ENVIRONMENTAL
MOLECULAR SCIENCES
LABORATORY

EMSL

Strategic Plan
2014

U.S. DEPARTMENT OF
ENERGY

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Our Mission

***EMSL's mission as a national scientific user facility
is to lead molecular-level discoveries for BER and DOE
that translate to predictive understanding and accelerated solutions
for national energy and environmental challenges.***

Our Vision

***EMSL's vision is to pioneer discoveries
and effectively mobilize the scientific community
to provide the molecular science foundations
for BER research priorities and our nation's critical
biological, environmental, and energy challenges.***

Director's Message

I am proud to introduce EMSL's decadal strategic plan. The advances and approaches you will read about here represent ***our vision for leading scientific discoveries that address significant global challenges in biology, environment, and energy***. Our vision reflects EMSL's commitment to leadership in molecular sciences, providing transformational discoveries for our sponsor, U.S. Department of Energy's (DOE) Office of Biological and Environmental Research, and cultivating novel methods of engaging the scientific community to harness the combined strengths of our users, our capabilities (staff, facilities, and instrumentation), and additional resources from DOE's system of scientific user facilities.

Our vision is shaped by major energy and environmental challenges facing DOE and our nation. These challenges defy efforts of a single discipline, a single institution, or a single capability. Our strategy draws together members of the scientific community and assembles resources and expertise necessary for each research problem. In service to and in partnership with our users and sponsors, we will apply this strategy to several energy and environmental "grand challenges"–those that require sustained vision, leadership, and world-class tools and talents of a national scientific user facility. As we discuss in the pages that follow, these grand challenges include efforts to understand foundational principles for predictive biodesign; impacts of aerosols and terrestrial systems on climate change; make clean, affordable, abundant energy a reality; and clean up our legacy wastes. In each of these challenge areas, a deep understanding of critical molecular-level processes is a necessary precursor to a predictive system-level understanding that accelerates environmental and energy solutions for our nation.

Addressing these challenges will also require clear understanding across a wide span of temporal and spatial scales. Today, science and technology must be integrated as never before to allow us to take full advantage of our unprecedented abilities to observe, simulate, and interpret phenomena at the molecular scale and relate them to larger complex systems from a single cell to the earth system. EMSL plays a unique role in the community in this regard, with its already distinctive capabilities and access to multiple suites of experimental and computational tools that allow scientific teams to experimentally test hypotheses, develop and run numerical models, and validate predictive simulations. New concepts, facilities, and instrumentation that push the limits of resolution, detection, identification, and quantification are required and must be pursued and developed in order to realize our aspirations.

This 10-year plan presents the challenges we will undertake, lays out aggressive goals, and charts a path for realizing our vision and goals. We are excited about EMSL's future and look forward to continuing to address scientific problems of consequence for the nation and the world.

Allison A. Campbell, Ph.D.
EMSL Director

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1.0 Introduction

The Environmental Molecular Sciences Laboratory (EMSL) is a U.S. Department of Energy (DOE) Office of Science (SC) Office of Biological and Environmental Research (BER) national scientific user facility with a vision to pioneer discoveries and effectively mobilize the scientific community by providing molecular science technologies for BER research priorities and our nation's critical biological, environmental, and energy challenges.

These scientific challenges include:

- Gaining systems-level knowledge of genomes to functional translations in cells to underpin a predictive understanding or redesign of metabolic processes for sustainable bioenergy and environmental purposes
- Understanding fundamental molecular-scale properties of natural and anthropogenic inputs to improve predictions of key atmospheric and environmental processes (**Figure 1.1**)
- Designing and characterizing new catalytic materials for improved energy storage and conversion (including biomass) processes to make clean, affordable, and abundant energy a reality.

To execute against these scientific challenges it is critically important to:

- Build EMSL's scientific leadership and impact, while advancing EMSL's molecular science capabilities and accelerating development and utilization for breakthrough science
- Develop effective and productive partnerships with other BER and SC national scientific user facilities, universities, other national laboratories, and industry in order to leverage the broadest set of capabilities across the nation to advance our scientific agenda
- Execute our user program with distinction through efficient, safe, and secure operations and management.

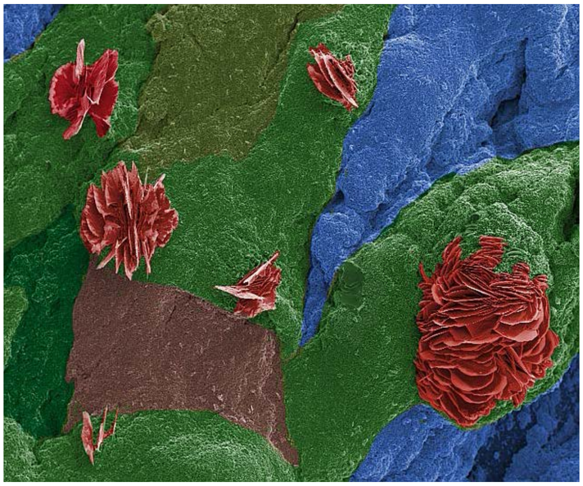


Figure 1.1. EMSL and Pacific Northwest National Laboratory (PNNL) researchers study how dust in the atmosphere can react with acids and the impact on rain and snow fall.

EMSL users and scientists are conducting groundbreaking research to address these scientific challenges. By connecting the scientific user community through our suites of scientific expertise, state-of-the-art equipment, and mission-ready facilities, EMSL provides a one-stop shop that enables and accelerates problem-solving beyond what is possible in a typical university, industrial, or even single national laboratory setting.

Our approach is to focus on compelling scientific questions in our four science themes and associated leadership areas (**Figure 1.2**) by coupling EMSL's capabilities (defined as a combination of world-class expertise, state-of-the-art equipment, and mission-ready facilities) with those of the scientific community. Each science theme was specifically developed to respond to the critical biological, environmental, and energy challenges articulated above. The science themes provide a framework and strategic direction for critical investments for innovative research as well as prioritization of user access. The leadership areas are specific areas where EMSL has sustained vision and leadership to create scientific breakthroughs that will substantially impact national priorities.

Figure 1.2 also shows the eight EMSL capability areas–each one is a powerful combination of scientific expertise, advanced (and often unique) instrumentation, and specialized laboratory space. EMSL's ability to integrate across these capabilities is also distinctive and provides leadership to the scientific community in specific scientific domains; for example, in radiochemistry, integrated omics, and dynamic and *in-situ* imaging. These domain areas have been specifically selected to create a comprehensive molecular science tool suite that supports our science themes and leadership areas.

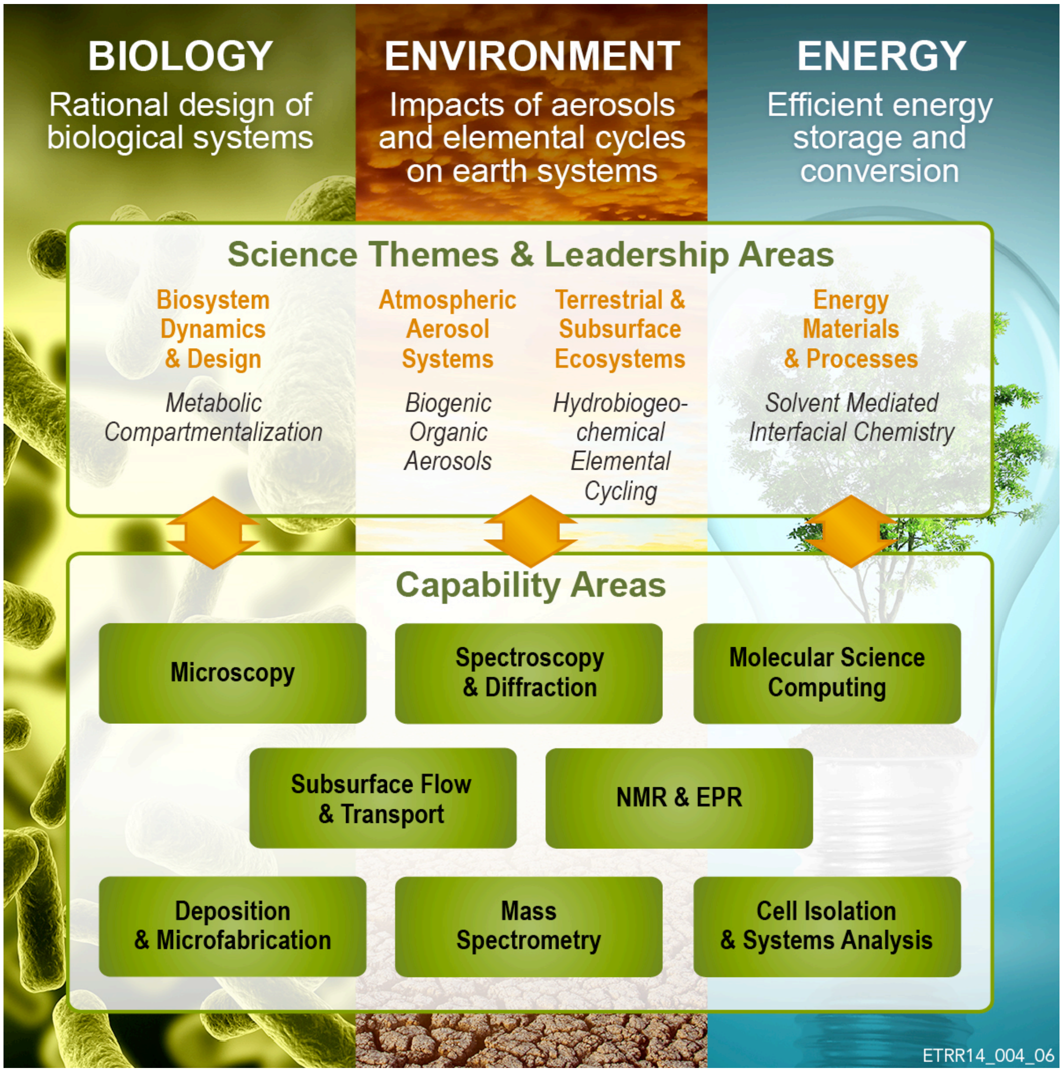


Figure 1.2. EMSL's science themes and leadership areas are focused on critical science challenges in biology, the environment, and energy. EMSL's eight capability areas are essential to meeting these challenges, and are unique in the world as a mix of capabilities found in one place.

As we evolve EMSL into the next generation molecular science user facility, we will invest in continued advancement of our capabilities to provide leadership to the scientific community. We will also develop new capabilities that integrate across our science themes. For example, the addition of a plant science phenomics component to the EMSL research portfolio will extend our leadership in integrated omics and build upon the Biosystem Dynamics and Design (BDD), Terrestrial and Subsurface Ecosystems (TSE), and Atmospheric Aerosol Systems (AAS) Science Themes in the context of carbon cycle interactions and dynamics.

To achieve our vision for EMSL, we must accomplish three strategic objectives:

1. Advance EMSL's scientific leadership, impact, and alignment to BER/DOE scientific missions through our science themes and leadership areas (EMSL Strategic Objective 1)
2. Advance EMSL's capabilities (a combination of world-class expertise, state-of-the-art equipment, and mission-ready facilities) and accelerate their utilization for breakthrough science (EMSL Strategic Objective 2)
3. Maintain an engaged and productive user community through sustained excellence in operations and management, including outreach and the user experience (EMSL Strategic Objective 3).

