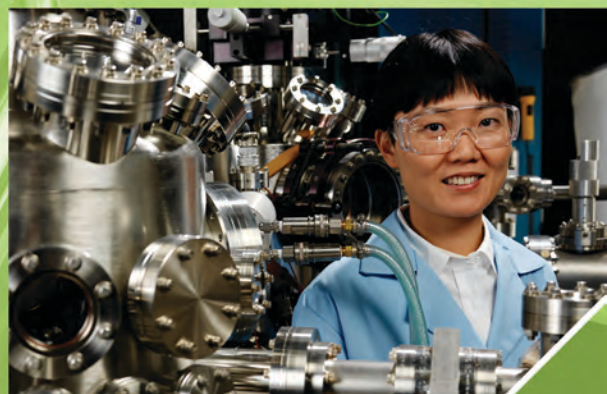
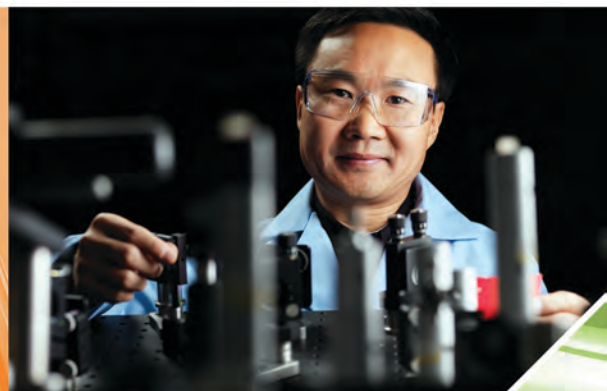


Environmental Molecular Sciences Laboratory



Strategic Plan

08



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EMSL Strategic Plan 2008

AA Campbell

August 2008

Prepared for the U.S. Department of Energy's Office of Biological and Environmental Research under Contract DE-AC05-76RL01830

Pacific Northwest National Laboratory
Richland, Washington 99352

Our Mission

EMSL, a U.S. Department of Energy national scientific user facility located 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

Director's Message



In this century, science and technology will be unified as never before because of our ability to image and interpret phenomena at single molecule scales combined with equally sophisticated methods for computational modeling at the same length scale. The challenge is to integrate this information into appropriate theoretical, experimental, and conceptual constructs, which transcend from atomic and molecular scales to bulk properties of matter and to complex and collective phenomena. The unprecedented power of modern spectroscopies and massively parallel supercomputers provide the essential tools, while interdisciplinary teams of scientists provide the intellectual leadership for addressing critical problems.

EMSL is well positioned to contribute to these challenges. In the coming years, we will contribute substantially to DOE's needs by integrating theoretical and computational approaches with experimental observation. Our researchers and user community will address critical environmental problems by investigating questions related to climate change, cleaning up the DOE weapons complex, and stabilizing waste forms. We will play a major scientific role in post-genomics biology by developing advanced tools that probe protein function in living cells and determine expression levels rapidly and with high accuracy, and then use this data to model cellular behavior. EMSL's development of tools and techniques for detection, characterization, and prediction of the behavior of biological and chemical species are vital aspects of our nation's security.

Today's research challenges require globally connected investigators working collectively and collaboratively across disciplines. Addressing these scientific problems demands the integration of transformational, high-resolution tools; massively parallel computational approaches; instantaneous access to public databases and digital libraries; and unique informatics and data visualization capabilities. These needs are well aligned with the historic strength of EMSL; its founding vision was bringing together scientists across disciplines to create a new paradigm of multidisciplinary science. The scientific challenges of the 21st Century will be solved using integrated and multidisciplinary methods—**an approach to which EMSL is extraordinarily well suited**. Our history in deploying multidisciplinary teams and integrated methods to solve scientific problems places EMSL in a unique position to solve some of the increasingly complex problems facing our world.

Allison A. Campbell, Ph.D.
EMSL Director

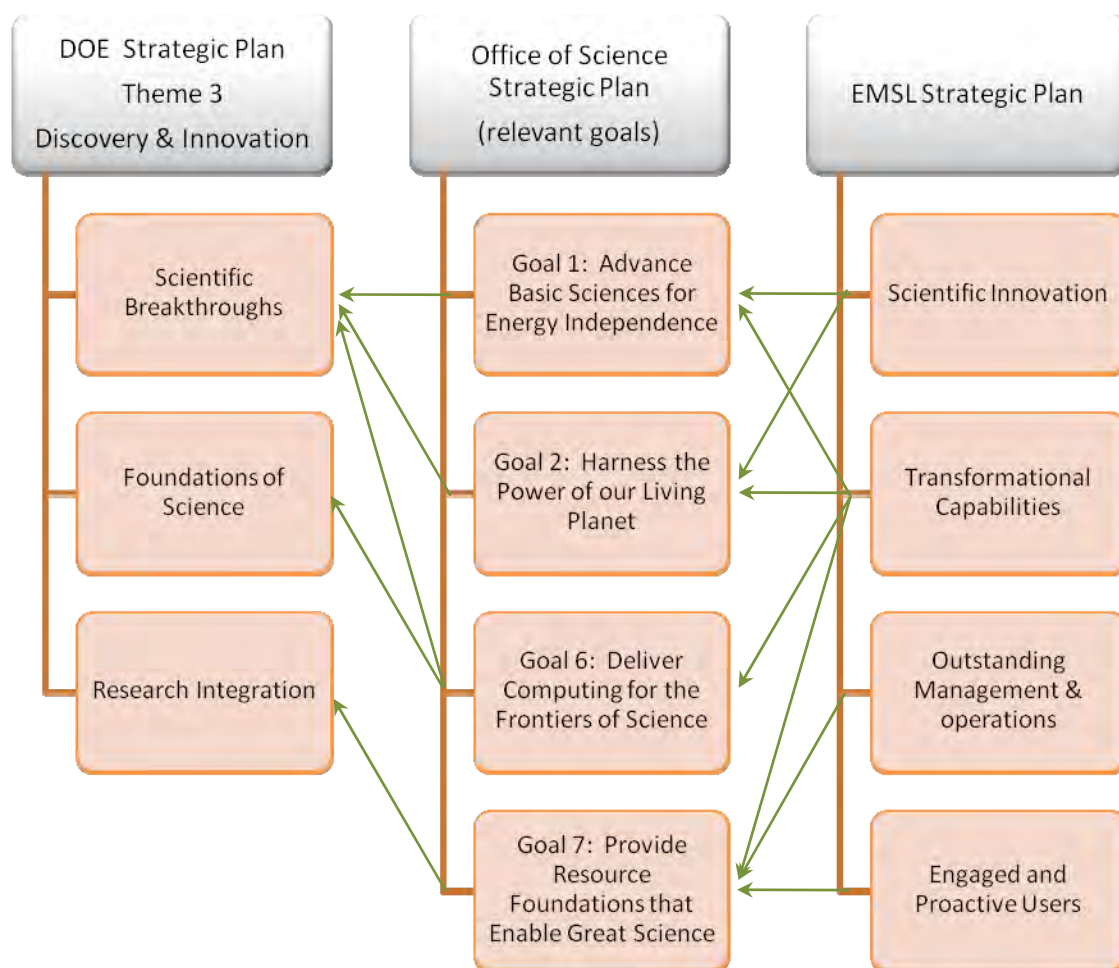
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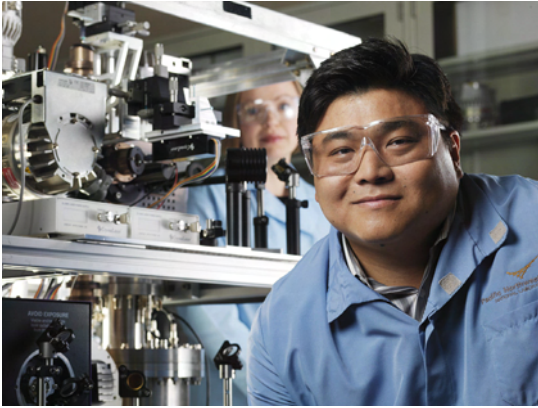
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1.0 Introduction

