addresses our customers' highest-priority challenges. Success in this objective will be indicated by a substantial increase in traditional metrics of scientific and technical impact, including publications, citations, invention reports, patents, and awards and recognition.

Publication of our findings and recommendations in the most appropriate and prestigious science and engineering journals is not only the primary method by which science and technology are impacted, but is also a critical means to increase our credibility as a leader in environmental molecular science. All publications demonstrate the accomplishments of EMSL's users and staff; however, a targeted approach to publications will more effectively reach the scientific community, potential clients, and other key audiences. EMSL management will establish metrics that quantify not only publications but the impact of these publications and the degree to which these publications are cited.

Goal 1.3 Identify and Implement EMSL's Scientific Grand Challenges

At EMSL, we are focusing groups of users on important scientific challenges that require a significant fraction of EMSL resources for considerable periods of time. This effort is being facilitated within our user model as Scientific Grand Challenges—coordinated, multi-investigator research focused on resolving a major scientific problem. These Scientific Grand Challenges will

- focus on critical milestones in the advancement or use of science
- support DOE mission areas
- be user driven
- take full advantage of EMSL's unique resources and technical expertise
- increase the scientific impact and robustness of EMSL as a user facility.

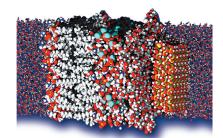
EMSL is the uniquely qualified scientific user facility that can serve as the resource and collaboration hub to address scientific investigations of massive scope. The Scientific Grand Challenges are expected to attract and involve users who are among the world's best scientists in the challenge area. The scope of the scientific problems to be addressed will involve multidisciplinary teaming, and the breadth of a challenge will be of such magnitude that it cannot be addressed at any other existing single facility. The Scientific Grand Challenges will require not only the capabilities of EMSL, but possibly other DOE user facilities and specialized instrumentation and capabilities at the participants' home institutions. They will also require significant management and coordination to meet their aggressive goals.

We will enable EMSL Scientific Grand Challenge efforts by allocating resources that support these efforts. Grand Challenge science will be given a high priority for time on our scientific resources, and we will dedicate a portion of our operating budget to work with Grand Challenge users. Finally, capital investments in support of EMSL's Scientific Grand Challenges will be a high priority.

2.2.2 Goal 2

Maintain EMSL's Strategic Capabilities at the Scientific Forefront

Today's revolutions in science are driven by rapidly advancing analytical capabilities and methodologies combined with the infusion of increasingly



The interaction of organics, metals, minerals, and microbes form a complex web that must be understood in order to design DOE environmental management strategies. For example, these electrostatic potential isocontours of the rough lipopolysaccharide membrane of *Pseudomonas aeruginosa* were obtained using molecular dynamics simulation techniques. This research fills a huge gap in our knowledge of the interaction of microbes with the subsurface. powerful information and computing technologies. Integrated investments in these advances are crucial for achieving the highest-value impact on a broad range of scientific frontiers and with a diverse user community.

Objectives

Goal 2.1 Develop and Maintain Unique Capabilities for Users

In EMSL's user environment, key instruments are highly used by scientists who are funded by diverse national sponsors. Consequently, investments made in upgrades to enhance productivity, efficacy, or new capability are heavily leveraged against the national investment in the user community. One of EMSL's strengths is providing high-demand capabilities that are not readily available elsewhere in the nation. Examples include high-throughput proteomics capability, a nuclear magnetic resonance spectrometer for use with radiological materials, and a 900-MHz wide-bore nuclear magnetic resonance spectrometer.

Anticipating opportunities and developing areas of science is often a difficult task. Our SFLs, working with EMSL's Chief Scientist and Lead Scientists, are charged with developing potential "Blue Sky" capability roadmaps, such as nextgeneration instrumentation and marquee capabilities, for new instrumentation ideas in support of our Scientific Grand Challenges, science themes, areas of interest to DOE BER programs, and EMSL's user community.

Goal 2.2 Provide an Integrated Problem-Solving Environment to Users

As a relatively new user facility with largely state-of-the-art equipment, EMSL provides an environment for many research activities that users could not accomplish elsewhere. A multifaceted approach to a particular scientific problem can be achieved by our users due to the ease and flexibility of integrating experimental and computational components of our core facilities. Additionally, staff quality and their willingness to advise, help, and assist users are key features that distinguish EMSL as a preferred location for users to pursue new or difficult scientific multi- or cross-disciplinary investigations.

In 2006, EMSL will make a concerted effort to market our capabilities as a collection of instruments and expertise that can be coupled to solve scientific problems. The desire is to enable users to use a suite of tools to solve a problem rather than use instruments in a "one-off" manner. Our science themes-based call for time allocation proposals will highlight the power of EMSL's collection of capabilities and that we allocate EMSL resources in a manner that facilitates this process.