1.1 Alignment with DOE and Office of Science Strategies

EMSL's strategic plan is fully aligned with DOE's strategic plan [1]. (**Figure 1.3**) At the highest level, the work conducted at EMSL primarily supports DOE Strategic Objective 3:

Figure 1.3 U.S. Department of Energy Strategic Plan 2014-2018

DOE Strategic Objective 3–Deliver the scientific discoveries and major scientific tools that transform our understanding of nature and strengthen the connection between advances in fundamental science and technology innovation.

In addition, the work conducted by EMSL users and scientists also contributes to aspects of several other DOE Strategic Objectives, including:

DOE Strategic Objective 1–Advance the goals and objectives in the President's Climate Action Plan by supporting prudent development, deployment, and efficient use of "all of the above" energy resources that also create new jobs and industries

DOE Strategic Objective 2–Support a more economically competitive, environmentally responsible, secure and resilient U.S. energy infrastructure

DOE Strategic Objective 8–Continue cleanup of radioactive and chemical waste resulting from Manhattan Project and Cold War activities.

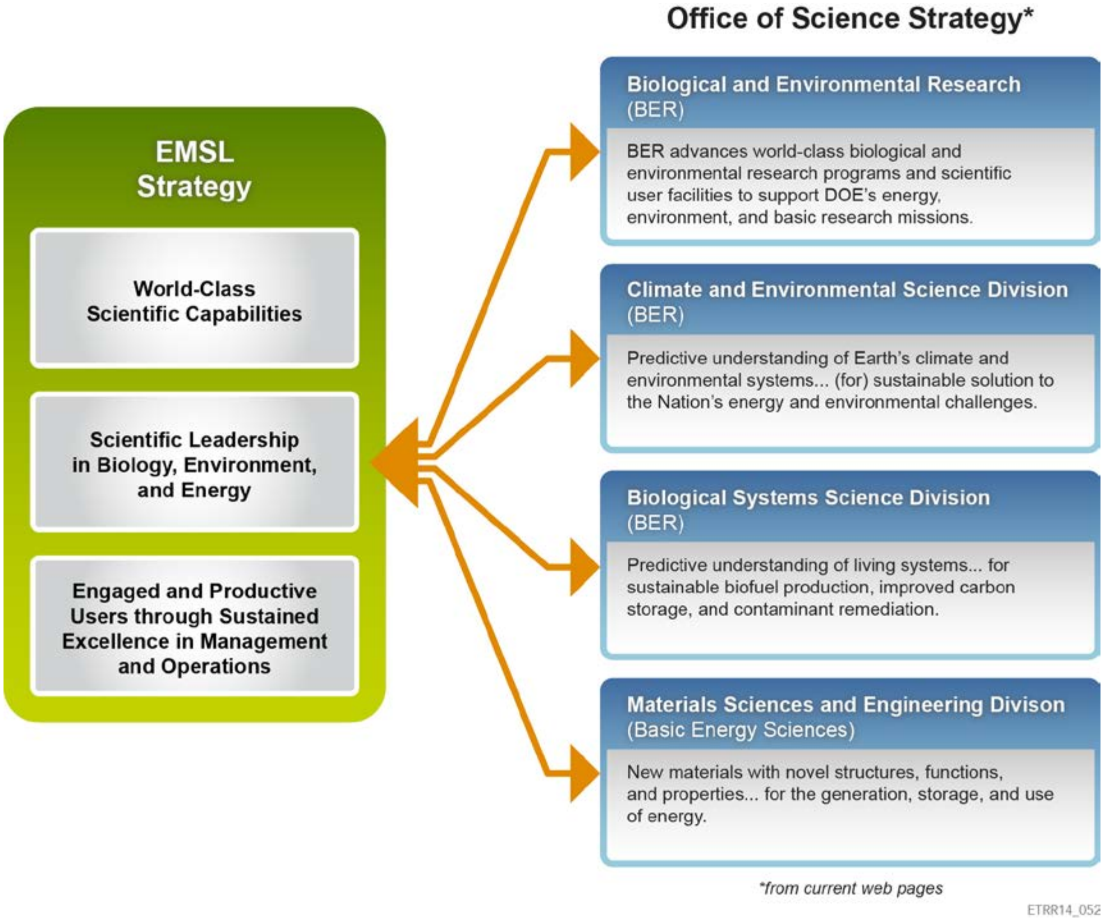
EMSL also is closely aligned with strategic goals and objectives of the Office of Science. **Figure 1.4** shows the alignment of EMSL's strategic objectives with the relevant goals and objectives of BER and BES as stated on their public websites [2-5]. These statements are also consistent with priorities stated in the President's FY 2015 budget submission [6]:

Biological and Environmental Research (BER) "Fundamental research and scientific user facilities to achieve a predictive understanding of complex biological, climatic, and environmental systems for a secure and sustainable energy future."

Climate and Environmental Science Division (BER) "Role of Earth's biogeochemical systems (atmosphere, land, oceans, sea ice, subsurface) … to predict climate … and inform … future energy and resource needs."

Biological Systems Science Division (BER) "How genomic information is translated into function … redesign of microbes and plants for sustainable biofuel production, improved carbon storage and … biological transformation … of nutrients and contaminants in the environment."

Basic Energy Sciences "Understand, predict, and ultimately control matter and energy at the electronic, atomic, and molecular levels … for new energy technologies and to support … energy, environment, and national security."



BER advances world-class biological and environmental research programs and scientific user facilities to support DOE's energy, environment, and basic research missions.

Predictive understanding of Earth's climate and environmental systems... (for) sustainable solution to the Nation's energy and environmental challenges.

Predictive understanding of living systems... for sustainable biofuel production, improved carbon storage, and contaminant remediation.

New materials with novel structures, functions, and properties... for the generation, storage, and use of energy.

**from current web pages*

Figure 1.4. EMSL's strategic goals and objectives are closely tied to BER and BES

This strategic plan is a living document. We will continually evaluate changing needs and opportunities posed by our stakeholders (i.e., BER, our scientists and users, and our advisory committees), work closely with them to understand and respond to those changes, and execute against our strategy accordingly.

1.2 Organization of This Strategic Plan

This document (**Figure 1.5**) is organized as follows: Section 2 briefly articulates the three critical biological, environmental, and energy challenges listed above, along with the science themes and leadership areas central to EMSL Strategic Objective 1. Included in this is a discussion of the rationale behind each challenge, the technical approach, why EMSL is well positioned to take on this challenge, and metrics by which success of each effort will be judged. Section 3 describes EMSL's capabilities, along with plans for their advancement and accelerating their use, supporting EMSL Strategic Objective 2. Section 4 discusses EMSL's vision for excellence in operations and user experience and EMSL Strategic Objective 3. A set of critical actions that support the vision and strategic objectives are in Section 5. Section 6 concludes with EMSL's commitment to translate the plan into action, with specific management processes included in the discussion to support that commitment.

The appendices contain supplementary materials. Appendix A contains a physical description of the EMSL facility. Appendix B contains the science theme implementation plans. Appendix C contains a capability development and implementation plan. Appendix D contains a summary of progress against the strategic objectives from the EMSL 2008 and draft 2011 strategic plans.

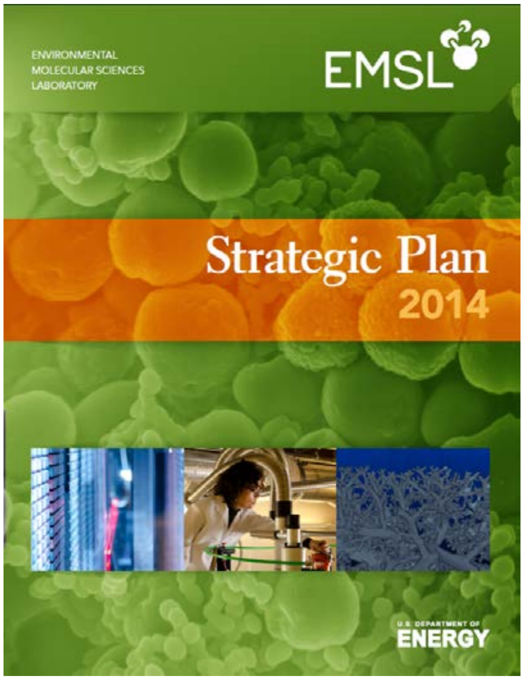


Figure 1.5. EMSL's Strategic Plan 2014

2.0 EMSL Leadership in Biology, Environment, and Energy

Science programs that are supported by BER and SC focus on understanding and providing sustainable solutions to the increased demand for energy worldwide. This demand affects the environment and climate while strengthening the need for clean alternative energy sources and superior energy storage strategies. Research projects supported by BER have a long history of both measuring and predicting biological and environmental impact of energy production and use on the environment and understanding the interplay of climate and energy. Over the next 10 years, scientific research at EMSL will be sharpened to focus on advancing the predictive understanding of key components of environmental, biological, and energy systems. Specifically, we will focus EMSL resources on the following three critical scientific challenges:

Biology

- **Understand the foundational biological principles for predictive biology.** Gaining systems-level knowledge of genome-to-functional translations in cells. Characterizing and analyzing, at the systems-level, cells, cell constituents, cell organization and processes to underpin a predictive understanding or redesign of metabolic processes for sustainable bioenergy and environmental purposes.

Environment

- **Understand the role of natural and anthropogenic inputs to climate, ecosystem, and earth-system processes.** Understanding fundamental molecular-scale properties of natural and anthropogenic inputs to improve predictions of key atmospheric and environmental processes. Measuring and analyzing fundamental molecular-scale properties of natural and anthropogenic inputs to improve predictions of key atmospheric and environmental processes.

Energy

- **Understand and control interfacial and molecular processes needed to design new materials for sustainable energy.** Designing and characterizing new catalytic materials for improved energy storage and conversion (including biomass) processes to make clean, affordable, and abundant energy a reality.

We have chosen to focus on these scientific challenges because they represent tremendous national needs and they align with BER and SC priorities. Most importantly, EMSL and its host laboratory, PNNL, have strength and depth (both scientific and operational) to address significant elements of these challenges, and our culture of a problem-solving multidisciplinary approach will accelerate meaningful progress. At the same time, it is not our intent to focus on these challenges to the exclusion of other important work that we and our users pursue using EMSL resources; rather, we will advance our overall impact by building scientific leadership in these areas, with benefits to our broader portfolio.

Within each of these scientific challenges we have chosen specific science themes and leadership areas (**Figure 1.2**). The science themes provide a framework and strategic direction for critical investments for innovative research, the development of innovative capabilities to support that research, and the prioritization of user access. The leadership areas are where EMSL has sustained vision, leadership, and world-class capabilities of an integrated molecular science national scientific user facility to create scientific breakthroughs with substantial impact to national priorities.

Our science themes and leadership areas, their 10-year goals, and metrics of success are outlined in **Table 2.1** (at the end of this section) and described in detail below. To maximize impact of these efforts, we have established aggressive goals, outlined paths and measures for ensuring success, and articulated why and how the EMSL user program will lead efforts to accomplish these goals. Through this strategy, EMSL scientists and users will have sustained scientific impact and will be at the center of a national and international network of scientists, capabilities, and facilities that is providing important and relevant solutions to challenges facing the nation.