This Strategic Plan is EMSL's template for achieving our vision of simultaneous excellence in all aspects of our mission as a national scientific user facility. It reflects our understanding of the long-term stewardship we must work toward to meet the scientific challenges of the Department of Energy and the nation. During the next decade, we will implement the strategies contained in this Plan, working closely with the scientific community, our advisory committees, DOE's Office of Biological and Environmental Research, and other key stakeholders.

This Strategic Plan is fully aligned with the strategic plans of DOE and its Office of Science. We recognize that shifts in science and technology, national priorities, and resources made available through the Federal budget process create planning uncertainties and, ultimately, a highly dynamic planning environment. Accordingly, this Strategic Plan should be viewed as a living document for which we will continually evaluate changing needs and opportunities posed by our stakeholders (i.e., DOE, users, staff, advisory committees), work closely with them to understand and respond to those changes, and align our strategy accordingly.





This Plan is organized around four strategic outcomes 1) Scientific Innovation, 2) Capabilities that Transform Science, 3) Outstanding Management and Operations, and 4) Engaged and Proactive Users. These outcomes provide the framework for the seven critical actions we must take over the next 3 to 5 years:

1. Establishing leadership in EMSL's science themes.
2. Building and deploying transformational capabilities.
3. Integrating computation with experiment.
4. Ensuring that EMSL's workforce meets the scientific challenges of the future.
5. Creating partnerships.
6. Attracting and engaging users in EMSL's long-term strategy.
7. Building a research infrastructure that meets users' emerging scientific needs.

Implementation of these outcomes and actions is grounded in Battelle's management principles of simultaneous excellence in all aspects of management and operations.



The vision outlined in this Strategic Plan is not an extrapolation of ongoing science but a visionary look towards new opportunities where advances in environmental molecular sciences and the tools that enable these advances can have a significant impact. Current and developing technologies can be combined in new ways to create a new generation of research tools, and this vision provides a roadmap for the next decade of scientific capabilities that can collectively position EMSL to meet challenges in the environmental molecular sciences.



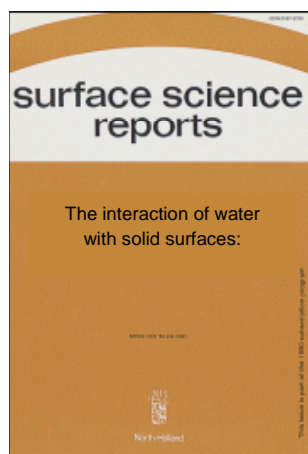
2.0 Our Impact

Our vision and strategy for the future is built upon a strong foundation of accomplishment. During the past decade, significant scientific progress has been achieved through development of new capabilities and by focusing combinations of EMSL's state-of-the-art tools and expertise on important scientific challenges. Below are past research highlights that exemplify scientific impact that EMSL has enabled to research important to DOE and the nation.



EMSL is a world-leading center for oxide and mineral surface chemistry research. The ability to synthesize unique oxide films and surfaces along with ability to characterize the physical structure and chemical properties has enabled EMSL to make significant contributions in catalysis, photocatalysis and new-generation oxide-based electronic materials as well playing an important role in advancing the understanding of model biogeochemical systems. Both the research and capability development have been recognized by national awards (2002 Federal Laboratory Consortium Technology Transfer Award and 2004 E.W. Muller Award for Outstanding Research in Surface Science). Recent work shows the impact of imaging technologies on our understanding of chemical transformations. Scanning tunneling microscopy measurements of oxygen molecules adsorbing on the surface of

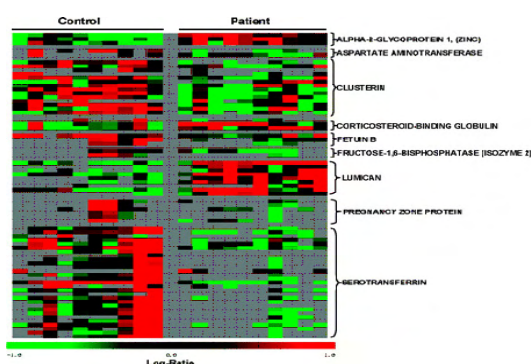
rutile [TiO₂ (110)] surface demonstrated that oxygen molecules dissociate only at specific sites (bridging oxygen vacancies) with one O atom healing a vacancy and another O atom bonding at the neighboring titanium site. This observation is of particular interest not only because it is a unique observation of site-specific adsorption, but because TiO₂ is an important catalyst substrate and the base material for photocatalytic destruction of contaminant molecules and the possible production of hydrogen. The research was published in *Journal of Physical Chemistry B* (110:21840-21845).



EMSL is a world leader in unraveling the complex interactions that occur in aqueous systems. Water occurs nearly ubiquitously in environmental systems, and unraveling the molecular-level interactions of ions and contaminants in water (both in solution, at surfaces, and in the atmosphere) is of fundamental importance in environmental molecular science. This unprecedented understanding of aqueous environments requires unique capabilities for studying ion-water clusters in the gas phase. Combining electrospray ionization with laser detachment anion beam photoelectron spectroscopy has enabled the production and spectroscopic characterization of multiply-charged, water solvated, gas-phase cluster ions ubiquitous in aqueous solution but unattainable in the gas phase. Using state-of-the-art molecular-, ion-, and electron-beam instrumentation in EMSL, scientific users have pioneered

the use of nanoscale amorphous solid water films to study ion solvation in solution and ice nucleation and crystallization in the upper atmosphere. Water interactions at solid and mineral surfaces are also

fundamental to unraveling the chemical behavior of environmental systems; this has been a focus of EMSL research from the beginning. As an example, EMSL user Mike A. Henderson published a comprehensive review of the work in this area which addressed such areas as how water is adsorbed, determining the chemical and electrostatic forces that constitute the adsorbed layer, and how coadsorbates influence these properties of water. Equally important are advances in the theory, modeling, and simulation of the properties of aqueous environments enabled by the world-class EMSL computational resources. Specifically, systematic approaches have been developed to assess the accuracy of various levels of electronic structure theory, and they have been applied to accurately evaluate several solute-solvent and solvent-solvent intermolecular interactions. This approach has paved the way for the development of a new generation of interaction potentials for water-water, ion-water and water-solute systems.