2.3 Outstanding Management and Operations

We provide our users with a positive and productive research experience through outstanding management and operations. Recognizing that world-class tools and capabilities alone will not ensure impact to the user experience, EMSL has developed tools and strategies to provide continuous improvement of the user experience. EMSL is an integral part of PNNL, and as such, benefits from myriad programs and activities that support PNNL overall. As a result, the scientific accomplishments and strategies of EMSL are robust management systems and operational tools. EMSL management is committed to operating BER's national scientific user facility with excellence through a strong management team; a focused strategy; and consistent policies and plans communicated to EMSL staff, PNNL staff, and DOE's BER and PNSO management and staff.

Outstanding Management and Operations – Strategic Goals

- Optimize management in support of the user program.
- Operate with excellence.

2.3.1 Goal 3

Optimize Management in Support of the User Program

Transparent, forward-focused management systems are vital to maximizing EMSL's impact to scientific endeavors undertaken using our resources.

Objectives

Goal 3.1 Develop and Maintain Robust Management Systems

In 2006, we are implementing a system for management and assurance that aligns governance, management, and performance functions within EMSL (Figure 2-2). The governance function focuses on our strategy. Management is accountable for translating strategic goals into tactical objectives and deploying resources to attain those objectives while managing performance within the limits set by governance. The performance level, where the work of the Laboratory is accomplished, is accountable to management for performing work within the established procedures and guidelines, with attention to minimizing risk.

• Governance - Set strategic direction. Governance, consisting of the PNNL and EMSL Directors, Battelle management, and senior EMSL management, sets the scientific direction of EMSL, aligns resource allocations with goals, approves operational and business boundaries, and monitors progress toward goals. Using knowledge of our customers' strategies, user needs, data and information on our past performance, and current capabilities, EMSL's senior managers set goals to be achieved and the strategies to employ. Governance sets operational expectations to provide management and staff with clear operating boundaries, and allocates resources to help achieve our goals and management of associated risks. Finally, governance monitors performance relative to goals and changes in the business environment, and adjusts budgets and guidance as needed to respond to significant changes.

- Management Translate strategy into tactics. Management translates goals into tactical objectives, deploys resources to achieve the objectives and manage within risk limits, and provides feedback to governance on performance. EMSL's mid-level managers (SFLs, Group Leads, and senior technical staff) perform this management function. With leadership direction on the EMSL strategy, they develop tactical objectives within EMSL's work plans to align resources to goals. After appropriate governance approval, management deploys resources to execute business plans and monitors performance, providing regular feedback to governance.
- **Performance Staff conduct the work.** Supervisors and staff use processes, procedures, and tools to perform day-to-day project activities to accomplish our tactical objectives, while managing within established operational limits. Performance data and trends relative to the goals and objectives are gathered from this level through the use of self-assessments and are summarized for management and governance to provide information essential for decision making.
- Assurance processes validate performance. Governance and management employ means such as audits, assessments, independent oversight, peer reviews, benchmarking, and external certifications to provide reasonable assurance that goals are being achieved within approved operational boundaries. We use self-assessments to obtain information on performance, to validate that management systems are performing effectively and efficiently, and to verify that accurate and reliable data are being delivered to decision makers and regulators. Assurance is also used to verify that our users are being provided high-quality products and services.



Figure 2-2. EMSL system for management and assurance.

Goal 3.2 Develop and Enable Engaged Leadership and Staff

EMSL scientific, technical, management, and support staff are vital to the facility's success. We are committed to continuing to attract, develop, and retain a diverse workforce of highly regarded staff, which is essential to the long-term health and growth of EMSL. Our future ability to provide leading-edge resources for environmental molecular sciences to users requires a stable workforce of capable and motivated professionals. Consequently, we must fully address the issues impacting retention and motivation of our staff.

Key to achieving these goals is creating and maintaining a quality work environment that enables staff to feel valued and work in a highly productive mode. We must provide the tools, support, and resources that enable staff to develop their careers to the fullest extent possible.

We are focused on creating a work environment that enables highly engaged staff to work with passion, drive innovation, and move the user program toward higher levels of scientific productivity. This includes a workforce characterized by staff members who are in roles that best suit their talents. We will continue to provide varied career path options and help staff identify their strengths, and then team them with outstanding managers to create an engaging work environment.

We will continue to develop our staff through active mentoring and participation in the Scientist and Engineer Development and Management Skill Development programs. We will continue to participate in PNNL's annual Quality of Work Life Survey to assess areas for improvement. Areas that raise concern due to statistically reduced scores will be an area of focus, and responding actions will be rolled into the EMSL Performance Management Plan for tracking and evaluation.