2.1 Scientific Challenge in Biology: Understand the Foundational Biological Principles for Predictive Biology

Science Theme: Biosystem Dynamics and Design **(Figure 2.1)**
Leadership Area: Metabolic Compartmentalization

10-year Goal: *Integrate molecular-scale structural information to characterize the nature, distribution, and variety of biological compartments, structures, and networks such as lipid particles and peroxisomes in plants, fungi, and the carboxysome in cyanobacteria.*

Success Metric: *Demonstrated the use of spatial and temporal metabolic pathway information for understanding the bases for, and improvement of, biofuels and bioproducts production by microbes, fungi, and plants.*

A recent BER workshop on Biosystems Design [7] concludes that research elucidating the biological sources of cell operations and behaviors would inform the "redesign" of biological systems in support of BER missions in biofuels and bioproducts and for carbon cycling by microbes and plants. Source-sink interactions in plants constitute a highly intra- and inter-cellular compartmentalized process, to a large extent controlled by transporters and sugar signaling. To lead the development of predictive biology, EMSL will enable understanding of the spatial organization and functional characteristics of eukaryotic organelles and bacterial microcompartments that are needed to significantly increase production and control of desired biomolecules. For example, *in-situ* studies at EMSL of spatial and temporal changes to metabolism in microbial communities, the dynamics of bacterial microcompartments organelle formation and function will increase our understanding and enable new approaches for

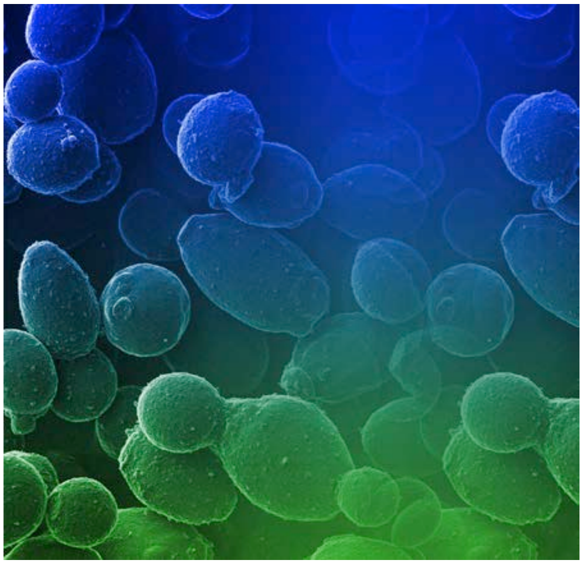


Figure 2.1. The BDD Science Theme focuses on regulation of spatial and temporal parameters of metabolic processes in microbes, fungi, and plants to advance systems biology for bioenergy and biorenewables.

optimizing microbial consortia and redesigning organisms for optimized or novel metabolic applications [8, 9]. To enable prediction, users must be able to model and simulate the current biological complexity of specific systems.

Compartmentalization establishes conditions that make metabolic and other cellular processes more efficient than they would be otherwise [7]. Moreover, the thermodynamic potential, determined by the redox state of the cell, is a crucial factor in determining whether reduced carbon compounds can be synthesized from precursors that are at a higher oxidation state. Modeling is required for using information from systems biology to facilitate synthetic biology, yet relatively few models include spatial localization. Of the few that do, many are flux-based models of metabolism, which are valuable for initial estimates of activity of metabolic pathways if growth rates and biomass measurements have been made. However, the real need is for models that can predict biomass production and growth rates. EMSL in combination with others at PNNL have capabilities to accomplish dynamic and thermodynamic modeling of redox processes, including spatio-temporal localization.

EMSL's Scientific Leadership

EMSL will serve as a hub for advancing biology that supports BER mission areas by working with users to generate omics and bioimage data with spatial and temporal information related to the genesis of cellular compartments and their associated metabolic pathways. These data will be used to develop new and modify existing metabolic models for microbes and plants involved in nutrient cycling and biofuel, and bioproduct production.

Figure 2.2. Once online, the 21T FTICR mass spectrometer will enable near-unequivocal identification of molecular constituents, and interactions and transformations in complex natural samples including soil organic matter (SOM), atmospheric organics, biofuels, and microbial community proteomes.

EMSL is a pioneering leader in proteomics with the High-Resolution Mass-Accuracy Capability known as the HRMAC project. Our 21 Tesla Fourier-Transform Ion Cyclotron Resonance (FTICR) mass spectrometer (to be known as the 21T FTICR mass spectrometer once it is online) will enable "top-down" proteomics of large complex proteins and protein complexes. (**Figure 2.2**) EMSL is also host to multiple mass-spectrometry-based imaging approaches that generate spatial information for a variety of molecules. Additionally, EMSL expertly characterizes primary mechanisms that regulate cell activities, including gene transcription (into mRNA), mRNA translation (into protein), and protein modification, with planned extension to single cells that will be key to addressing cell heterogeneity.

Measurements of metabolite levels (metabolomics) and locations as well as rate of change (fluxomics) also provide critical data to test and refine predictive models of plant and microbial metabolism (both single-cell models and community models). New metabolomics capabilities are needed and have been identified in Science Theme Advisory Panel (STAP) meetings [10]. EMSL's plans for strengthening both nuclear magnetic resonance spectroscopy (NMR) and MS metabolomics capabilities, in addition to the accompanying data and informatics needs, are described in Section 3.3. EMSL's ability to generate spatial information is also critical for understanding where the different components of the regulatory system are located and how they change with time. The development of the Dynamic Transmission Electron Microscope (DTEM) and our proposed ultrafast microscopy capability will enable dynamic *in-situ* observation of cellular systems and their components at near atomic spatial resolution and nanosecond time resolution (see Section 3.3).

Moving into the future, EMSL plans to extend our leadership in integrated omics to plant sciences, developing the ability for high-throughput phenotyping of plant traits and chemistry. The ultimate goal of this research is the development of a prognostic model of plant growth, performance, and composition as a function of genotype and environment. This is a knowledge base urgently needed for research, for applications on sustainable and resource-efficient crop production in the context of climate change and changing agricultural production, and for comprehensively predicting effects on plant performance in synthetic biology approaches.

Finally, understanding systems-level regulatory processes requires computational models and the infrastructure to collect, convert, and integrate data into a form suitable for model building and testing. Because of the extremely large volumes of data involved, as well as the complexity of the models, EMSL's scalable data storage, software, and high-performance supercomputing capabilities are needed. The planning process for EMSL's next generation of supercomputing hardware includes evaluation of design features needed for metabolic modeling and bioinformatics. EMSL will continue to work with users from both academia and industry to develop new approaches to metabolic modeling with the goal of moving biology from qualitative and descriptive to quantitative and predictive.

2.2 Scientific Challenge in the Environment: Understand the Role of Natural and Anthropogenic Inputs on Climate and Subsurface Systems

In this challenge we focus on processes both above ground and below ground. Above ground, our AAS Science Theme focuses on scientific studies that target biogenic aerosols, while below ground, our TSE Science Theme focuses on hydro-biogeochemical elemental cycling.

Science Theme: Atmospheric Aerosol Systems **(Figure 2.3)**
Leadership Area: Controllable Biogenic Organic Aerosols

10-year Goal: *Develop a molecular-scale understanding of the processes that enhance Controllable Biogenic Organic Aerosol (CBOA) formation and determine their radiative properties to improve the accuracy of climate model simulations.*

Success Metric: *Developed a quantitative molecular-scale understanding of the processes controlling Biogenic Volatile Organic Compounds (BVOC) emission, anthropogenic enhancement of biogenic organic aerosol, brown carbon and ice nucleation that reduces the related uncertainties in climate model simulations by 50 percent.*

One of the greatest challenges to accurately predicting regional climate change on decadal timescales is quantifying the role of human activities in enhancing Secondary Organic Aerosol (SOA) formation from BVOC emitted by terrestrial ecosystems. There is growing evidence that anthropogenic pollution greatly enhances the production of SOA from BVOC and thus this organic aerosol can be controlled by reducing anthropogenic emissions. We refer to the ultimate products as CBOA and considering the large contribution of organic aerosol to the total aerosol burden, we must understand their mechanisms of formation and determine their radiative properties to improve the accuracy of current climate model simulations. Incorporating a molecular-scale understanding of the production and radiative characteristics of aerosols and how they change throughout their life cycle would significantly reduce uncertainties in current climate simulations and would transform our ability to develop accurate predictive global climate models.

On a global scale, the dominant source of organic aerosol is BVOCs emitted from terrestrial ecosystems [11]. Through their atmospheric oxidation reactions, these contribute more than half the mass of all airborne particles, are physically and chemically complex [12], significantly impact key climate processes, and represent an important influence on climate that is not adequately accounted for in climate model simulations [13]. To incorporate quantitatively the effects of CBOAs on climate requires appropriate parameterization of their production in terrestrial ecosystems, atmospheric transformations, chromophoric properties, and influence on clouds. The development of model algorithms that can use these parameters is critical to quantitatively incorporate such information into climate system models. Conceptually, the potential linkages and feedbacks among ecosystem-atmosphere organic fluxes, CBOA formation, and the influence of temperature and precipitation on all these processes are obvious. Yet there are major gaps in understanding how these processes and feedbacks control the fundamental molecular-scale properties of BVOCs and CBOAs, as well as how to link this molecular-scale knowledge to the mesoscale characteristics and behavior of such atmospheric components [12].

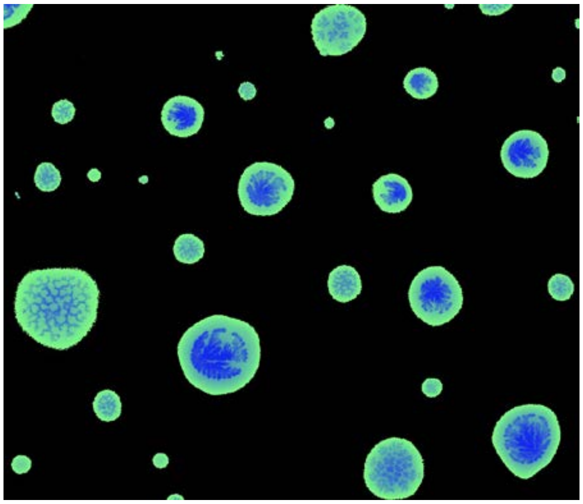


Figure 2.3. The AAS Science Theme focuses on chemistry, physics and molecular-scale dynamics of aerosols to improve accuracy of climate model simulations and develop predictive understanding of climate.

EMSL's Scientific Leadership

EMSL's scientists and users will focus on understanding and characterizing molecular-scale properties and behaviors of CBOAs by conducting both laboratory and field studies and incorporating mechanistic information and empirical constraints from these studies into aerosol and cloud model components that inform Earth System Models (ESM). Studies will be conducted with the goal of determining specific constituents of CBOA materials and processes that control CBOA precursors. The knowledge gained from these studies will be used to develop and parameterize numerical algorithms that capture the molecular-level knowledge that can be implemented to improve DOE climate model simulations of organic aerosol production, lifetime, and impacts on climate.

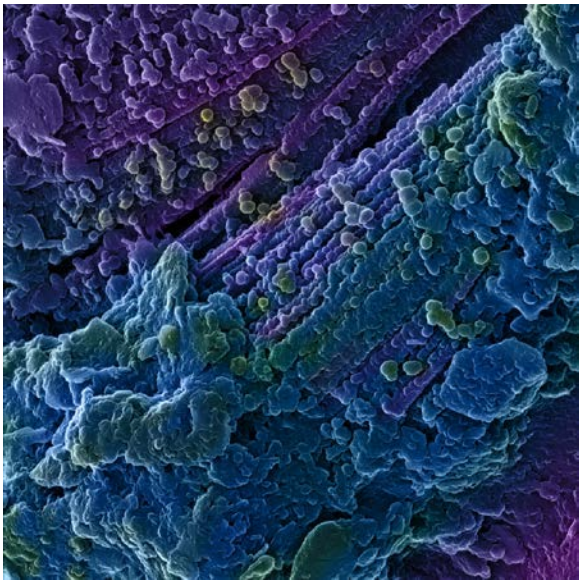


Figure 2.4. EMSL users' early research on uranium-contaminated wetlands used EMSL's helium ion microscopy in the Quiet Wing to image biogenic nano-iron oxides oriented along a root recovered from a wetland plant from the Savannah River Site.