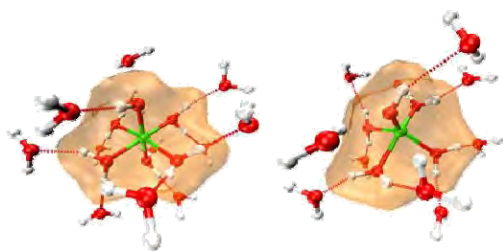
Using EMSL proteomics capabilities, users from the Centers for Disease Control and Pacific Northwest National Laboratory discovered five proteins that could help predict type 1 diabetes with higher sensitivity and specificity than current methods. Research results were published in the *Journal of Proteome Research* [7(2):698-707].

EMSL's high-throughput proteomics measurement and characterization capabilities are world-leading.

Developed using EMSL and programmatic resources, the capabilities are based on customized high-performance liquid ion cyclotron resonance (FT-ICR), time-of-flight, and Orbitrap™] instrumentation, and complemented with comprehensive data interpretation and informatics software and tools. A current throughput of approximately 100 proteome samples per day can be accommodated, and a database of nearly 1 million peptides enables comprehensive eukaryotic and prokaryotic protein identification. A particularly strong capability in microbial proteomics has been developed and is being applied to environmental remediation, carbon sequestration, and energy development problems.

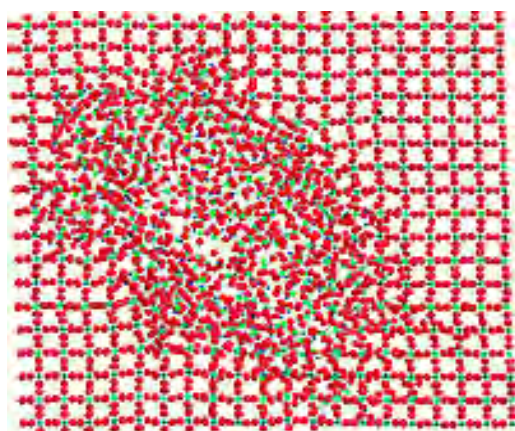
EMSL's high-performance computational capabilities and specialized software enable major scientific progress.

EMSL scientists lead the development of DOE's premier computational chemistry tool (*NWChem*) to enable researchers to solve scientific questions in areas such as catalysis, solar energy, hydrogen economy, environmental remediation, and biology, while including the complex dynamical behavior of nature in realistic environments. *NWChem* is a leading high-performance computational chemistry software suite that provides researchers with the unique capability to understand complex challenging scientific problems at the molecular level by coupling the power of advanced computational chemistry techniques



EMSL's high-performance, 11.8-teraflop supercomputer combined with its premiere computational chemistry software, *NWChem*, allowed a research team from the University of California, Davis; University of Calgary; PNNL; and State University of New York to determine the structure of a five-coordinate aluminum ion in solution. The results were published in *Science* [308(5727):1450-1453].

with existing and rapidly evolving high-performance, massively parallel computing systems. *NWChem* has been recognized with prestigious national awards (R&D 100 and Federal Laboratory Consortium for excellence in technology transfer). Running on EMSL's supercomputing hardware, *NWChem* has enabled the reliable modeling of the thermodynamics cycle of hydrogen release and uptake for chemical boron-nitrogen hydrogen storage compounds, a critical part in the development of environmentally friendly hydrogen-based fuel cells as a power source. It was also used to confirm the discovery of a five-coordinate $\text{Al}(\text{H}_2\text{O})_4\text{OH}^{2+}$ ion as the predominant form in biochemically and geochemically relevant solution environments such as natural bodies of water.



An improved understanding of how alpha particles decay waste forms is leading to enhanced predictive models that support informed decisions on long-term storage of radioactive isotopes. Results of this research, led by a scientific user from the Cambridge University using EMSL's radiological NMR capabilities, were published in *Nature* [445(7124):190-194].

EMSL is a world leader in enabling high-field nuclear magnetic resonance (NMR) to be applied to a wide range of complex systems. EMSL houses a suite of cutting-edge magnetic resonance spectrometers, including a powerful 900-MHz system and the world's only NMR spectrometer and laboratory that are dedicated to the study of solid-phase radiological samples. This unique suite of instruments has contributed broadly to the characterization of biomolecules, surface chemistry, and catalysis research. Special emphasis has been placed on use of high-field capabilities to determine hard-to-examine nuclei such as isotopes of alkaline earth elements, strontium and calcium. These investigations contributed to an improved fundamental understanding of the long-term stability of materials proposed for waste immobilization and this is leading to improved predictive models that support informed decisions on long-term storage of radioactive isotopes. For example, EMSL users from

Cambridge University and the Pacific Northwest National Laboratory published a paper in the January 11, 2007, issue of *Nature* that describes the impact of alpha emitters on the crystal structure of zircon. The dedicated radionuclide NMR was instrumental in demonstrating unequivocally that radiation effects rapidly degrade the crystal structure of the mineral.

This Strategic Plan builds on these and past accomplishments of developing transformational capabilities and integrating them to create problem-solving environment for our users. The long-term outcomes of our strategy—scientific innovation, transformational capabilities, outstanding management and operations, and engaged and proactive users—underscore the value we provide to DOE and the nation.

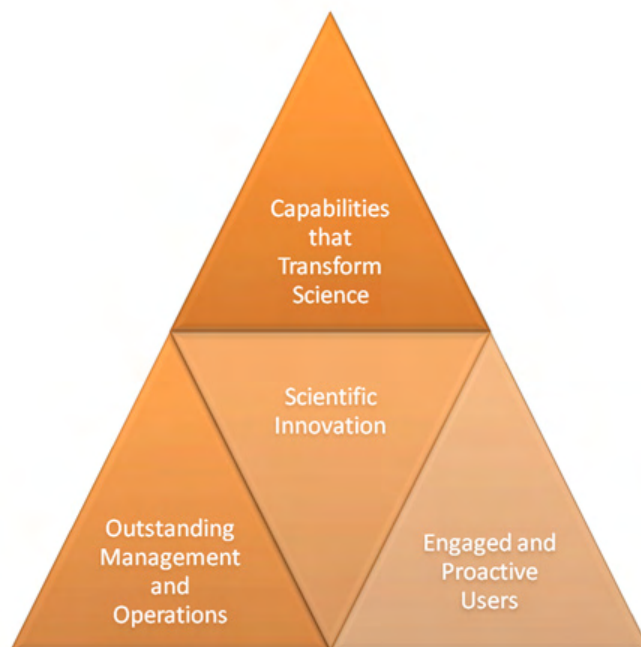
3.0 Our Vision

3.1 Delivering Scientific Innovation through Integration

Our vision is that EMSL develops and integrates, for use by the scientific community, world-leading capabilities that transform understanding in the environmental molecular sciences and accelerate discoveries relevant to DOE's missions. We will accomplish this through multidisciplinary collaborations between an engaged user community and expert scientists and staff.