Goal 3.3 Engage Advisory Committees

To secure EMSL's success scientifically and in terms of excellence related to the user experience, we have formed two advisory committees: the User Advisory Committee (UAC) and the Science Advisory Committee (SAC).

The User Advisory Committee is an independent body charged with providing objective, timely advice and recommendations to EMSL leadership with respect to the user experience. The UAC and the UAC Chair report directly to the EMSL Director.

The Science Advisory Committee is chartered by the EMSL Director to render advice, guidance, and counsel on the effective management and strategic objectives of EMSL. This committee, which reports to the PNNL Director, serves as the key external advisory body for stakeholder advocacy of EMSL strategy, operations, and scientific relevance and quality.

We will engage these committees to improve the user experience and evaluate the processes and procedures developed to enable user access to EMSL. We will engage the user community through user workshops led by the UAC. We will seek the advice and guidance of the SAC in evaluations of the EMSL strategy



The Scientist and Engineer Development Program is intended to strengthen and diversify science and engineering leadership by providing opportunities for mid-level researchers to network and present their work with peers and senior researchers, and receive in-depth training on management skills. and in critical decisions in the area of science themes that define the capabilities and capital investments of EMSL. Details of the construction and operations of the advisory committees can be found in Appendix E and F of the User Operations Manual.

2.3.2 Goal 4

Operate with Excellence

Excellent research facilities enable and encourage excellent research results. EMSL will concentrate on refreshing and maintaining a "mission-ready" infrastructure and equipment in support of a productive user community.

Objectives

Goal 4.1 Ensure Safe, Secure, and Compliant Operations

EMSL's goal is to provide our users and staff with the highest-quality and most efficient services in support of research activities. A key aspect to achieving this goal is to continue to involve staff in the development, improvement, and ownership of environment, health, and safety practices. We will continue to seek methods for streamlining and improving staff and user training, waste management, and hazard identification and tracking.

EMSL has a long history of outstanding safety and security. We will continue to build on our record by implementing leading indicators for safety, holding meetings to discuss best practices, conducting management walkthroughs of all laboratory space, and benchmarking with other national user facilities.

Goal 4.2 Enhance EMSL's Infrastructure

Implementation of Scientific Grand Challenge research and the maturation of EMSL's capabilities in our science themes provide opportunities that place a high premium on both capability and capacity dimensions of EMSL facilities. Additional pressure will be felt when PNNL facilities in the Hanford Site's 300 Area are closed and transferred for cleanup. This closure will impact several EMSL capabilities, including three nuclear magnetic resonance spectrometers that are currently located in the 300 Area's 331 Building.

Vital to the successful operation of EMSL is providing our staff and users with quality facilities and adequate laboratory and office space. Currently, the EMSL building is fully occupied. As we continue to build new capabilities or enhance existing facilities, we must establish a clear plan for space allocation and identify options for increasing available space.

EMSL management is working closely with PNNL's Research Campus of the Future staff to develop long-term facility plans to meet EMSL's growth

needs. Of critical importance is additional office space. An additional office wing, expected to begin construction in 2006, will only reduce overpopulation in an already dramatically overcrowded facility. Also needed is space for our expanding scientific capabilities. In the near term, we will work to consolidate similar capabilities and eliminate redundant and underused capabilities.

Goal 4.3 Provide Efficient and Effective Utilization of EMSL Resources

One of EMSL's primary responsibilities is the management of its resources, including the scientific instrumentation and the financial resources to operate these instruments. In order to continually improve the efficiency and effectiveness of these instruments, we developed the EMSL Resource System (ERS) to track use of all major instruments within EMSL. The ERS provides the data necessary to evaluate our performance in terms of instrument availability, downtime for maintenance, and user demand. The ERS is also designed to assist with scheduling access to these instruments.

The ERS also allows EMSL management to assess user demands on all instruments in EMSL and is valuable in determining when additional assets are needed or when to consider retiring underused systems. Additionally, maintenance costs for each instrument can be determined, which is useful in determining the level of maintenance contracts that are required.

We will use the data obtained from the ERS to evaluate all EMSL assets and develop life-cycle plans for each instrument. These life-cycle plans will address long-term maintenance and upgrades as well as retirement of aging and underused systems.

2.4 Exceptional User Outreach and Services

EMSL strives to attract high-impact scientists through the development of outreach programs and the active involvement of the user community. To strengthen EMSL's research program and its scientific impact, we must develop methods to engage our user community.

EMSL's vision requires an engaged and proactive user community. The EMSL Strategic Plan has identified two strategic goals to address this facet of our vision.

Exceptional User Outreach and Services – Strategic Goals Attract the best users and user research. Optimize services to users.