Gathering information on the physical and chemical properties of CBOA and precursors is challenging because no single analytical method is capable of providing the full range of necessary information. Instead we will use our demonstrated ability to integrate across multiple domains to provide comprehensive information that ranges from the microscopic characterization of individual particles and cells to advanced molecular characterization of complex organic matter. The microscopes housed in the Quiet Wing are well-suited for characterizing these aerosols at high-spatial resolution and under dynamic conditions. (**Figure 2.4**) We will also complement the existing suite of in-house instrumentation with both deployable field instruments to provide fundamental observations for BER community studies, such as the GOAmazon study, and higher resolution laboratory-based instrumentation that will enable the more exact molecular identification and determination that is needed to conclusively elucidate atmospheric transformation dynamics and to validate and expand on field measurements.

There is no adequate facility in the U.S. for investigating biosphere-atmosphere interactions, including biogenic emissions and aerosol production and growth, in a chamber system that does not have significant wall effects. A chamber that would combine both plant and aerosol components into a single system has particular interest and no known precedence in other user facilities. This concept of a community aerosol and earth-system chamber, (i.e., a chamber that would enable observation, measurement, and evolution of vapors, aerosols, and particles in a controlled, monitored environment) was identified in AAS's STAP meeting in 2013 [14]. A community chamber could diminish disparities between lab and field research. Although several chambers have been built in Europe and Japan, they do not cover the entire scope of aerosol and earth-system research and do not solve key experimental concerns, such as avoiding wall effects and contamination.

EMSL scientists and users will lead the scientific community in investigating CBOA processes and accurately representing them in climate models by coupling this experimental expertise with our expertise in theoretical modeling (e.g., with NWChem simulation codes and the recently enhanced high-performance computer system). As a result, EMSL will enable complementary simulations of BVOC production and CBOA formation and transformations and the properties of organic chromophores.

Science Theme: Terrestrial and Subsurface Ecosystems (Figure 2.5)
Leadership Area: Hydro-biogeochemical Elemental Cycling

10-year Goal: *Develop a molecular-to-pore-scale mechanistic understanding of the coupled biogeochemical controls, reactions, hydrologic inputs, and elemental cycling to advance a predictive understanding of the feedbacks between the water cycle and ecosystem biogeochemistry and inform biogeochemistry components of ESMs.*

Success Metric: *Developed hierarchical models representing key hydro-biogeochemical processes (the chemical form, distribution, and transformation of soil carbon) that control elemental cycling to inform and improve the Community Land Model component of ESMs.*

Current ESMs include a terrestrial (land surface) modeling component that represents key fluxes (water, energy, carbon dioxide) across the land surface-atmosphere interface. Unfortunately, a formidable disparity exists between the temporal and spatial scales of the fundamental processes that govern carbon and water cycling at the land surface and those represented in ESMs. This mismatch results in increased model uncertainty and prediction error for carbon dynamics under changing climatic conditions. For example, it is well known that predictions of future net land carbon uptake vary widely in both magnitude and sign among various land surface models, even though those models all reasonably reproduce historical trends [15]. A critical need exists for an improved understanding of pore-scale hydro-biogeochemical processes, their behavior across ecosystem boundaries, and their connections to larger-scale phenomena.

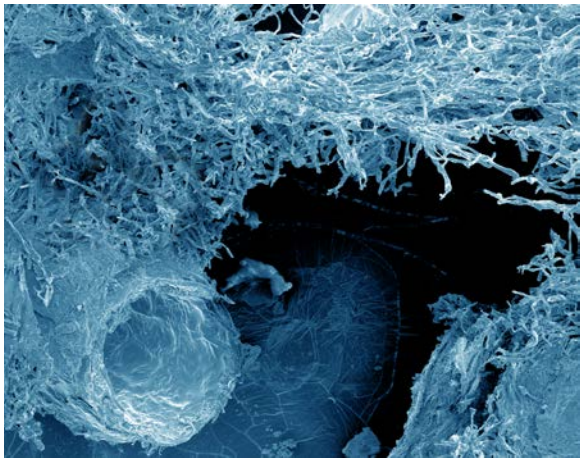


Figure 2.5. The TSE Science Theme focuses on dynamics of nutrients, metabolites, and contaminates at biogeochemical interfaces in heterogeneous environments.

Recent efforts to improve the fidelity of land models have focused on coupling them with more highly resolved reactive transport models (RTM) which can incorporate highly resolved process understanding in three dimensions. There are many examples in which molecular- and pore-scale information has qualitatively informed process descriptions in RTMs, and recently there have been several efforts to directly incorporate quantitative molecular- and pore-scale information into RTM processes [16-18]. To the extent that pore- and molecular-scale information is incorporated in RTMs, the coupling of RTMs with land models offers an avenue to impact land modeling process representations.

These same RTMs also apply directly to modeling radionuclide mobility in terrestrial and shallow subsurface environments for the remediation of legacy waste and design of waste repositories [19]. The fate and transport of radionuclides is fundamentally similar to other multivalent elements and is dependent on the interplay of a complex array of variables such as the oxidation state of the radionuclide, the reducing or oxidizing conditions of the subsurface sediments, the native microbial community, and the hydrologic characteristics of the sediments.

EMSL's Scientific Leadership

Using a systems approach, we will develop a mechanistic understanding of the complex processes that regulate biogeochemical elemental cycles and dynamics that can be used to improve information in land process models. Our research teams will include specialists from biological, geochemical, and hydrologic scientific communities and will encompass laboratory, field, and modeling studies. This collaborative framework provides an interdisciplinary, hypothesis-driven systems approach to the research. We will integrate results from molecular-scale laboratory studies and observations from field studies to inform and improve process representation in biogeochemistry components of land process models.

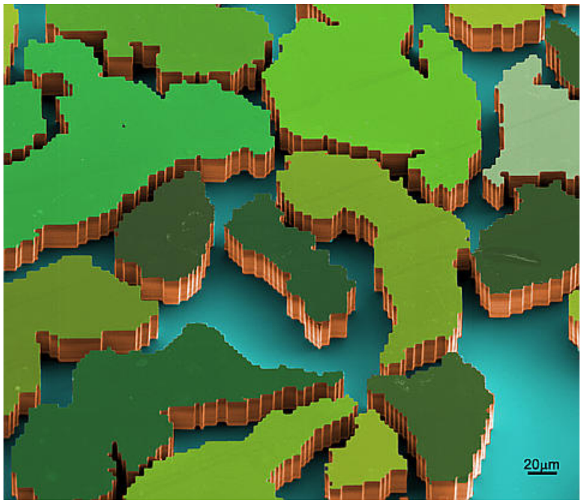


Figure 2.6. EMSL users are developing micromodels to understand multiphase flow, diffusion, and reactions processes at the microscopic scale (μm to cm) that affect the fate and transport of contaminants in the subsurface and geological sequestration of CO_2. Micro-Elecro-Mechanical Systems devices are prepared in the EMSL clean room and can aid in the development of these micromodels.

EMSL's pore-scale to intermediate experimental and modeling platforms are critical to understanding the impact of these processes on carbon dynamics, elemental cycling, and contaminant transport at larger scales. (Figure 2.6) The radiochemistry facility, known as RadEMSL, is purposefully equipped with advanced spectroscopic and imaging instrumentation to provide molecular-level chemical speciation information needed to develop mechanistic models of radionuclide chemical behavior under environmental conditions. Our development of a suite of *in-situ*, spatially-resolved chemical imaging and spectroscopic capabilities at the pore-scale and in the acquisition and interpretation of high-resolution mass spectral data on soil carbon species creates an exciting new opportunity to understand the molecular chemistry of these complex and multi-dimensional problems at the relevant spatial and temporal scales. New radiological and MS capabilities are needed to achieve these goals, including additional basic radiochemical and radioanalytical instrumentation, capabilities to enable preparation of non-dispersible samples, auxiliary equipment to fully capitalize on EMSL's radiological NMR, electronic paramagnetic resonance (EPR), and X-Ray Photoemission Spectroscopy (XPS) capabilities, and the acquisition of sensitive imaging capability for visualizing the distribution of Tc and other radionuclides in complex environmental and processing samples. These needs all derive from recommendations made by EMSL's STAPs in the TSE Science Theme [20].

2.3 Scientific Challenge in Energy: Understand and Control Interfacial and Molecular Processes Needed to Design New Materials and Catalysts for Sustainable Energy

Science Theme: Energy Materials and Processes **(Figure 2.7)**
Leadership Area: Solvent-mediated Interfacial Chemistry

10-year Goal: *Develop sufficient understanding of the dynamic and emergent processes that occur at solvent-mediated interfaces to predict the transformation mechanisms and physical and chemical properties needed to design advanced batteries and new catalysts for degradation of biomass and upgrading of bio-produced fuels and renewable chemicals.*

Success Metric: *Contributed to principles for achieving the Joint Center for Energy Storage Research (*JCESR*) goals.*

Sustained economic progress depends on secure, reliable, and affordable energy supplies. Existing approaches will not be adequate to meet the size and scope of the challenge, and a range of new technologies for producing, storing, and using energy will be required [21]. A conference report on Materials Challenges for Alternative and Renewable Energy stated, "We have no hope of solving the daunting energy requirements of the developed and developing world without new materials and chemistry that will increase capacity while simultaneously reducing environmental damage." [22]

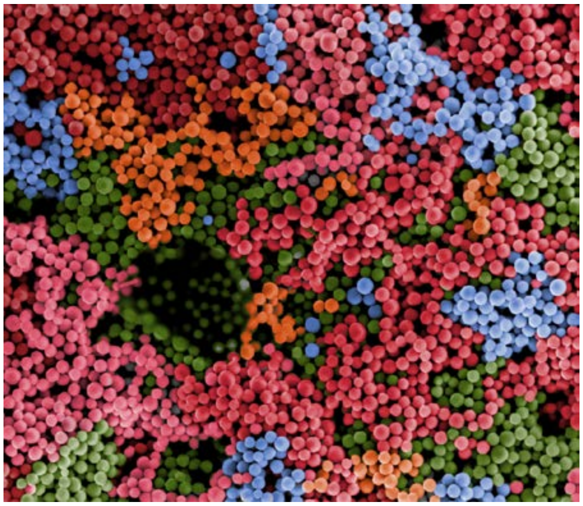


Figure 2.7. The EMP Science Theme focuses on dynamic transformation mechanisms and physical and chemical properties at interfaces in catalysts and energy materials.

Interfacial chemistry and new materials are priority research areas for battery systems where understanding charge and mass transport at interfaces, electrochemical over potential, and the nature of solid/electrolyte interactions need both advanced characterization methods and the development of predictive models [21-25]. It has been noted that improving the efficacy of catalysts for production or upgrading of biofuels or bio-derived chemicals would significantly enhance the economic viability of biofuel production [26]. BER's Bioenergy Research Centers have the technology goal of enabling sustained and viable biofuel technologies through a better understanding of the biological mechanisms underlying biofuel production [27]. Chemical catalysis can play a useful role in enhancing the quality and value of biofuel and other bioproducts.