Achieving this vision means that EMSL is widely recognized for:

1. **Developing transformational tools that advance scientific frontiers** in EMSL's molecular science themes.
2. Adding exponential value by **integrating science and technology** across disciplines and scientific capabilities.
3. Empowering a **distinguished community of users** that is invested in and advocates the long-term use and success of EMSL.
4. **Ensuring management excellence** that propels EMSL into a long-term, upward path of accomplishment and performance.



In achieving this vision, we commit to **advancing the scientific reputation of EMSL and our users** by engaging some of the best and brightest scientists from around the world who seek out EMSL to accomplish their scientific objectives.

Increased involvement of renowned scientists, high-impact publications, strategic partnerships, and recognition by the scientific community are key metrics for our progress.

4.0 Our Strategic Outcomes

This Strategic Plan builds on EMSL's strengths in building transformational capabilities and integrating them to create a problem-solving environment for our users. The long-term outcomes of our strategy—scientific innovation, transformational capabilities, outstanding management and operations, and engaged and proactive users—underscore the value we provide to DOE and the nation.

4.1 Scientific innovation:

EMSL will advance fundamental understanding in the environmental molecular sciences and produce accelerated leadership class discoveries for DOE mission-relevant applications.

With more than 2500 user and staff publications in peer-reviewed scientific journals during EMSL's first decade of operation, EMSL is enabling users to make significant contributions to the scientific understanding of the nation's complex energy and environmental problems. In Fiscal Year 2007, EMSL staff and user research appeared in more than 300 articles, including many in prestigious journals such as *Science*, *Nature*, *Proceedings of the National Academy of Science*, and *Journal of the American Chemical Society*.



As we look forward into the next decade of operation, we will establish a world-class research presence in key science themes of importance to DOE and the nation. Advances in understanding aqueous systems and cluster chemistry will enable us to focus on **atmospheric aerosol chemistry** and help decrease uncertainties in predicting climate change. Increased knowledge regarding **biological interactions and dynamics** and advances in our understanding of oxide materials and **interfacial science** will impact both the development of clean and secure energy and environmental cleanup solutions. Predictive knowledge of **geochemistry/biogeochemistry and subsurface science** will enable safe and predictive management of legacy and hazardous waste.

4.2 Capabilities that transform science:

EMSL will develop, integrate and deploy transformational tools that accelerate scientific discovery and innovation; provide a pillar in the nation's scientific infrastructure, and attract and retain the best and brightest scientists as staff and users.

During the past decade, EMSL has established a leadership position in building transformational capabilities in areas such as mass spectrometry based proteomics, magnetic resonance and high-performance computing software.

Moving forward and building upon the past accomplishments, EMSL will, in the next decade, build and deploy new transformational capabilities that will provide researchers with new approaches to view

chemical and biological systems—from **single molecules or organisms to complex structures or communities**, from **static to dynamic** processes, from *ex-situ* systems to *in-situ* observation. These capabilities are transformational because they transcend the envelope of current ability—they attract the brightest scientific minds in the world and enable discoveries that change the face of science.

Development and integration of these tools requires access to a wider range of resources and capabilities than typically available to individual researchers and research institutions. However, they comprise a set of capabilities appropriate to a national scientific user facility that can equip many extramural scientists to conduct truly unique and transformational research.

“We need TRANSFORMATIONAL discoveries, leading to what I call DISRUPTIVE technologies—technologies that fundamentally change the rules of the game—and that means we need fundamental breakthroughs.”

*Dr. Raymond Orbach,
Under Secretary for Science,
U.S. Department of Energy*



4.3 Best-in-class management and operations:

EMSL operations and management systems will be the most effective and efficient in delivering outstanding research; providing a world-class research infrastructure; and supporting a highly productive, world-class staff and user community.

EMSL management is committed to operating the DOE Office of Biological and Environmental Research’s national scientific user facility with excellence through strong management, premier facilities, a focused strategy, and consistently communicated policies and plans.

During the past decade, EMSL has built and deployed several management systems that streamline the user proposal and access processes. We have adopted and embedded strong project management principles into our everyday operations, and we have completed the first expansion onto the facility to provide additional raised floor computing space as well as office space for our staff and users.



In the coming years, EMSL will continue to embrace best management practices by improving processes and performance, staff and user engagement, and costs and effort efficiencies. EMSL management will employ a well-structured, integrated management approach with clear roles, responsibilities, and expectations to result in effective line management oversight. EMSL will have a robust system of clear, consistent performance objectives and measurements so that resources are more effectively focused on key objectives and continued improvements are made to meet those objectives.

We will continue to expand and improve our research infrastructure to meet the demands of our users. Our facilities will remain best in class through preventative maintenance efforts, and we will continue to identify future infrastructure needs.

Our environment, health and safety program will remain best in class through active participation in human performance assessments and waste minimization and risk assessment programs.

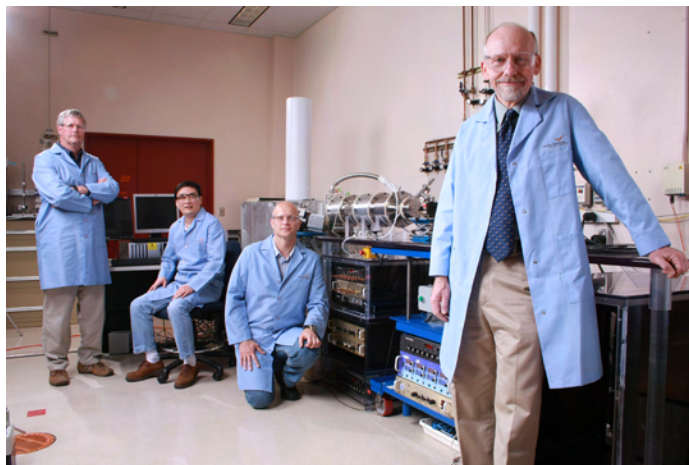
We will continue to engage our staff through active recruitment of senior leadership and providing staff with the tools that help them to advance their careers.

4.4 Highly engaged and satisfied user community:

EMSL's user program will attract the best and brightest scientists who produce scientific discoveries and are engaged in the long-term success of the user program.