2.4.1 Goal 5

Attract the Best Users and User Research

Objectives

Goal 5.1 Establish and Expand Peer Review of User Proposals

Potential users may at any time submit a proposal through the EMSL external website (http://www.emsl.pnl.gov). To select the best and most appropriate science, all EMSL proposals are reviewed using specific criteria, which include scientific merit with respect to EMSL and DOE missions; technical approach; potential environmental, safety and health hazards; proprietary status; appropriateness of requested instrumentation; contributions that EMSL can make in bringing the research to fruition; and availability of resources and personnel.

To assist in the work associated with the peer review of proposals, we developed the web-based EMSL Proposal-Review System (EPRS). This system will reduce the burden on the reviewers and Scientific Facility Leads by capturing all of the review data and automating much of the process. The EPRS allows the SFLs to maintain a list of internal and external proposal reviewers and select the most appropriate reviewers for each proposal. EMSL will provide an external review for all capabilities deemed to be over-subscribed.

All of EMSL's research facilities will use the EMSL Peer-Review System as a required peer-review tool for all user proposals. In addition, our Scientific Facility Leads will strive to increase the use of our unique capabilities through outreach and calls for proposals.

Goal 5.2 Establish a Robust User Outreach Program

The goal of EMSL's outreach strategy is to enable its vision to be recognized as a scientific solutions leader, providing the catalyst for assembling teams of expert scientists to address challenging research objectives that demand multidisciplinary approaches. To achieve this vision and establish an engaged, proactive user community, EMSL has designed the following outreach strategies:

- Attract high-profile users. Attracting high-profile scientists to EMSL will enhance our scientific reputation and increase its visibility and appeal to the scientific community. Through their research activities and collaborations at EMSL, these high-profile scientists will help further develop the distinctive signature scientific areas for which EMSL is known. Additionally, these scientists bring to EMSL mentoring and scientific collaboration opportunities for early-career staff and users.
- **Build visibility within the scientific community.** EMSL is well known among select groups in scientific and/or regional domains, but the user facility is not widely known among all of the scientific communities that represent EMSL's main science themes. Communication and demonstration of

EMSL's scientific capabilities and research accomplishments to the scientific community will result in the recognition of EMSL as a unique user facility—which in turn will result in advocacy for EMSL's capabilities at external institutions and to EMSL sponsors and stakeholders.

- Foster collaborations with PNNL researchers. PNNL is rich with scientific expertise and technology development abilities. Development of leading-edge capabilities at EMSL requires collaboration with PNNL scientific leaders. Promoting collaborations among EMSL staff and other PNNL researchers will enable new capability development through joint grant proposals and more efficient use of PNNL-wide resources and intellectual pool—resulting in a strengthened EMSL user program.
- Promote educational outreach. A critical element of furthering environmental molecular science is to educate and train the next generation of researchers. EMSL is committed to supporting science and engineering education. To maximize impact, EMSL will leverage its activities with those of PNNL's Partnership groups. This collaboration will in turn maximize the use of EMSL/PNNL resources and focus on areas of mutual interest, such as outreach to regional universities and enhancement of EMSL visibility to academic scientists.

2.4.2 Goal 6

Optimize Services to Users

Objectives

Goal 6.1 Outstanding User Satisfaction

We continually seek a high level of user satisfaction. To assess the quality of a user's experience, we annually ask for user feedback through an online user survey. Historically, our response return rates have been low (20%). Therefore, we have revised our user survey to reduce the level of effort needed from responders and maximize the significance and impact of their responses to survey questions by removing from the survey collection of data that can be obtained from sources other than the respondent. Additionally, we will investigate other routes for obtaining feedback, such as onsite exit interviews and evaluations.

Goal 6.2 Provide a Transparent and Seamless Environment to Users

We strive to provide seamless mechanisms for users to access and use EMSL capabilities for problems that range from small research projects involving a single principal investigator to large, complex, multi-institution scientific challenges. Users may access EMSL facilities via unsolicited proposals, calls for proposals, or Scientific Grand Challenges. Regardless of access type, all users and their institutions must sign an EMSL User Agreement and agree to abide by the terms of the User Agreement prior to use of EMSL facilities or

capabilities. All users must also be cognizant of, and abide by, EMSL standard practices and procedures.

3.0 IMPLEMENTING THE STRATEGIC PLAN

Central to the integrated effort to manage EMSL as a best-in-class national scientific user facility is a cyclic process that involves refreshment of this strategic plan annually in response to DOE and PNNL strategic direction, execution of the plan, assessment and reporting of performance, decisive and effective corrective action, and reevaluation to assure continuous improvement. The Integrated Planning and Assessment Management System (IPAMS), found in PNNL's Standards-Based Management System (SBMS), provides the process and procedures to accomplish these steps.

This section describes these planning, performance measurement, and feedback processes, and displays the strategic plan dashboard and the timeline of expected outcomes from implementing EMSL's Strategic Plan.