The ability to predict solvent-mediated interfacial chemical processes is limited. Such interfaces present experimental and computational challenges and play critical roles in energy conversion and storage technologies. Although they may be expressed in different ways, solid electrolyte interfaces in battery systems, and catalysts operating in liquid environments relevant to upgrading the quality of biofuels share important scientific unknowns. These unknowns include how molecules are attached at the solvent-solid interfaces, how solvent properties alter chemical properties, and how external electrical or photo-energy impact relevant molecular interactions such as reactivity and charge transfer.

EMSL's Scientific Leadership

We plan to focus EMSL scientists and users on understanding the dynamic transformation mechanisms and physical and chemical properties at interfaces critical to the function of catalysts and energy materials. This improved understanding will enable the design of new systems for sustainable energy applications. The discovery of molecular-level information that enables the development and testing of predictive models of interfacial properties will provide the fundamental understanding needed to design and develop practical, efficient, environmentally benign, and economical energy storage and energy conversion systems. Through our engagement in the Office of Energy Efficiency and Renewable Energy's Batteries for Advanced Transportation Technologies program and the Office of Basic Energy Sciences' JCESR Hub, these predictive models can be extended to those designing next generation batteries and catalysts.

EMSL brings a unique and important suite of experimental and computational capabilities to this problem and will team with other user facilities (e.g., synchrotron light and neutron sources) to obtain additional important *in-situ* real-time information. Over the past five years, EMSL has developed electron microscopy and magnetic resonance approaches to examine solid-liquid interfaces in catalytic and battery systems. These award-winning advancements have enabled highly cited publications highlighting new types of battery electrodes and played an important role in JCESR. These methods in combination with *in-situ* mass spectrometry, "near" *in situ* and important *ex-situ* tools, provide comprehensive information needed to understand the structure and function of the relevant materials, solvents, and resulting interfaces. Multi-modal experimental and theoretical tools will be used to develop and test theoretical models at the extended length and timescales that are needed to shed light on these complex interfacial phenomena in order to obtain the desired predictive understanding for the design of new materials and systems.

To effectively understand the role of dynamic structures and processes, the Energy Materials and Processes (EMP) Science Theme STAPs [28] have recommended that EMSL build on its current strengths and continue to invest in new microscopies that provide more rapid observation and reduced beam exposure; develop an *in operando* flow reactor; develop the ability to interrogate specific catalytic sites using multi-modal techniques including computational simulation; strengthen EMSL's non-linear vibrational spectroscopy; and obtain new NMR (e.g., dynamic nuclear polarization (DNP)) and mass spectrometry (e.g., differential electrochemical mass spectrometry) capabilities.

EMSL's premier computational chemistry code, NWChem, enhanced to take full advantage of the advanced architecture of the Cascade supercomputer, provides the platform needed to model these interfaces. Enhancements are underway to allow NWChem to deal with fluctuations in charge and structure and larger relevant distance and timescales. EMSL will lead in the application of semi-empirical models to these interfaces by providing complex quantum mechanical approaches in NWChem and coupled cluster theory within the same program allowing a unique ability to test, validate, and develop new Density Functional-based Tight Binding (DFTB) parameter sets that will be important for solvent-mediated interfaces and a wide class of other systems. The coupling to accurate many-body methodologies at small and medium scales also offers the opportunity to propagate accurate high-level corrections across length scales. Within such a many-body corrected protocol we will be able to extend the applicability of DFTB methods to describe the collective behavior and emergent properties of interfaces at very large and long timescales.

Table 2.1. Summary of EMSL's Leadership Areas, 10-year Goals, and Success Metrics

Scientific Challenge	Science Theme and Leadership Area	10-year Science Goals and Metrics of Success	Key Partnerships
Biology	BDD Science Theme and Metabolic Compartmentalization Leadership Area	Integrate molecular-scale structural information, to determine principles underlying compartmentalization in biological systems, from cells to microbial communities and plants. Demonstrated the use of spatial and temporal metabolic pathway information for the redesign and improvement of biofuels and bioproducts production by microbes, fungi, and plants.	**Bioenergy Research Centers**–Bioenergy Science Center, Great Lakes Bioenergy Research Center, and JBEI **JBEI**–generating and integrating omics data into metabolic models that will inform biofuel production by microbes. **JGI**–collaborative science focused on carbon cycling biogeochemistry and biofuel production. **LANL SFA**–identifying secreted proteins from fungi to better understand dynamic processes involved in soil carbon cycling. **Iowa State**–identifying microbial community members who deconstruct and/or consume cellulose.
Environment	AAS Science Theme and CBOA Leadership Area	Develop molecular-scale understanding of processes that enhance CBOA formation and determine radiative properties to improve accuracy of climate model simulations. Developed a quantitative molecular-scale understanding of the processes controlling BVOC emission, anthropogenic enhancement of biogenic organic aerosol, brown carbon and ice nucleation that reduces the related uncertainties in climate model simulations by 50 percent.	**ARM**–molecular characterization of aerosols for field campaigns (including 2010 CARES and ongoing 2014 GOAmazon studies). Developing field-deployable instruments and novel observational approaches for the BER ASR program. Exploring mechanisms to facilitate user requests for both ARM and EMSL use.
	TSE Science Theme and Hydro-biogeochemical Elemental Cycling Leadership Area	Develop a molecular-to-pore-scale mechanistic understanding of coupled biogeochemical controls, reactions, and elemental cycling to advance predictive understanding of feedbacks between the water cycle and ecosystem biogeochemistry, and inform biogeochemistry components of ESMs. Developed hierarchical models representing key hydro-biogeochemical processes (the chemical form, distribution, and transformation of soil carbon) that control elemental cycling that inform and improve the Community Land Model component of ESMs.	**JGI**–determining microbial community structure and function on biogeochemical processes. **SSRL**–probing molecular speciation of contaminants and critical biogeochemical elements that impact chemical state, cycling and transport.
Energy	EMP Science Theme and Solvent-mediated Interfacial Chemistry Leadership Area	Develop sufficient understanding of dynamic and emergent processes that occur at solvent-mediated interfaces to predict transformation mechanisms and physical and chemical properties needed to design advanced batteries and new catalysts for degrading biomass and upgrading bio-produced fuels and renewable chemicals. Contributed to principles for achieving the JCESR goals.	**JCESR Hub**–new energy storage materials and design concepts. **Advanced Light Source**–development of Advanced Materials Beamline for Energy Research. **NorthEast Center for Chemical Energy Storage EFRC**–understand changes in electrode structure that occur during battery operations.

3.0 EMSL's Scientific Capabilities

As a national scientific user facility, EMSL must continue to develop, and provide our users and scientists with, the capabilities–world-class staff, state-of-the-art equipment, and mission-ready facilities–for sustained scientific impact. EMSL's capabilities are developed and built using the following approach:

- *Science drives the capabilities*–EMSL's science needs drive capability investments and actions–our capabilities are built with strategic goals and scientific needs as the forefront drivers.
- *The scientific community validates the needs*–Capabilities are closely vetted and developed through engagement with the scientific community–we use the scientific community to refine, improve, and validate our capability needs and concepts.
- *The user community benefits*–EMSL's capabilities are selected and integrated with each other to provide distinctive tools for its user community–we strive to provide unique, sought-after, distinctive tools and tool sets that can advance our science achievements.
- *EMSL provides lifecycle management*–EMSL manages its capabilities using a lifecycle approach; managing capabilities from cradle to grave, conception to disposal, maximizing utility and efficiency of our capability suite.

EMSL currently has eight capability areas. Each capability is a powerful combination of scientific expertise, premier instrumentation, and specialized laboratory space, and each one is specifically designed to support EMSL's science themes and leadership areas. We also integrate across these capabilities to provide leadership to the scientific community; for example in radiochemistry, integrated omics, and dynamic and *in-situ* imaging.

As we evolve EMSL into the next generation molecular science user facility, we will invest in continued advancement and integration of our capabilities to provide leadership to the scientific community. We envision this integration to take place on a larger scale, involving not only instrument integration, but development of new specialized facilities like the Quiet Wing and RadEMSL. For example, the addition of a plant science/plant phenomics component to our research portfolio will advance EMSL's leadership in integrated omics and integrate the BDD, TSE, and AAS Science Themes with carbon dynamics as well as integrate the BDD and EMP Science Themes in attacking major challenges in production of plant-based biofuels and bioproducts.

Development of a community aerosol research capability that can monitor biogenic emissions and correlate those emissions with subsequent evolution of SOAs is another example. The description of true biological diversity and its molecular-level cause and effects can only be determined through development of single-cell analyses and observations. This is another capability goal for EMSL. All of these ideas derive from workshops, STAP meetings, and other discussions and interactions with the science community, and will be described in more detail later in this plan.

3.1 Premier Capabilities

EMSL's current capabilities are organized into eight areas, listed below. Each of these areas possesses a critical mass of staff expertise, unique and specialized instrumentation, and specialized facilities. An illustrative unique aspect of each capability area is provided, and a more comprehensive description and listing of instrumentation and associated representative capability are available on the EMSL capabilities web page.

These capabilities provide the foundation for EMSL's scientific vision and mission as a national scientific user facility. EMSL plays an important role in the scientific community: providing distinctive molecular science capabilities and access to multiple suites of experimental and computational tools that allow scientific teams to experimentally test hypotheses, develop and run numerical models, and validate predictive simulations. New concepts, facilities, and instrumentation that push the limits of resolution, detection, identification, and quantification are required and must be developed. Our specific strategic capability integration and transformational aspirations, their 10-year goals, and success indicators are summarized in **Table 3.1** (at the end of the section) and described in additional detail below.

Cell Isolation and Systems Analysis (CISA)

Cell and organelle isolation–Resources are available at EMSL for detecting and isolating distinct cells and organelles for further single-cell and other analyses. In addition to cell and organelle isolation, CISA provides quantitative and super-resolution fluorescence microscopy, as well as transcriptomic analyses of complex microbial communities to better understand cellular processes at the molecular level.

Deposition and Microfabrication

Pore-scale flow laboratory–Custom pore structures approximately 10-100 µm in size are etched into silicon or similar substrates in our clean room facility with flow through these pores studied using optical microscopy or Raman spectroscopy. Fundamental relationships governing fluid flow can feed directly into large scale models that predict changes in the natural environment.

Mass Spectrometry

Proteomics mass spectrometry–Cutting-edge proteomics tools and methods available at EMSL facilitate advanced global proteomics research and allow detailed visualization and analyses of cellular proteins at large sample scales, and at both the peptide and intact protein levels.

Microscopy

Multi-modal microscopy–EMSL hosts a variety of sophisticated microscopy instruments, including electron microscopes, optical microscopes, scanning probe microscopes, ion microscopes, and computer-controlled microscopes for automated particle analysis. EMSL specializes in environmental, *in-situ* microscopy, and is developing new dynamic (time-resolved) microscopy capabilities.

Molecular Science Computing

Integrated production computing environment–The MSC capability includes Cascade (a supercomputer with theoretical peak performance of 3.4 petaflops), NWChem (an award-winning community computational chemistry code developed at EMSL), and Aurora, a 15.8 petabyte data storage system.

Nuclear Magnetic Resonance and Electron Paramagnetic Resonance Spectroscopy

Solid-state, interfacial and in-situ NMR–EMSL offers users solid-state NMR techniques for low-gamma nuclei detection and a full range of magic angle spinning methodologies to study biological, geochemical, catalytic, and advanced material systems in their near-native state and in real time. NMR systems up to 850 MHz are available, including a “hot” 750 MHz NMR system capable of investigating radioactive samples.