EMSL's vision cannot be realized without an engaged, satisfied, and proactive user community, the hallmark of a successful user facility. EMSL's goal is to attract and foster a user community that conducts outstanding research and is actively involved and engaged in EMSL's success. Our goal is to advance the impact of EMSL's scientific accomplishments to the extent that some of the most prestigious scientists from around the world will seek to become users. To that end, we will continue to embrace ideas that build strong user communities. One example is to build upon the EMSL Scientific Grand Challenges that focus multidisciplinary groups of users on challenging scientific problems. The primary purpose of these grand challenges is to answer important scientific questions through a collaborative user-driven approach, using the comprehensive capabilities of EMSL. The scope of the scientific problems to be addressed requires multidisciplinary teaming, and the breadth of a challenge will be of magnitude such that it cannot be addressed at any other existing single facility.

Other approaches for building user engagement include focused workshops and tutorials that bring communities of users together to learn about EMSL capabilities and science themes; use of competitive analysis capabilities to obtain information on top universities where research is conducted that is compatible with EMSL's science themes, and then put into place mechanisms to target the heads of those academic departments with information about EMSL; and identification of one major professional society meeting (e.g., American Chemical Society, American Geophysical Union) per science theme per year where targeted, streamlined outreach efforts—such as a Director's Seminar Series—can be conducted towards relevant technical programs.



5.0 Critical Actions

The actions outlined below represent areas where EMSL management will focus effort and resources over the next 3 to 5 years in order to meet our vision and strategic goals. They cross cut and enable all of our strategic outcomes.

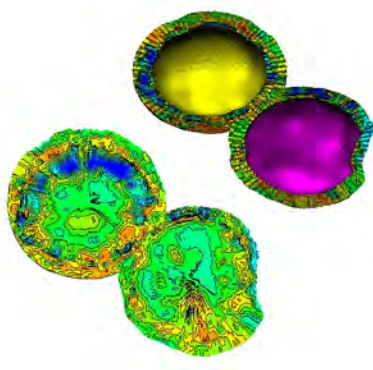
5.1 Establish scientific leadership in EMSL's science themes

EMSL science themes are areas where EMSL can make significant scientific contributions. Current science themes build upon and expand the historical scientific expertise of EMSL. They were evaluated against key criteria including DOE and national relevance, contribution to impactful environmental molecular science, strong national science and technology programs, and the ability to grow a vibrant national user program, and they were selected with broad input and support from the scientific community and EMSL advisory committees. As scientific advances are made, the nature and elements of EMSL's science themes will evolve to reflect both scientific gains and changing societal needs. New areas will be explored and evaluated during annual business planning.

In the next 3 to 5 years, EMSL will establish scientific leadership in its three mature science themes. Measures of success in the area of scientific leadership will include publications in top-tier journals, external reviews, and the ability to attract leading scientists as staff and users.

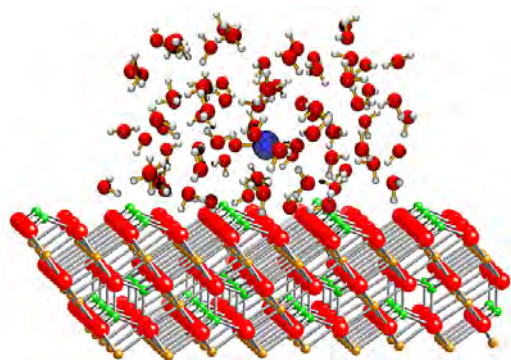
During the next 5 to 10 years, EMSL will drive scientific progress by creating a cohesive portfolio of user projects under its science themes by issuing annual calls for proposals for user projects that fill gaps in understanding and focus on key scientific questions of importance to DOE and the nation. In doing so, EMSL will make significant scientific contributions in each area as outlined below.

Current Science Themes

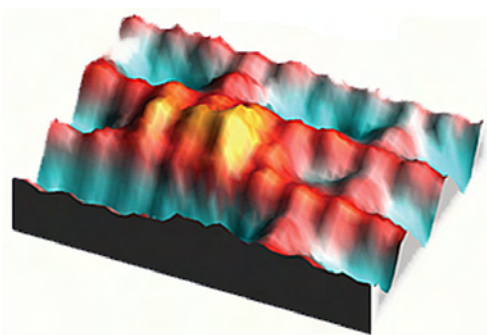


The **biological interactions and dynamics** theme emphasizes a systems-level understanding of microbes and microbial communities. The unique biological function, interactions and community dynamics of extremophiles will receive special emphasis. This work will be facilitated by establishing a new capability for culturing and sampling of microbes under precisely controlled conditions and for the isolation and analysis of individual cells and their components. Coupling EMSL's signature strengths in proteomics and metabolomics with the Joint Genome Institute's unique strengths in genomics will provide a breadth of molecular detail never previously achieved. Combining

these measurements with high dimensional data management, modeling, and simulation will, in turn, allow for the **first time a predictive understanding of microbial regulatory networks that will enable optimization and manipulation of microbial processes such as CO₂ sequestration.**

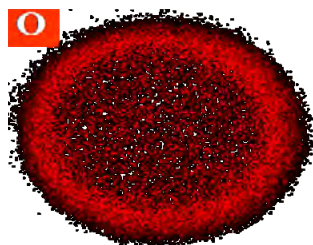


EMSL's **geochemistry/biogeochemistry and subsurface science** theme advances a core strength of EMSL and focuses on one of DOE's singularly important challenges—the cleanup of legacy waste. EMSL's emphasis on molecular-scale understanding of the complex transport and reactive processes taking place in the migration of plumes from nuclear waste sites has the promise for dramatically reducing the costs of cleanup. The understanding of such fundamental processes as proton and electron transfer in complex mineral environments mediated by microbial metabolism is a key scientific challenge. Molecular-level measurements coupled with sophisticated modeling of transport and chemical conversion processes as a function of environmental parameters is our signature approach to solving this problem. To that end EMSL shall, within the next decade, focus user projects in areas that will **improve our ability to predict and modify pollutant transport or transformation in the subsurface.**



The **science of interfacial phenomena** theme exploits signature strengths of EMSL staff and users and focuses on developing an understanding of molecular structure-function relationships at the atomic level that will allow precise control of interfacial activity and selectivity. This science theme 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 research areas, including surface chemistry and catalysis. To this end, EMSL will focus user projects on the **development of new understanding that enables the optimization of interfacial properties, such as the control of catalytic activity and longevity.**

Emerging Science Theme



EMSL has also identified an emerging area in **atmospheric aerosol chemistry** that focuses on **establishing a molecular-scale, predictive understanding of the principal chemical and physical processes of aerosol formation, growth, and decay.** Among all the forcing factors in global climate, aerosols stand alone in that the knowledge of their chemical and

physical properties are so poorly defined that even the sign of the impact factor is unknown. The greatest uncertainty is the chemistry and physics of organic aerosols, and tracing their life cycle, from molecular to cluster to nanoparticles to many microns, is virtually undefined scientifically. To fully realize this science theme, cohesive and robust science and technology programs are needed within DOE's Office of Biological and Environmental Research and scientific leadership is needed at EMSL. During the next several years, **EMSL will work with BER program managers to identify new science and technology programs that can support user research areas, work to attract scientific leadership to EMSL, and focus user projects around highly focused calls for proposals** to establish a critical mass of user projects, capabilities and expertise that enable a fully mature science theme.