3.1 Strategic Planning Process

Strategic planning processes (Figure 3-1) and tools enable development and documentation of EMSL's mission, vision, and strategy. Performance against the

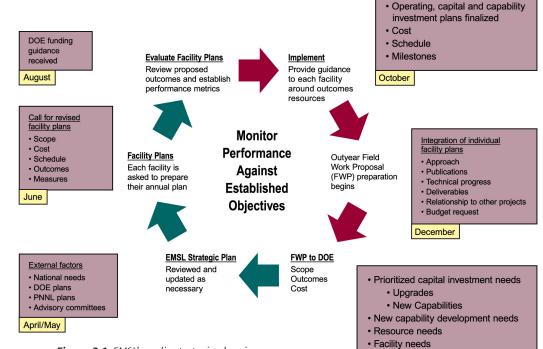


Figure 3-1. EMSL's cyclic strategic planning process.

strategy is monitored and reviewed on an ongoing basis throughout the year, and the overall strategy is refreshed as needed. EMSL's strategic plan provides the foundation for EMSL's business planning and resource allocation processes.

3.2 Strategy Dashboard

EMSL's strategic plan is maintained by the EMSL Director based on collaboration and concurrence with BER, PNSO, PNNL, and EMSL's Science Advisory and User Advisory committees. The strategic plan amalgamates EMSL's, PNNL's, and DOE's vision of EMSL's future. It describes EMSL's strategy in terms of our model for simultaneous excellence in science, management and operations, and user outreach. EMSL's strategy is depicted using a "bubble chart" dashboard (Figure 3-2) containing our strategic goals and objectives. Under each strategic goal are objectives to guide and inform EMSL management of progress toward our goals.

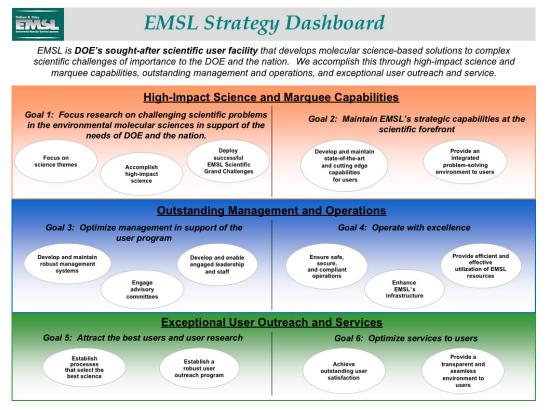


Figure 3-2. The EMSL Strategy Dashboard.

The dashboard shows the alignment of the goals and objectives within the three tenets of the vision statement to provide high-impact science and marquee capabilities, outstanding management and operations, and exceptional user outreach and services. Supporting each strategic goal is a set of strategic objectives, displayed as "bubbles" on the dashboard. The objectives have been developed to monitor and address all aspects of EMSL performance. Behind

each objective are supporting management systems and procedures in place or in development to ensure the successful implementation of the objective, and there are defined schedules, performance metrics, and assessment processes to review and document the progress on meeting the objectives. This dashboard is used to monitor the status and effectiveness of EMSL's Strategic Plan in accomplishing our vision and mission.

The following is further clarification of some of the strategic elements displayed on the dashboard:

- **Strategic Goals** are long-term goals (5 years) toward the future of EMSL. The six goals discussed in this strategic plan are aligned with the three facets of the EMSL Vision Statement and are the targets toward which our strategic objectives are directed.
- **Objectives** are used to track the intermediate-term (3 to 5 years), tangible results that relate directly to achieving our strategic goals. Objectives may evolve over time with changes in DOE's or our own priorities, but are intended to embody the enduring actions needed to meet our goals.



Accountable to PNNL through IPAMS

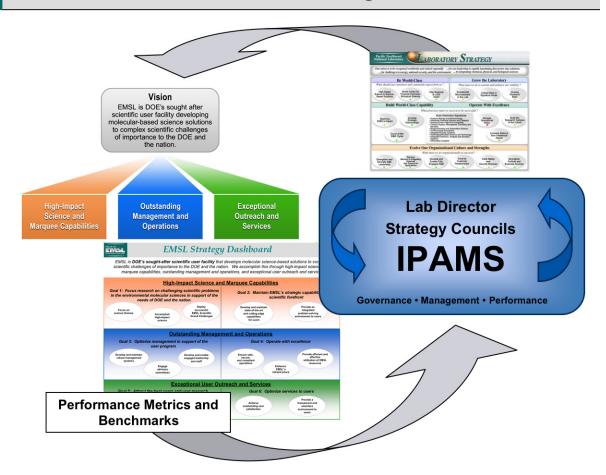


Figure 3-3. PNNL's Integrated Planning and Assessment Management System.