Spectroscopy and Diffraction

NanoSIMS–Capable of sub-micron level chemical and isotopic imaging, the NanoSIMS is revolutionizing fields as diverse as microbial ecology and atmospheric chemistry.

Subsurface Flow and Transport

Pore- and intermediate-scale flow cells–EMSL’s approach to subsurface flow and transport studies is unique and holistic, integrating flow cells, analytical tools, tomographic imaging, and predictive modeling capabilities to study subsurface phenomena. Truly unique are EMSL’s custom-designed and fabricated pore- and intermediate-scale flow cells, used in conjunction with a suite of reactive transport simulators, which enable multiscale study of flow, transport, and biogeochemical reactions (metals and radionuclides, non-aqueous-phase liquids, carbon transformation, and microbial activity).

Capabilities have helped thousands of researchers use a multidisciplinary, collaborative approach to solve some of the most important national challenges in energy and environmental sciences.

3.2 Increasing Scientific Impact through Integration

By integrating across EMSL’s capabilities, we enable increased scientific impact and provide unique toolsets to our users and scientists. In addition, we leverage and integrate resources from across PNNL, other BER and SC user facilities, and user/collaborator laboratories. Within EMSL we focus on four areas of integration:

Radiochemistry–The caliber of scientists, instrumentation, and specialized laboratories available at RadEMSL is building an engaged and productive user community comprising the world’s leading radiochemists. The co-location at a user facility for radiochemistry and a full suite of state-of-the-art instrumentation is unique in the United States, and it is one of just a few such user facilities worldwide.

An action plan is in place to maximize the scientific impact of RadEMSL. This plan was written in order to jumpstart interest within the scientific community (particularly in the BER community), accelerate the impact of the capability, and maximize the scientific benefit of that investment. It includes a science vision for the facility, a set of strategic actions, and success metrics. This acceleration plan model is one we intend to follow for future instrument-focused and application-focused capabilities.

Integrated Omics–EMSL is internationally recognized for leadership in mass spectrometry-based proteomics. Contributing to this success is an expansive mass spectrometry capability that enables high-throughput, high-resolution analysis of complex mixtures of many sample types. These world-class instruments and techniques are part of an unparalleled collection of capabilities that include high-performance separations, mass spectrometry, and data informatics packaged together to generate the most sophisticated proteomics profiles available anywhere.

Building upon our expertise in proteomics, we are expanding this application-focused capability to include transcriptomics and metabolomics along with the necessary informatics tools that enable translating large sets of data into scientific understanding. In FY 2015, we will deploy the 21T FTICR mass spectrometer, which will be the world's highest field FTICR mass spectrometer. This instrument, currently under development, will provide the unequivocal ability to discern and identify molecular species in complex systems and will enable researchers to tackle analytical challenges in omics and systems biology, intact proteins and protein assemblies, microbial communities, fossil fuels, organic aerosols, and other natural organic matter (NOM) to address DOE mission needs. An action plan is also in place for maximizing the impact of the 21T FTICR mass spectrometer.

Dynamic and *In-situ* Imaging–EMSL's scientists and users have access to some of the most advanced dynamic and *in-situ* imaging systems in the world. The Quiet Wing is one of the most vibrationally and electromagnetically quiet places on earth for extremely sensitive characterization and imaging instrumentation. Our marquee DTEM instrument will enable scientists to visualize complex systems dynamically in real time under realistic conditions–at atomic spatial resolution with nanosecond temporal resolution, opening the door to understanding protein conformational changes, the aging and transformations of aerosols, and the mechanisms of battery and catalytic function.

Coupling our high-resolution instruments with unique custom cells that enables the study of aerosols, cells, and energy materials helps distinguish EMSL, and we will also work to establish formal partnerships with other user facilities that house complementary imaging modalities. An action plan for maximizing the impact of the EMSL Quiet Wing, which houses these capabilities, has been developed and submitted to BER for approval.

Computation–EMSL's scientists and users are encouraged to couple high-performance computation with experimentation to broaden research impact. BER's strategic emphasis on development of robust predictive capabilities provides a mandate to incorporate experimental results into simulation tools for BER science applications. An example is the integration of experimental photoelectron spectroscopy measurements with theoretical descriptions (based on quantum and statistical mechanical theory) embodied in the NWChem simulation code to provide new fundamental understanding of molecular-level effects that drive the formation of common multicomponent aerosol particles. Molecular-scale calculations of aerosol properties (such as energy absorption spectra) can directly support parameterization of atmospheric aerosol models and their influence on earth's energy budget. Integration can also take the form of experimental interpretation; for example, the calculation of theoretical NMR spectra to guide interpretation of NMR measurements of soil organic carbon composition. Finally, numerical simulations can be used to guide experimental design, and experimental results in turn can be used to improve numerical models. An excellent example of this is the Pore-scale Research Campaign, in which experiments were designed to test a suite of pore-scale models, leading to significant improvement in model representations of solute dispersion processes[29].

3.3 Aligning Capabilities with Future Scientific Challenges

As we move into the future we must continue to provide EMSL's scientists and users with capabilities necessary for sustained scientific impact. This includes the need to advance capabilities, as well as continue to integrate capabilities and provide leadership to the scientific community. As stated in the Introduction, we recognize we exist in a highly dynamic planning environment in which we must continually evaluate and respond to changing needs and opportunities. In particular, we must work with our BER sponsors and users, from academia, national laboratories, and industry to understand what potential scientific and/or technological innovations exist that we can adapt or adopt for the benefit of our user program.

In addition to the continued development described in Sections 3.1 and 3.2, we plan to take the following capability development actions:

Molecular Science Computing–Expand existing, and develop new, computational capabilities to advance the predictive simulation objectives of BER and the Office of Science. Advancement of predictive simulation capabilities requires complementary development of software, data managements systems, and supporting hardware and infrastructure. (**Figure 3.1**)

Software: The EMSL software strategy has three major components:

1. Expand the NWChem software development paradigm (high-performance open-source community tools for computational chemistry) to broader computational targets of importance to BER, including subsurface RTMs, atmospheric aerosol models, and models of biological function (genotype to phenotype). NWChem is a high-performance computational chemistry suite that enables study of complex molecular systems, and is well positioned for powerful application to larger scales (i.e., mesoscale science) by using high-accuracy computationally intensive methods to inform and parameterize computationally efficient semi-empirical methods. Investments are being made to expand its applicability to aerosol and biological processes that require fundamental molecular understanding, and to further enhance the integration of EMSL's experimental and modeling capabilities for increased scientific impact.

2. Develop new computational capabilities in areas other than computational chemistry that are motivated by BER science objectives and crosscut the three BER-focused EMSL science themes. Because of its identity as a scientific user facility, its expertise in high-performance computing operations and software development, and its science themes that span a broad range of BER science, EMSL is uniquely positioned to meet an emerging need for an integrated community software ecosystem directly

supporting BER objectives. EMSL aspires to lead the development of such a community framework, built around the concept of the Virtual Plant-Atmosphere-Soil System (VPASS). This virtual laboratory will comprise a suite of connected software, to be developed and applied in collaboration with the BER community, capable of simulating critical hydrologic, soil microbiologic, plant, and atmospheric aerosol systems at multiple integrated scales ranging from molecular (microbial and plant omics) to pore (soil hydrology and carbon transformations) to plant (including biogenic aerosol emissions) to watershed ecosystems (large-scale hydrology and biology interactions) and beyond (e.g., impacts of biogenic aerosols on cloud formation). The VPASS will build on existing expertise in, and provide integration across, the three BER-focused science themes (TSE: pore- and continuum-scale reactive transport and soil carbon transformations; AAS: biogenic organic aerosol formation and property simulations; BDD: omics-informed soil microbial community dynamics and simulation of microbial metabolic function). The proposed VPASS is inherently multiscale in nature, and therefore its development is closely related to the multiscale modeling strategy being developed based on the results of the recent EMSL workshop on “Multiscale Computation: Needs and Opportunities for BER Science.”

Figure 3.1. Environmental molecular research is accelerated when combined with leading-edge hardware, efficient parallel software, predictive theories and visualization capabilities. Users are encouraged to combine computation with other state-of-the-art experimental tools, providing an integrated platform for scientific discovery.

3. Modernize codes to take full advantage of emerging computational architectures, particularly the Intel Xeon Phi coprocessors that comprise a significant portion of Cascade’s computational capacity. Utilization of the coprocessors requires significant code refactoring, and many current codes are unable to take full advantage of Cascade’s power. EMSL is engaged in multiple collaborations to ensure NWChem remains at the forefront of high-performance computational chemistry, including: a) Intel Parallel Computing Centers program (adapt all NWChem modules to utilize Phi coprocessors); b) participation in the NERSC Exascale Science Application Program (facilitate execution of NWChem on the planned Cori system comprised of self-hosted Xeon Phi processors); and c) participation in the OLCF Center for Accelerated Application Readiness Program (facilitate execution of NWChem on GPU-based systems).

Data Management: Complete deployment of the MyEMSL system, which provides mechanisms for collection and archival of EMSL’s experimental data and associated metadata efficiently and in a manner that facilitates data access by a broader scientific community. Expand current efforts to provide EMSL’s scientists and users intuitive analysis tools for the resulting large, complex data sets. Integrate these tools with our high-performance molecular science computing infrastructure to better convert raw data into discoverable, reusable information products with rich, descriptive metadata and semantic content. This will reduce dramatically the time and effort needed to understand data from experiments, help design new/follow-up experiments, and facilitate and simplify the use of data from multiple capabilities and physical locations.

Hardware and Infrastructure: Prepare infrastructure for, design, procure, and begin operations of HPCS-5 (targeted user readiness in January 2018), the next generation EMSL supercomputing system. Coordinate infrastructure development with PNNL Information Technology and High-Performance Computing organizations to take advantage of potential synergies and economies of scale. Consider the early procurement of small testbed systems to facilitate early adaptation of key codes to new hardware architectures. Evaluate and address user needs for computational capabilities to complement current and future supercomputers, potentially including data-intensive computing needs, private cloud computing architectures, and data analytics and visualization support. Addressing these needs will facilitate design flexibility to accommodate multiple needs across the science themes.