Potential Future Science Themes

As science and technology programs evolve along with the scientific needs of the nation, we will identify potential new areas to focus EMSL resources, including nuclear waste form science, actinide science, and trace detection. During the next several years, EMSL scientific leadership will evaluate the feasibility and potential scientific impact of these areas.

5.2 Develop and deploy transformational scientific capabilities to the scientific user community

Scientific advancements cannot be made without similar advances in the capabilities used to make discoveries. New tools being developed at EMSL will enable researchers to change how they view chemical and biological systems—from **single molecules to communities of species**, from **static to dynamic processes**, from **ex-situ systems to in-situ observation**, and will also enable the type of discoveries that truly change the face of science.

Working with users, science advisors, and other scientific leaders, EMSL has identified emerging needs and new scientific tools and resources that will advance scientific discovery in EMSL's science themes. The results of this analysis and a variety of other indicators, including the 2006 National Academies study of advanced research instrumentation and facilities, suggest that there will be fundamental changes in the way science is conducted. These trends and advances define several important technology challenges and opportunities that will be used to focus EMSL capability development activities. These opportunities include tools and techniques for:

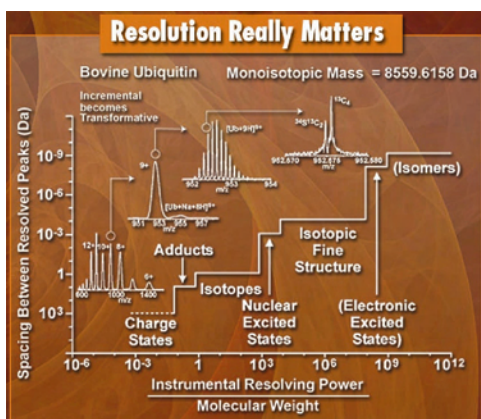
1. Moving from Statics to Dynamics in Native Environments.
2. Characterization of Surfaces and Interfaces with Unprecedented Resolution.



3. Design and Synthesis of Increasingly Complex Materials.
4. Predicting Biological Functions from Molecular and Chemical Data.
5. Rapidly Linking Theory with Experiment.
6. Bridging Scales: Bridging the Gap between Molecular and Continuum Understanding.

These challenges, coupled with the directions outlined in the science themes, provide the basis of a vision that will be used to guide capability development in EMSL during the next decade, the details of which are outlined in the EMSL document, “Recapitalizing EMSL: Meeting Future Science and Technology Challenges.” As part of this effort, several major new and exciting development opportunities are envisioned.

1. **Development of the world’s highest-field FT-ICR mass spectrometry system with unprecedented speed and resolution.** Advances in mass spectrometry will bring analytical capabilities for top-down



proteomics to a much higher level than is presently possible. Critical information on the proteomic and metabolomic profiles is thought to reside in the minor constituents that are currently below the level of detection of existing mass spectrometers. The challenge is to advance the mass resolution and mass range of mass spectrometry by as much as an order of magnitude while more than doubling the dynamic range (ratio of most abundant to least abundant ions detectable in a given scan) and the sensitivity of ICR analysis. Scientific challenges in the environmental molecular science addressed by this capability involve analyzing the most complex molecules and mixtures

imaginable and creating a measurement tool that dramatically extends the range of problems that are amenable to molecular-level investigation.

2. **Integrated capabilities for systems microbiology and extremophile research.** Microbial communities can be considered a network of cells that are controlled by their individual gene and protein regulatory networks. Mapping community function to the properties of their underlying networks requires the growth and sampling of microbes under a wide range of different, and sometimes extreme, conditions. Each sample must then be analyzed using technologies that can reveal the network structure at particular scales (from the community to molecular level). To address this challenging goal, EMSL will develop an integrated capability that will allow the parallel culturing of microbes under a wide range of different controlled conditions coupled with automated and remote



controlled capabilities that will allow users to run long-term experiments remotely. A new generation of flow cytometers and laser dissection equipment will allow the isolation and analysis of individual microbial cells. High-speed microscopes with single-molecule resolution will enable the resolution of cellular structures below the diffraction limit. Multimodal instruments, including a combined NMR and confocal microscope, will reveal the metabolic and gene expression profile of cells within a community. A comprehensive data management system will be developed to link experimental conditions to the compositional analysis of cells and communities. This will enable entirely new computational approaches to be used for the analysis and simulation of microbial function.

3. **Next-generation surface science capabilities.** The need to characterize and then tailor surfaces and interfaces require unique instrumentation in materials synthesis, the ability to probe reaction *in situ* in real time, and new limits of spatial and energy resolution. To address these needs, EMSL will, over the next decade, make substantial investments in the development of:

- A suite of complementary *in situ* and real-time methods to collect high-resolution structural and chemical information, such as can be accomplished using high-resolution transmission electron microscopy with environmental cells
- Combined spectroscopy and microscopy for three-dimensional analysis of structures, including buried interfaces
- A range of unique and state-of-the-art capabilities to advance understanding of complex interfaces and surfaces. New capabilities important in this area include *oxygen plasma-assisted molecular beam epitaxy and high-throughput materials production and analysis*.



4. **Move EMSL's scientific computing to the petascale.** EMSL's high-performance scientific supercomputer is a unique capability tailored to address computational challenges in the environmental molecular sciences. The computational hardware resource science drivers that formed an integral part of the procurement of EMSL's next-generation high performance scientific supercomputer (called Chinook) were derived from EMSL's vision and science themes, solicited white papers, and a technical workshop on scientific computing held at EMSL in December 2004, which were collected in the document "Scientific Challenges: Linking Across Scales."



The next-generation supercomputing hardware, Chinook, will consist of tens to hundreds of thousands of processors, a scale that could hardly be envisioned when EMSL's premier computational chemistry code *NWChem* was conceived fifteen years ago. These huge computing resources will enable researchers to tackle scientific problems that are larger and more realistic than ever before, to include more of the complex dynamical behavior of nature, and will allow researchers to ask new and different scientific questions. However, both the changes in scientific needs and computing technology require that we also examine our software capabilities to ensure that *NWChem* and other EMSL-developed software will provide its users with the cutting-edge capabilities they need for next-generation platforms. Bringing *NWChem* to petascale platforms will be a major effort that will require a community of computational chemists, mathematicians, and computer scientists to join forces.