During annual strategic plan reviews, wording and intent of these objectives are reviewed for continued applicability and alignment with any higher-level direction.

- In order to gauge our progress and effectiveness, we select **performance metrics** appropriate to the current year's expectations for each objective. These are reported internally monthly, with quarterly summaries provided to PNNL management, BER, and PNSO. Tracking and reporting of these metrics provides EMSL management with the performance data streams necessary to refocus attention or efforts as necessary and also provides timely feedback to the PNNL Director for oversight functions within the Laboratory.
- EMSL uses **Performance Assessment and Analysis Systems** that are part of PNNL's IPAMS to gather and combine EMSL data with similar data streams from the other PNNL directorates to compare EMSL performance against other Laboratory organizations, determine trends, and provide PNNL-view feedback to support high-level direction from the Laboratory Director to the Directorates (Figure 3-3).

3.3 Project and Performance Measurement

EMSL measures the effectiveness of defined plans and strategies, operations, and overall organization health, and drives improvement through our performance management process. Performance against defined goals, objectives, metrics, and risk limits across EMSL line organizations and management systems is assessed and evaluated using self, independent, internal, and external assessments, audits, and reviews (including peer review of research results). These tools are described more fully in PNNL's SBMS IPAMS. Outcomes of these processes are used 1) to perform strategy development and management decision making and 2) to identify and enable improvement.

Monthly reporting and presentations by the EMSL management team provide a standardized approach to monitoring progress. This approach provides for early detection and tracking of issues and timely corrective action where needed.

3.4 Strategic Timeline and Deliverables

Each objective for the goals of EMSL's strategic plan is accompanied by specific actions and timelines in which these actions will be delivered. The following tables depict the deliverables and timelines related to each of EMSL's strategic tenets and subsequent goals and objectives.

3.4.1 High-Impact Science and Marquee Capabilities

Goal 1: Focus Research on Challenging Scientific Problems in the Environmental Molecular Sciences in Support of the Needs of DOE and the Nation

2006 2010			
OBJECTIVE	'06 - '07	'07 - '09	ʻ09 - '10
Identify and Implement	Implement a 3-year Biogeochemistry Scientific Grand Challenge to explore the molecular basis of electron transfer across microbe-mineral interfaces	Complete the Biogeochemistry Scientific Grand Challenge and publish the results	
EMSL's Scientific Grand Challenges	Implement a 5-year Membrane Biology Scientific Grand Challenge in biological membrane processes in cells		Complete the Membrane Biology Scientific Grand Challenge and publish the results
	Develop scientific concepts for new Scientific Grand Challenges	Implement at least one new Scientific Grand Challenge	Implement at least one new Scientific Grand Challenge
	Develop and refine the themes		Reevaluate the science themes
Focus on	Establish a call for proposals		
Science Themes	Perform user outreach around the science themes		
	Invest in science theme capabilities		
Accomplish High- Impact Science	Develop list of targeted journals		
	Develop metrics of publications, citations, invention reports, patents, awards and recognition		

Goal 2: Maintain EMSL's Strategic Capabilities at the Scientific Forefront

2006 2010				
OBJECTIVE	'06 - '07	ʻ07 - ʻ09	ʻ09 - <mark>'1</mark> 0	
Develop and Maintain Unique Capabilities for Users	Establish a recapitalization plan	Refresh high-performance	Invest in next-generation high-	
	<i>Operando</i> transmission electron microscope	supercomputing capabilities	performance mass spectrometer	
Provide an Integrated Problem-Solving	Molecular Science Computing Facility calls for proposals will encourage an experimental component			
Environment to Users	Cross-facility capability development			

3.4.2 Outstanding Management and Operations

Goal 3: Optimize Management in Support of the User Program

2006			
OBJECTIVE	'06 - '0 7	'07 - '09	ʻ09 - '10
Develop and Maintain Robust Management Systems	Implement a performance management system		Reevaluate EMSL's management systems
Develop and Enable Engaged Leadership	Hire a computational science lead	Hire a biology science lead	
and Staff	Enroll staff in skill development courses		
Engage EMSL's Advisory Committees	Repopulate the advisory committees	Hold a user meeting	

Goal 4: Operate with Excellence

2006			
OBJECTIVE	'06 - '07	'07 - '0 9	ʻ09 - '10
Ensure Safe, Secure, and Compliant Operations	Develop leading indicators	Consolidate similar capabilities	Benchmark the next- generation DOE Office of Science user facility's safety and health program
Enhance EMSL's Infrastructure	Construct a raised floor in the Molecular Science Computing Facility		Construct an office module
	Construct an office module		Construct a lab module
Provide Efficient and Effective Utilization of EMSL Resources	Fully implement and use the EMSL Resource System	Develop systems to increase efficiency	Analyze the EMSL Resource System and revise as required