Soil Biogeochemistry of Carbon and Transport and Radiological Chemistry–Develop new expertise and instrumentation for the molecular characterization of NOM, its spatial distribution within soil pores, and its transformations to improve understanding of the biogeochemical processes that transform and stabilize carbon in the belowground terrestrial ecosystem. (**Figure 3.2**) This understanding can provide a basis for better using and manipulating this large carbon reservoir for both climate change and bioenergy/bioproduct research. The SOM is a complex, heterogeneous mixture of above and belowground plant litter and animal and microbial residues at various degrees of decomposition and is a reservoir for carbon (C) and other elemental nutrients needed for ecosystem services. Surprising little is known about the molecular composition of SOM and its response to changing climatic conditions or land use. SOM structural and molecular analysis is critically needed to decipher chemical processes within soil and predict changes in the sign and magnitude of terrestrial carbon fluxes in a changing environment. High-resolution mass spectrometry, including the 21T FTICR mass spectrometer (to be available in late 2015) facilitates the assignment of molecular formula (elemental composition) to soil organic molecules. By establishing the identity of most of these compounds in highly correlated samples we will be able to discern signatures of biological activity and follow the flow and transformation of carbon (nitrogen) through the terrestrial ecosystem. Current chemical characterization of SOM is inadequate to discern the biological processes that result in either the respiration or stabilization of carbon. Mechanistic description of these processes is important to a broad spectrum of scientists including agriculturists, soil ecologists, and climate scientists who need to predict how these processes, or their rates, will change under different climatic or cropping conditions. The molecular complexity of SOM is truly extraordinary–metabolic products of higher plants, soil microbial communities and mycorrhizal fungi all mixed together in a complex inorganic soil matrix. With high-

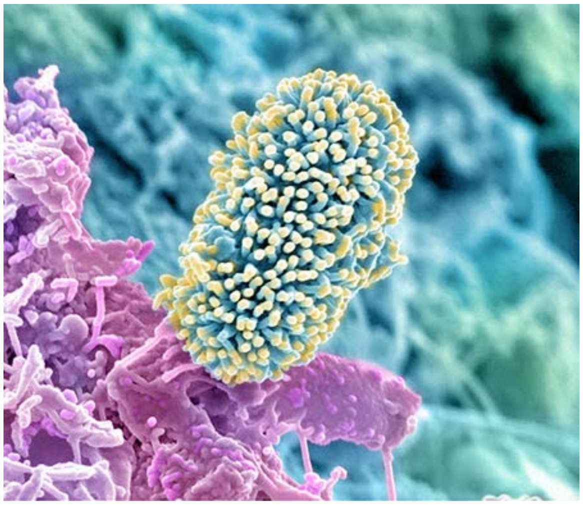


Figure 3.2. An intricately structured soil bacterium, less than a micron in size, makes its home on the root surface of an Arabidopsis plant. Much remains to be learned about the plant root zone and its microbial communities and influence on environmental processes.

resolution MS techniques we will for the first time be able to identify intact molecular species in soil in a high-throughput fashion. This is a major step toward implementing a systems biology approach in soils. When combined with imaging techniques, the 21T FTICR mass spectrometer will also enable *in-situ* chemical analysis to address spatial relationships and heterogeneity assessments. When combined with fluorescent *in-situ* hybridization (FISH) and ^{13}C measurements using NanoSIMS, the 21T FTICR mass spectrometer will enable linking biota with processes at the sub-µm scale.

RadEMSL houses many spectroscopic and imaging components needed for radiochemistry fate and transport studies. These include the sub-ppm O_2 environmental chambers to conduct solubility studies under controlled redox conditions and for sample preparation. The radiological NMR, EPR, and XPS capabilities provide characterization of the oxidation state and coordination environment (bonding, number, and identity of nearest neighbors) of both solid and solution phases. However, with few exceptions, the current experimental capabilities are limited to relatively high-radionuclide concentrations (millimolar) and solutions of simple chemical complexity. The capabilities in RadEMSL need to be expanded to facilitate speciation of nuclides such as ^{99}Tc and others under a wider range of controlled redox conditions where intermediate oxidation states and associated complexes can be stabilized and ascertained. Specifically, electrochemical capabilities for NMR and EPR experiments are needed to exploit the synergy with the two techniques to cover the range of possible Tc and other radionuclide oxidation states. Currently only a few spectra are available in the literature for the less common radionuclide oxidation states. In addition, synthetic capabilities for the preparation of many radionuclide solid-state compounds are needed as reference compounds for the calibration of spectroscopic techniques available at EMSL and elsewhere. Other routine capabilities (e.g., FT-IR, UV-Vis spectrophotometry) also need to be added to the RadEMSL suite of instrumentation.

Integrated Omics–Expand current scientific leadership in global proteomics beyond transcriptomics and basic metabolomics to include greatly enhanced metabolomic capabilities and also include metallomics and glycomics. This is part of a long-term strategy to create and demonstrate a comprehensive, integrated omics capability to address both peptide-level and intact-level proteins, metabolite measurement and flux analyses, protein and metabolite localization and visualization, and the deep, quantitative multi-omics measurements coupled with informatics/bioinformatics/modeling approaches that will accelerate insights into biological system mechanics and principles. EMSL possesses the requisite NMR and MS framework on which to build a substantive metabolomics capability to complement its current world-class proteomics capability. Additional, specific instrumentation that is needed in this area is GC-based MS capability that will allow improved characterization of low-molecular weight metabolites. Additional LCMS instrumentation is also needed to provide dedicated and high-throughput metabolomics capacity. Both targeted and untargeted metabolomics capabilities are needed. Spatially resolved metabolomics is also an area where EMSL is uniquely poised for development and contribution. The metabolomics field is currently constrained by the availability, quality, and extent of metabolite library information, and a leadership opportunity exists here if EMSL can develop techniques or approaches that provide freedom from library and/or standards dependencies. Investments are needed in metabolomics data management and flux modeling software to achieve this goal, and also to take ultimate scientific advantage of new metabolomic capabilities that are projected.

Dynamic and *In-situ* Imaging–Extend current scientific leadership from static atomic-scale imaging to dynamic and fast time-resolved imaging at the atomic to near-atomic scale. (**Figure 3.3**) EMSL is developing a dynamic transmission microscopy (DTEM) capability that will provide real-time (µsec timescales) structural and biochemical information with sub-molecular size resolution. Both “snapshot” (single pulse) and “movie” (stroboscopic pulses) observations of live biological activity can potentially be made. EMSL also has plans to extend and further develop this dynamic microscopy approach to the nsec-psec timescale with a proposed ultrafast microscopy capability. This effort will require a major equipment proposal to DOE. Ultrafast microscopy can provide direct observations of energy transduction mechanisms, including assembly and molecular interactions of supramolecular protein machines in plant and microbial biology. A better understanding and visualization of the life cycle of aerosol particles from nucleation and growth to aggregation and dissolution could facilitate more reliable models for environmental research. The proposed ultrafast microscopy capability would open novel opportunities to fundamentally understand components of atmospheric samples and processes involved in chemical reactions contributing to climate change. Ultrafast microscopy would also provide insights into interfacial electron transfer to mineral surfaces in biogeochemistry and dynamic and time varying processes in catalysis. In addition, incorporation of true multi-modality microscopy techniques (optical, ion, electron, and x-ray) and integration of large data set and computational modeling techniques will provide an imaging capability unique in the world.

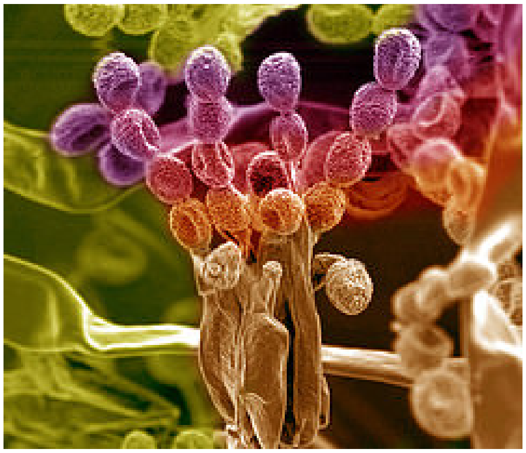


Figure 3.3. Scientists are studying the mineral and biological associations in the plant root systems to better understand the role of soil microbes in the soil-mineral weathering process. Pictured here are conidia (spores) of Penicillium sp., a ubiquitous soil fungus that lives mainly on organic biodegradable substances. The spores were imaged with a Helios 600 Nanolab dual-beam scanning electron microscope.

Single-cell Analysis–Predicting, manipulating or preserving biological systems to achieve sustainable solutions to the nation's energy and environmental challenges requires understanding principles of these complex systems at the molecular level. Because biological systems are highly heterogeneous, averaged cell population measurements, which often detect the most robust or abundant processes, provide only part of the picture, leaving critical processes undetected due the dilution of signals in the averaged measurements. By interrogating individual cells, it will be possible to understand the complexity of the population and achieve the required level of molecular accuracy and details needed to predict and efficiently redesign or preserve the system.

Building on EMSL’s strong biology and technology expertise, we will develop and integrate techniques that preserve the entity of the individual cell to unmask cellular heterogeneities and molecular details hidden otherwise in averaged cell population measurements. These single-cell analysis techniques will make it possible to identify individual cells and their unique functions within microbial communities, where the complex relationships between multiple members make it impossible to regrow isolated cells in culture, or identify key molecular players in metabolic pathways to enable the design of specialized cells for bioproducts.

We will solve technological challenges inherent to single-cell analysis approaches and provide integrated tools needed to interrogate individual cells in heterogeneous biological systems. Super resolution fluorescence, atomic force, electron, ion and x-ray microscopy, as well as NanoSIMS, will be integrated with molecular biology techniques to detect and quantify the expression of multiple genes or proteins in individual intact cells and provide chemical flux and spatial context to omics with nanometer resolution. For example, super-resolution fluorescence techniques which enable imaging with 20-30 nm resolution in intact hydrated cells will be used to quantify the expression of multiple genes in individual cells by a combinatorial barcoding of FISH probes. This approach provides quantitative gene expression while preserving the spatial information within microbial communities or across plant-microbe interactions. FISH will be also used with NanoSIMS to quantify gene expression in metabolically active cells to understand the community function at the molecule level. These techniques can also be correlated with atomic force microscopy to provide 3D maps of distinct proteins, identified by fluorescent tags within the intact cell surface or membrane. A new approach for quantifying gene expression in single cells in high throughput will be developed using combined cytometry and mass spectrometry techniques to follow protein changes at the single-cell level. This will be done in combination with *in-situ* hybridization probes that will be tagged with metallic elements, such as rare earth elements, which will be detected and quantified with high accuracy using TOF and ICP-MS. This approach will enable the quantification of gene expression for more than 50 different genes per cell in high throughput to better understand the role of individual microbes in the function of the community. Single-cell NMR techniques will be developed to identify molecular structures in metabolic pathways, and single-cell RNA sequencing (RNA-Seq) will be established to quantify the expression of critical proteins or enzymes that might be buried otherwise in the averaged measurements. With the aid of computational and modeling methods, these integrated techniques will enable predictive understanding of complex biological systems across scales–from molecules to pathways within cells, microbial communities and organisms.

Plant Phenomics–EMSL has bold plans to develop entirely new scientific expertise, instrumentation, and facilities that will support several BER-relevant biology programs, including a newly envisioned plant phenomics capability that would greatly broaden the reach of the BDD Science Theme. EMSL has recently hired a senior plant scientist and is in the early stages of conceptualizing and planning a high-throughput (HTP), image-based, non-invasive plant phenomics capability to serve as a filter and allow the screening of extensive germplasm and mutant collections to identify a limited number of potential candidates at a pool size suitable for interrogation using EMSL’s extensive analytical and imaging platforms. Under this approach, HTP phenomics under controlled environmental conditions followed by high-precision phenotyping will be conducted. This approach will be critical for obtaining detailed insights into plant performance, function, and composition in order to build an envisioned ‘virtual plant’ model. We propose the development of a plant phenotyping capability platform to be housed together with the plant and aerosol labs within recently vacated EMSL space. An initial capability can be built to accommodate handling of approximately 100 plants simultaneously. Equipment for such non-invasive plant phenotyping is commercially available and will be acquired soon. Additionally, other greenhouse, growth chamber and laboratory space will be needed for generation and cultivation of plant lines, for plant transformation, and for HTP sampling of plant tissue for quick freezing and subsequent metabolite, protein, and RNA analyses.

The long-term goals of such a facility are to help develop a capability to predict plant growth, performance, and composition (phenotype) for selected model plants from their genotype and simulated environment, i.e., bridging the genome-plant-environment knowledge gap, and to better understand and exploit the exceptional metabolic diversity between and within plant species. This capability, once developed, will enable prediction of climate change drivers on potential biofuel crops, future design of adapted new crop species, routes to enhanced production of plant fuels and chemicals, and useful new metabolic pathways and metabolites.