5.3 Fully integrate scientific computing and information technologies with experiment to accelerate scientific innovation and demonstrate the value of multidisciplinary approaches to science



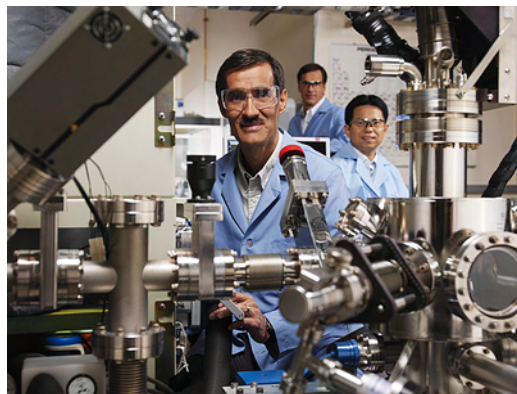
The 21st century brings a new way in which science is conducted, due, in large part, to the expansion of the internet and new technologies that enable observations of unprecedented quality, resolution and accuracy. At EMSL, we will explore new modes of conducting science that will couple, in near real time, revolutionary new experimental systems with massively parallel supercomputers, digital libraries, and unique visualization environments. These advances will make it possible to accelerate discovery and increase by orders of magnitude the levels of complexity open to exploration and experimentation.

Evolving in parallel with these new capabilities are different ways of working across science disciplines. Increasingly, scientific discovery involves the expertise of individuals from different disciplines, and often from different nations, who work together to address the complexity of today's challenges. The need for multidisciplinary science has made collaboration a centerpiece of the science enterprise. At EMSL, we will demonstrate the value of integrated multidisciplinary science by focusing our user program on the integration of computing and experiment, and through focused calls for proposals and scientific grand challenges.

5.4 Ensure EMSL's workforce meets the scientific challenges of the future

People are EMSL's most important resource. 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. Key to achieving these goals is creating and maintaining a quality work environment

that enables staff to feel valued and to work in a highly productive mode. As we move forward, we must provide the tools, support, and resources that enable staff to develop their careers to the fullest extent possible. We will focus on creating a work environment that enables highly engaged staff to work with passion, to drive innovation, and to move the organization forward toward higher levels of scientific productivity. Key to these actions are active participation in PNNL's Scientist and Engineering Development Program and EMSL Intramural Research Program.



5.5 Create partnerships across the Department of Energy, National Science Foundation, National Institutes of Health, and other user facilities and targeted universities

EMSL currently enjoys several partnerships with the NSF, including the NSF-sponsored Environmental Molecular Science Institute and a new PNNL/NSF collaborative program that provides supplemental awards to NSF grantees to support travel for graduate students, postdoctoral fellows, and staff to EMSL. NSF's Integrative Graduate Education and Research Training Grant programs at collaborating universities bring students to EMSL for advanced scientific training, as do traditional grants from other agencies.

In addition, a partnership with NIH's Proteomics Research Resource for Integrative Biology will extend EMSL's base of

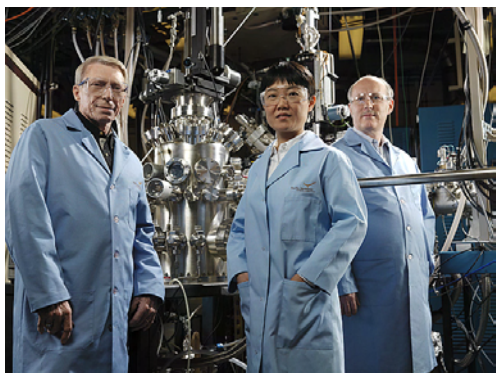


high-impact users as well as attract students and postdoctoral fellows to EMSL for advanced education and training in molecular science. Finally, strategic partnerships with universities, such as the University of Washington in nanoscience and technology and the Oregon Health Sciences University in applied biosciences, serve to further expand EMSL's user base.

EMSL will build upon these partnerships and develop new collaborations across agencies, organizations and corporations, identifying common goals that can drive scientific and technological innovation. We will work across agencies to identify opportunities for co-investment in new discovery-class tools. We will establish programs that facilitate long-term collaborations between distinguished scientists and young researchers using EMSL.

5.6 Attract and engage users in EMSL's long-term strategy

Highly engaged, satisfied users are a hallmark of a successful user facility. EMSL's goal is to attract and foster a user community that is engaged beyond the user's individual research efforts. This will enable us to more effectively involve the user community in EMSL's future directions as well as build advocacy for EMSL and user facilities broadly.



Attracting high-profile scientists as users will enhance EMSL's scientific reputation, increase its visibility, and appeal to the scientific community. Through their research activities and collaborations at EMSL, these high-profile users will help further develop the distinctive scientific areas for which EMSL is known. Additionally, these users will bring to EMSL mentoring and scientific collaboration opportunities for early-career staff and users.

In addition, EMSL needs to continue to foster collaborations with PNNL researchers—PNNL is rich with scientific expertise and technology development abilities. Promoting collaborations among EMSL and PNNL researchers will enable new capability development through joint grant proposals and more efficient use of PNNL-wide resources and intellectual pool—resulting in strengthening both EMSL and PNNL.

Engagement of the user community (both external and internal) in the long-term planning for EMSL is vital to our success. To that end, EMSL has established programs aimed at attracting and engaging its user community.



- **Wiley Research Fellow Program**—recognizes users who make significant contributions to the EMSL user program above and beyond their research involvement.
- **Wiley Distinguished Visiting Scientist Program**—recognizes and encourages distinguished scientists to come to EMSL and make significant contributions to the EMSL user program as well as provide input to and recommendations on the path forward for EMSL.

5.7 Build a research infrastructure that meets emerging scientific needs

As EMSL moves to build new transformational tools that push the limits of sensitivity and resolution, probe dynamic processes and examine materials in complex native environments, new challenges in infrastructure requirements will emerge. Tight controls on vibration, electromagnetic, and thermal parameters will be required. Networking and cyber requirements will be required to enable the close collaboration of individuals between distant locations. Laboratory environments that allow for the study of radiological materials in native and simulated environments are needed. To address these needs, EMSL has established a long-term vision for future facility enhancements.

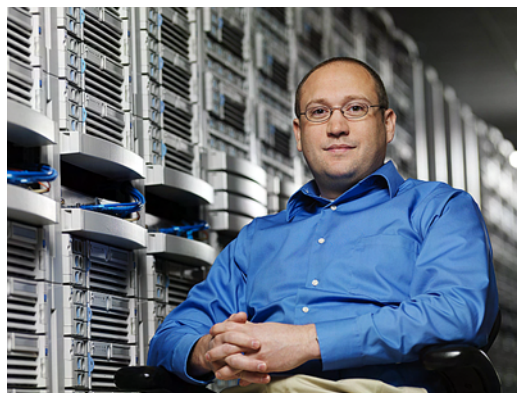
Radiological Annex. Access to specialized equipment for the study of radiological materials is in decline nationwide, and a user facility with these capabilities would provide an important resource to scientists

throughout the country. In addition, providing training for the next generation of radiochemists and associated nuclear sciences is important to the long-term mission of DOE. Expanded radiochemical capabilities in EMSL would provide these opportunities and allow contribution of high-quality science to areas of importance to DOE's mission. The EMSL Radiological Annex will support enhanced research and radiological actinide capabilities via a complement of unique research capabilities housed in the annex. The annex is planned to be physically separate from the EMSL facility, thus isolating radiological activities, and relying only on the main EMSL facility for support infrastructure such as compressed air, nitrogen, and electrical power. This annex is being proposed at \$4.9 million with an expected completion date of FY 2010.