3.4.3 Exceptional User Outreach and Services

Goal 5: Attract the Best Users and User Research

	2006		<u>2010</u>
OBJECTIVE	0 - 2 years	2 - 4 years	4 - 5 years
Establish and Expand Peer Review of User Proposals	Institutionalize EMSL's Proposal Review System		
Establish a Robust User Outreach Program	Present at two national meetings	Host a user workshop	

Goal 6: Optimize Services to Users

2006 2010			
OBJECTIVE	0 - 2 years	2 - 4 years	4 - 5 years
Outstanding User Satisfaction	Validate user satisfaction instruments		
Provide a Transparent and Seamless Environment to Users	Centralize user services	Revisit the User Agreement	

APPENDIX A EMSL SCIENCE THEMES

The William R. Wiley Environmental Molecular Sciences Laboratory (EMSL) is establishing key scientific theme areas in order to focus the strengths of EMSL and the user program to increase scientific impact. The objective of developing science themes is to define and develop key collections of user projects that, taken together, can have a significant impact on an important area of environmental molecular science. The current focus areas of the science themes are

- Biological Interactions and Interfaces
- Geochemistry/Biogeochemistry and Subsurface Science
- Atmospheric Aerosol Chemistry
- Science of Interfacial Phenomena.

Following is a brief overview of these science themes.

Biological Interactions and Interfaces

Developing a Molecular-Scale Understanding of Cells and Biomolecules to Provide a Scientific Solutions Approach to Biological Systems.

Understanding and optimizing the response or performance of biological systems to the interaction with its environment can have a significant impact on achieving viable solutions to several problems of national concern. For example, anaerobic microbial metabolism is of direct relevance to U.S. Department of Energy (DOE) missions in environmental stewardship, clean and secure energy, and basic science. Thus, molecular-level measurements and the corresponding insight into biochemical processes could lead to new predictive computational models that provide a more solid basis for using microbes effectively and safely to mitigate the impacts of energy-production activities on the environment and human health.

Recent advances in whole genome sequencing for a variety of organisms and structure/function relationships of proteins have contributed to a rapid transition of the biological research paradigm towards understanding biology from a global perspective. As a result, biology is evolving to a quantitative and ultimately predictive science in which the ability to collect and productively use large amounts of biological data is crucial. This new approach requires a global measurement of proteins because of their primary role in almost all cellular processes.

This science theme will focus EMSL scientific resources on three key topical areas:

- Understanding translation of the gene product
- Understanding the activation and regulation of protein activity
- Determining the structure, function, and dynamics of protein complexes.

Understanding the translation of the gene product, the activation and regulation of protein activity, and determining the structure, function and dynamics of protein complexes will provide a more solid basis for using microbes effectively and safely to mitigate the impacts of energy-production activities on the environment and human health. EMSL already has an outstanding record of accomplishments in the area of biological interactions and interfaces, and significant improvements in the instrumentation and their use on increasingly difficult problems will enable our user community to significantly advance the state of the art in this science theme area.

Geochemistry/Biogeochemistry and Subsurface Science

Expanding a Molecular-Level Understanding of Subsurface Fate and Transport and Biogeochemical Cycling.

One of the most challenging and pressing issues confronting DOE and the nation is the safe and cost-effective management of environmental pollutants and the remediation of hazardous waste sites. DOE is responsible for managing some 40-million cubic meters of contaminated soils and 1.7-trillion gallons of contaminated groundwater. Across the United States, thousands of Superfund sites exist with various levels and types of contamination (e.g., organic materials, heavy metals, inorganic materials, radionuclides).

Atmospheric pollution also is of great concern because it contributes to groundwater and soil contamination. Activities such as petroleum refining, use of fossil fuels, deforestation, landfill operations, and use of chlorofluorocarbons in refrigeration systems produce a variety of pollutants (e.g., carbon dioxide, nitrogen oxides, gaseous hydrocarbons, carbon monoxide) and large quantities of particulates. Airborne pollutants from other sources include insecticides, herbicides, radioactive fallout, and dust from fertilizers, mining operations, and livestock feedlots. The fate and transport of these pollutants on biogeochemical cycles directly and indirectly affect ecological systems and human life. These cycles are strongly interconnected and, ultimately, have important regional- and global-scale climatic or ecological impacts.

This science theme will focus EMSL's scientific resources on the following key topical areas:

- Interfacial molecular geochemistry and biogeochemistry
- Understanding the chemistry of radionuclides in the subsurface
- Understanding the fate and transport of chemical and microbial species in the subsurface.

Research in the science theme area of biogeochemistry and subsurface science is well established at EMSL. We propose to build on our strength in that area by focusing on key scientific questions/challenges in the area of molecular geochemistry and biogeochemistry, linking Subsurface Flow and Transport Experimental Laboratory capabilities to molecular-science capabilities, and gaining better access to use of radioactive materials (including establishment of an EMSL Radiochemical Annex).

Atmospheric Aerosol Chemistry

Expanding a Global- to Molecular-Scale Understanding of Aerosol Processes and Their Impacts.

Atmospheric aerosols play an important role in global climate change. Variations of aerosols are recognized as a significant forcing factor that alters the planetary radiation balance onto and away from the Earth, thus contributing to global temperature change. The effects of climate forcing caused by aerosols are not well understood, especially in the case of anthropogenic aerosols. Indeed, the effect of aerosols has been one of the greatest sources of uncertainty in efforts to interpret climate change that occurred in the past century and to project future climate change.

This science theme is designed to advance the state of knowledge of aerosol physics and chemistry from the molecular level to regional and global scales and their impacts on climate change. State-of-the-art instrumentation at EMSL will be used to characterize the size, composition, density, morphology, chemical reactivity, and cloud interactions of aerosol particles. The research will employ a collaborative, comprehensive, and interdisciplinary approach that will combine both the unique analytical capabilities of EMSL and the research expertise of EMSL scientific staff and the user community.

This science theme is formulated around the following specific, key scientific topical areas that the aerosol chemistry and atmospheric science communities face today and will continue to face in the future:

- Developing a novel analytical platform for comprehensive chemical and physical characterization of organic aerosols
- Evaluating dynamics of cloud-aerosol interactions and their climatic impacts
- Gaining critical knowledge of life cycle and long-term aging of aerosols in the atmospheric environment.

Understanding the role of aerosols in climate change is an important scientific challenge that is critical to more accurately predict the environmental impact of future energy technology options. This science theme addresses the chemical and physical properties of organic aerosols that are of key relevance to cloud formation and climate change. Aerosols are constantly evolving, and the changes they undergo profoundly alter their impact and even how long they live or how far they travel. Providing the scientific foundation to better predict how and when these properties change is necessary so policy makers can make environmentally sound decisions about processes that generate aerosols.

Science of Interfacial Phenomena

Tailoring Interfacial Structures for Dynamics, Reactivity, and Transport.

Relevant to a secure environment and energy future for the nation is the understanding of scientific issues associated with designing surfaces and interfaces for selective reactivity and processes. Specifically, hydrogen-fuel and solid-oxide fuel cell research and development activities directly related to clean energy production and storage, hydrogen production, cleanup efforts associated with high-level wastes throughout the DOE complex, development of next generation nuclear reactors for energy production, material science associated with these activities, and development of radiation detection materials will all rely on a greater molecular-level understanding of catalytic design and function and photochemical and reactive transport properties.

Because EMSL is a premier laboratory for the study of oxide materials, our main focus would be these materials. As such, it is crucial to understand the scientific issues associated with designed surfaces and interfaces that can be effectively used in a particular physical and chemical process. Compared to what is known at the atomic and molecular levels for metal and semiconductor materials, little is known about metal oxides. The complexity of the structures involved often makes them difficult to study, both theoretically and experimentally. The scientific expertise developed over the past years and the research capabilities available at EMSL are ideally suited to helping advance our understanding of these scientific issues.

Some of the interfacial research activities associated with environmental geochemistry, biology, and atmospheric chemistry are not covered here because these are being captured under the science themes of Biogeochemistry and Subsurface Science, Biological Interactions and Interfaces, and Atmospheric Chemistry. In particular, this science theme will focus on the following topical areas:

- Catalytic structure-function relationships to allow precise control of catalytic activity and selectivity
- · Gaining critical knowledge of photocatalysis and photochemistry
- Design material systems with specialized transport properties.

This science theme focuses on developing an understanding of catalytic structurefunction relationships at the atomic level that will allow precise control of catalytic activity and selectivity. In addition, the science will address in a definitive and comprehensive way, for the first time, the effect of nanoscaling on the surface chemistry of well-defined metal oxides. Highly controlled experiments in the growth, characterization, and reactivity of oxide nanodots and continuous films of nanometer thickness will elucidate the effects of quantum-confined and strain-driven electronic structures on the thermal and photochemistries of select materials. The research capabilities and expertise in EMSL will also enable the design of material systems with specialized atomic, electronic, and ionic transport properties. EMSL is an ideal place for this research to be performed because it is a premier oxide laboratory and has provided the foundation for several current research areas including surface chemistry and catalysis. As part of this research, several one-of-a-kind capabilities are planned for development in the near future. These capabilities will make EMSL a unique facility that will attract many world-class scientists as users.

EMSL Strategic Plan 2006





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