EMSL Quiet Wing. The Quiet Wing will support future capabilities within EMSL that require tight controls on electromagnetic interference, vibration and thermal tolerances. The new Chemical Transmission Electron Microscope, planned for arrival in early FY 2009, will require space of this nature as will future planned investments such as NanoSIMS and other microscopes.

South Electrical Plant. The south electrical plant will support current and future supercomputer capabilities within EMSL. The major need for power and cooling is driven by future computer needs. This \$4.9 million building is expected to be constructed by the end of FY 2011 and is being coordinated in conjunction with the PNNL campus electrical infrastructure enhancement planned with the City of Richland.

Computer Room Addition. The computer room addition will support the next-generation supercomputer, High Performance Computing System-4. The future space will lend itself to next-generation technologies of condensed computer arrangements with proper cooling and short-run cable connections, with the existing space used for other computer housing. The expansion is planned for FY 2012 and is also expected to be a \$4.9 million project.



EMSL North Addition. Long term, EMSL is looking to expand its footprint to the north to meet emerging demands. More and more environmental specifications around vibration, electromagnetic isolation, temperature, and atmospheric parameters need to be controlled within very tight tolerances. The proposed EMSL North Addition would include construction of two laboratory modules on the north end of the building with an accompanying office pod extending east. This 55,000-square-foot addition is proposed to be initiated in FY 2012, with completion in FY 2014.

6.0 Translating the Plan to Action

This Strategic Plan guides EMSL's annual planning. The Annual Plan translates EMSL's mission, vision, strategic outcomes and critical actions into tactical actions. Implementation of this Plan is the responsibility of EMSL's Director, Associate Directors, Chief Officers and internal groups responsible for planning and performance. Individual performance appraisals will measure staff accountability and alignment with organizational goals, while annual metrics will track our progress.

6.1 Annual planning process

This Strategic Plan is EMSL's template for achieving our vision of simultaneous excellence in all aspects of our mission as a national scientific user facility. It provides the foundation for EMSL's annual planning, budget, and performance assessment processes and documents. Through our annual planning process, we solidify the objectives, measures, and targets that will guide our work during the next several years.

6.2 Making investment decisions

Based on our strategic outcomes, EMSL management identifies key areas for future investment by balancing a variety of concurrent and equally important factors. These areas may reflect emerging opportunities, address pressing challenges, or responding to critical needs. They may require sustained levels of investment over many years, or they may be more narrowly focused and change from year to year. Proposed investments will be evaluated against this matrix of considerations.



Alignment: Alignment with EMSL's mission, vision, and goals. Deciding factors include whether investments lie within the bounds established by the EMSL Strategic Plan, effectively address multiple goals, and do not duplicate the efforts of other institutions.

Impact and Transformation: Promote ideas that are intellectually compelling, innovative and transforming. Deciding factors include the extent to which investments may transform a field of science; are broadly significant or of great interest to DOE; position EMSL at the forefront of an emerging field; contribute to national research and development priorities; or enable scientifically important outcomes.

Budget: Balance investments with funding levels. Deciding factors include whether the proposed level of investment is commensurate with opportunity, level of risk, relevance, and potential impact.

Leveraging Collaborations: Create opportunities for collaboration. Deciding factors include whether investments augment other DOE activities; leverage other community or federal agency investments in research and infrastructure; and broaden participation in EMSL's user program.

Urgency and Readiness: Capture timely opportunities. Deciding factors include whether timing is critical to achieve optimum results, or investment is necessary to maintain long-term stability and progress in critical areas.

6.3 Performance and assurance management

EMSL uses a model for performance management and assurance, which aligns governance, management, and performance functions within EMSL.

- Governance – Set Strategic Direction.** Governance, consisting of EMSL senior management, with input from EMSL’s advisory committees, PNNL senior management and DOE, sets the direction of EMSL, aligns resources with goals, approves operational and business boundaries, and monitors progress.
- Management – Translate Strategy into Tactics.** Management translates goals into tactical objectives, deploys resources to achieve the objectives, manages within risk limits, and provides feedback to governance on performance. With direction on strategy, they develop tactical objectives within EMSL’s work plans to align resources to goals. After governance approval, management deploys resources to execute business plans and monitors performance, providing regular feedback to governance.
- Performance – Conduct the Work.** Staff use processes, procedures, and tools to perform day-to-day activities to accomplish tactical objectives, while managing within established operational limits.



Assurance Processes Validate Performance. Governance employs means such as internal audits and assessments, independent oversight, peer reviews, and benchmarking to provide reasonable assurance that goals are being achieved within approved operational boundaries. Self-assessments are used 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. Assurance is also used to verify that our users are being provided high-quality products and services.

EMSL measures the effectiveness of defined plans and strategies, operations, and overall organization health, and drives improvement through our performance management process. Each fiscal year, EMSL management develops an annual Performance Management and Assessment Plan with associated Dashboard that evaluates and tracks performance against defined goals, objectives, and metrics across EMSL line organizations and management systems. Assessments and evaluations are performed using self, independent, internal, and external assessments, audits, and reviews (including peer review of research results). Outcomes of these processes are used 1) to perform strategy development and management decision making and 2) to identify and enable improvement.

6.4 Strategic timeline and resource requirements

Critical Action	As measured by	1-2 YEARS	2-4 YEARS	Steward
Establish scientific leadership in EMSL's science themes	Total and top 10 publications SAC ad hoc reviews	SAC as hoc review of each science theme (1 per year)		Chief Scientist
		Assess Aerosol science theme		
		Deep Dive new Science Themes area		
Develop and deploy transformational scientific capabilities to the scientific user community	New capabilities	FTICR (CD0 in FY09)		Chief Technology Officer
		Make decision on NanoSIMS		
		2nd recapitalization workshop		
		SFG/SHG		Science Lead for Biology
		Build and deploy STORM		
		Build and Deploy SMERF		AD Enabling Technologies
Integration of computing with experiment	Proposals and publications with integrated capabilities	Call for proposals that focus on integration		User Support Specialist
Create partnerships		MOA with NHFMF		EMSL Director
		Travel funding from NIH for users	Co-funding of next Grand Challenge	
Ensure the scientific leadership meets the challenges of the future	New senior hires Awards and recognition First Authorship	Hire SFG/SHG lead		Associate Directors
		Hire TEM Lead		
			Hire NMR Lead	
Attract and engage users in EMSL's long-term strategy	Distinguished Users	Appoint 6 Wiley Fellows	Appoint 6 Wiley Fellows	EMSL Director
		Award 2 Wiley Visiting Scientist	Award 2 Wiley Visiting Scientist	
Build a research infrastructure that meets emerging scientific needs		Rad Annex		Chief Operations Officer
		Q Wing		
			South Electrical Plant	
			Data center Expansion	