Aerosol/Earth System Chamber–Investigations of the processes controlling atmospheric composition have identified many major factors controlling climate change. For example, there is growing evidence that interactions of anthropogenic pollution and BVOC emissions are a major source of atmospheric aerosol and may be responsible for strong feedback with the climate system. The quantitative understanding required for representing these processes in numerical climate models remains elusive due to immense complexity of the relevant earth-system components. A laboratory chamber facility for quantifying these processes under controlled environmental conditions was eagerly discussed at this year's AAS STAP meeting [30]. Such a chamber facility could serve a number of purposes including developing analytical approaches and reducing disparities between theoretical, laboratory and field investigations of interactions between biogenic emissions and anthropogenic pollution. Environmental chamber facilities for investigating biogenic emissions and aerosol production have been built in Europe and Japan, but they neither cover the entire scope of biogenic aerosol and earth-system research nor fully solve key experimental concerns, such as avoiding wall effects or the influence of growing plants in simulated environments. There is no adequate facility in the U.S. for investigating the full range of biosphere-atmosphere interactions including biogenic emissions and uptake, aerosol production and growth, and feedbacks to biogenic emissions. Thus, an opportunity exists to build a novel EMSL facility that would complement and integrate EMSL laboratory capabilities with DOE BER field study approaches. EMSL proposes to investigate design and construction of a highly instrumented aerosol chamber system, one that would include high quality core measurements (e.g., VOC, ozone, NO, and particle numbers) that are readily available from commercial instruments, but are challenging to obtain the high quality sensitive measurements required for many studies, as well as provide innovative aerosol and gas measurement on-line monitoring capability and off-line analysis. In addition, the facility would enable researchers to bring their own unique instruments to the chamber for specific, tailored experiments.

In addition to an aerosol/earth-system chamber (i.e., an earth-system simulator), additional investments are needed to bring the AAS capabilities more in balance with EMSL's other science theme areas. This includes capabilities that can further AAS goals requiring advanced microscopy and mass spectrometry. Currently researchers investigating molecular-scale aerosol processes typically perform *ex-situ*, "post mortem" experiments, figuring out what happens only after the fact. To adequately understand atmospheric aerosol systems and improve their representation in climate models, some experiments need to be performed *in situ*, with multi-dimensional imaging in real time so dynamic processes and transformations can be observed, measured, and chemically correlated or synchronized. This requires a breed of microscopes that can handle and adapt to different simulated environmental conditions and perturbations. Mass spectrometry applied to aerosols and their precursors has advanced significantly over the last decade, but higher resolution and sensitivity measurements are still needed to accurately quantify many aerosol constituents, particularly the organic components of secondary aerosols or SOA's. EMSL's 21T FTICR mass spectrometer was developed for this kind of application and should be particularly useful in characterizing atmospheric aerosols and particulates. There is also a need for EMSL to develop field-deployable mass spectrometry instruments for aerosol research with high resolution and wide mass ranges along with flexible, streamlined data analysis to manage and interpret large data sets.

Table 3.1. Summary of EMSL's Capability Development Areas, 10-year Goals, and Success Metrics

Scientific Challenge	Science Theme and Leadership Area	10-year Capability Goals and Metrics of Success	Key Partnerships or other Needs
Biology	BDD Science Theme and Metabolic Compartmentalization Leadership Area	**Metabolomics**–Add new MS and NMR, and integrate use of MS/NMR to augment EMSL's omics capabilities. **Metabolomics**–Add 2-3 new FTEs with metabolomics expertise (including at least one FTE in statistical and modeling areas). **Metabolomics**–Develop recognized capability and reputation for spatially-resolved metabolomics in concert with compartmentalization leadership goals. **Single-cell Analysis**–Develop and apply new, integrated microscopy techniques to interrogate single-cell biology and diversity (e.g. FISH-NanoSIMS). **Plant Phenomics**–Add 2-3 new FTEs in plant science to enhance plant scientist research with users and to develop a strong plant science and phenomics platform.	**Bioenergy Research Centers**–BioEnergy Science Center, Great Lakes Bioenergy Research Center, and JBEI **JBEI**–Collaborate with JBEI personnel on metabolomics techniques, applications, and flux balance analyses. **Academia**–Engage new postdoctoral researchers or recent graduates with metabolomics expertise (University of California, Irvine; Imperial College London) **LLNL**–Collaborate on biological NanoSIMS.
Environment	AAS Science Theme and CBOA Leadership Area	**Aerosol Characterization**–Develop high-resolution MS capabilities for comprehensive ID of aerosol molecular species (the 21T FTICR mass spectrometer and/or Orbitrap MS). **Aerosol Characterization**–Develop new field-deployable instruments and novel observational platforms BER ASR program objectives. **Aerosol/Earth System Chamber**–Develop concepts, designs, and facility for aerosol/plant/terrestrial chamber to support earth-systems science research.	**ARM**–Combine and integrate field and lab measurements and comparisons for molecular characterization of aerosols for field campaigns (including 2010 CARES and ongoing 2014 GOAmazon studies). **Aerodyne Corporation**–Co-develop improved aerosol measurement techniques and correlated atmosphere/aerosol composition changes. **Other aerosol chamber facilities**–Identify facilities within and outside U.S. (benchmarking institutions TBD).
	TSE Science Theme and Hydro-biogeochemical Elemental Cycling Leadership Area	**NOM Characterization**–Develop new approaches and capability for SOM characterization, add 1-2 new experienced FTEs, and add dedicated environmental MS/NMR capabilities. **Radiological Capabilities**–Round out RadEMSL's capabilities with electrochemical, *in-situ* sampling, IR and UV spectrophotometry instrumentation.	**Academia**–Work with recognized academic leaders in NOM/SOM area (e.g. Old Dominion University, Florida State University). **SSRL**–Probe molecular speciation of contaminants and critical biogeochemical elements that impact chemical state, cycling and transport. National laboratories: Work with major Scientific Focus Area and Next-generation Ecosystem Experiment projects funded by BER Environmental Systems Sciences program (PNNL, LBNL, ORNL).

Table 3.1. (cont'd)

Scientific Challenge	Science Theme and Leadership Area	10-year Capability Goals and Metrics of Success	Key Partnerships or other Needs
Energy	EMP Science Theme and Solvent-mediated Interfacial Chemistry Leadership Area	**Catalysis**–Continue development and application of new TEM and non-linear spectroscopy techniques. Acquire DNP capability. **Energy Storage**–Liquid, *in-situ* cell TEM developments are still needed. A direct electron detector should be acquired so TEM capability remains competitive. Sample interchangeability (between microscopes/techniques) can be optimized better. **Computation**–Develop and implement hierarchical methods with increased accuracy and complexity; provide workflows to guide usage of NWChem (and other codes); develop/deliver easy-to-use interfaces.	**Ames Laboratory**, NHMFL, Bruker–DNP capability development and application **Hummingbird Corp**–liquid, specialty cells **FEI, Direct Electron Corp**–direct electron conversion detectors **User community**–NWChem development

4.0 Outreach and User Experience

An engaged and productive scientific user community is critical to accomplishing our mission and vision, and we actively build our user community by seeking scientists for their scientific leadership, alignment to our values and objectives, and commitment to mutual success. EMSL's users are leaders from academia, industry, and PNNL and other national and international laboratories providing solutions to the world's most daunting scientific challenges.

4.1 Outreach

Our outreach strategy is focused on building sustainable relationships with a diverse mix of high-impact researchers who are funded by BER programs or whose work is relevant to those programs, and is based on communications best practices, and on the direct feedback our users provide through our communication surveys. Our approach proceeds in three distinct phases, starting with raising awareness, shown in Figure 4.1, with activities that indirectly reach users (such as social media). These activities receive a lower level of effort because they are focused on raising awareness. As individuals move through the circle to credibility and interest, we invest in activities that more directly reach users. Throughout these phases, we focus on building communities around specific areas of research and/or research campaigns.

The first phase is to *raise awareness* within the scientific community about EMSL's science and capabilities. This is done primarily through our website, social media, virtual tours, and users and staff. Over 125,000 unique visitors viewed the EMSL website in CY 2011. Our Facebook follows have increased by nearly 300 percent in the past three years (3,800 in 2014). EMSL's users and staff members also raise awareness through their presentations at scientific meetings and conferences, journal publications, and discussions with colleagues, as indicated by 77 percent of responders to our October 2013 survey question to users "How did you learn about EMSL?"

The second phase of our outreach strategy is to *reinforce credibility* through our presence at BER PI meetings, presentations at scientific meetings, electronic newsletter, science highlights, and other approaches. For example, we increased our outreach at multiple BER PI meetings in FY 2014, including plenary presentations of EMSL's science at the Genomic Science Program and the Subsurface Biogeochemical Research and Terrestrial Ecosystem Science Programs PI meetings. Additionally, we reach scientists conducting research relevant to BER through leadership or commentary pieces published in key professional society publications, such as the American Society of Microbiology's *Microbe* magazine. Efforts will be accelerated in FY 2016 to place additional authored pieces in these types of magazines, including the American Geophysics Union's Eos magazine. The EMSL Science and Technology Council also will develop strategies for enhancing involvement and visibility at key scientific meetings, including but not limited to: American Geophysical Union (AGU), American Society for Microbiology (ASM), the American Meteorological Society, Society for Industrial Microbiology, Plant and Animal Genomics, and the International Society for Microbial Ecology. New digital communications efforts will better demonstrate how EMSL's capabilities of people, instruments and facilities can address challenges within BER's mission and how users can engage to apply them to their research.

The third phase of our outreach strategy is to *secure interest* of users by a variety of methods outlined in **Figure 4.1**. For example, EMSL maintains significant outreach programs to engage and develop long-term relationships with high-impact users. In FY 2015, EMSL created a Director's Year of Soils Seminar Series to celebrate and leverage the International Year of the Soils. Distinguished professor Rattan Lal of The Ohio State University kicked off the seminar series in February 2015. The Wiley research programs, including the Wiley Visiting Scientist and Wiley Research Fellow, create strategic partnerships with current and potential users whose expertise benefits the user program. These programs encourage distinguished scientists to stay at EMSL for extended periods of time and participate on partner proposals to develop new capabilities, mentor staff, and assist in long-term planning. The Wiley Distinguished Postdoctoral Program is a competitive program designed to attract high-performing, newly graduated Ph.D. scientists who collaborate with EMSL scientists in a research area that aligns with our science themes, and who have potential to become full-time scientific staff at EMSL.

4.2 User Experience

EMSL was founded as a multidisciplinary facility focused on solving large, complex challenges. As such, teaming, partnerships, and collaboration are key components of all our activities. Our approach is to create a flexible and dynamic experience that allows the user to tailor the resources and assets available to them based on the needs of their research. This is a powerful approach that greatly increases the productivity of users when they are onsite.

Based on results of formal satisfaction surveys and informal unsolicited feedback received throughout the year, EMSL's users are satisfied with the quality of the facility and staff support they receive. Overall satisfaction ratings consistently exceed our BER target of 90 percent, and none of the areas surveyed have scored below 80 percent. We rely on user surveys to gauge the level of satisfaction with facility operations, including scientific and administrative staff support, readiness of capabilities, and proposal access and training. Regardless of scores, we closely review individual user comments to identify recurring themes or issues that need to be addressed. Over the next decade, we will build on our strong foundation in user experience and continue to look for ways to improve it.

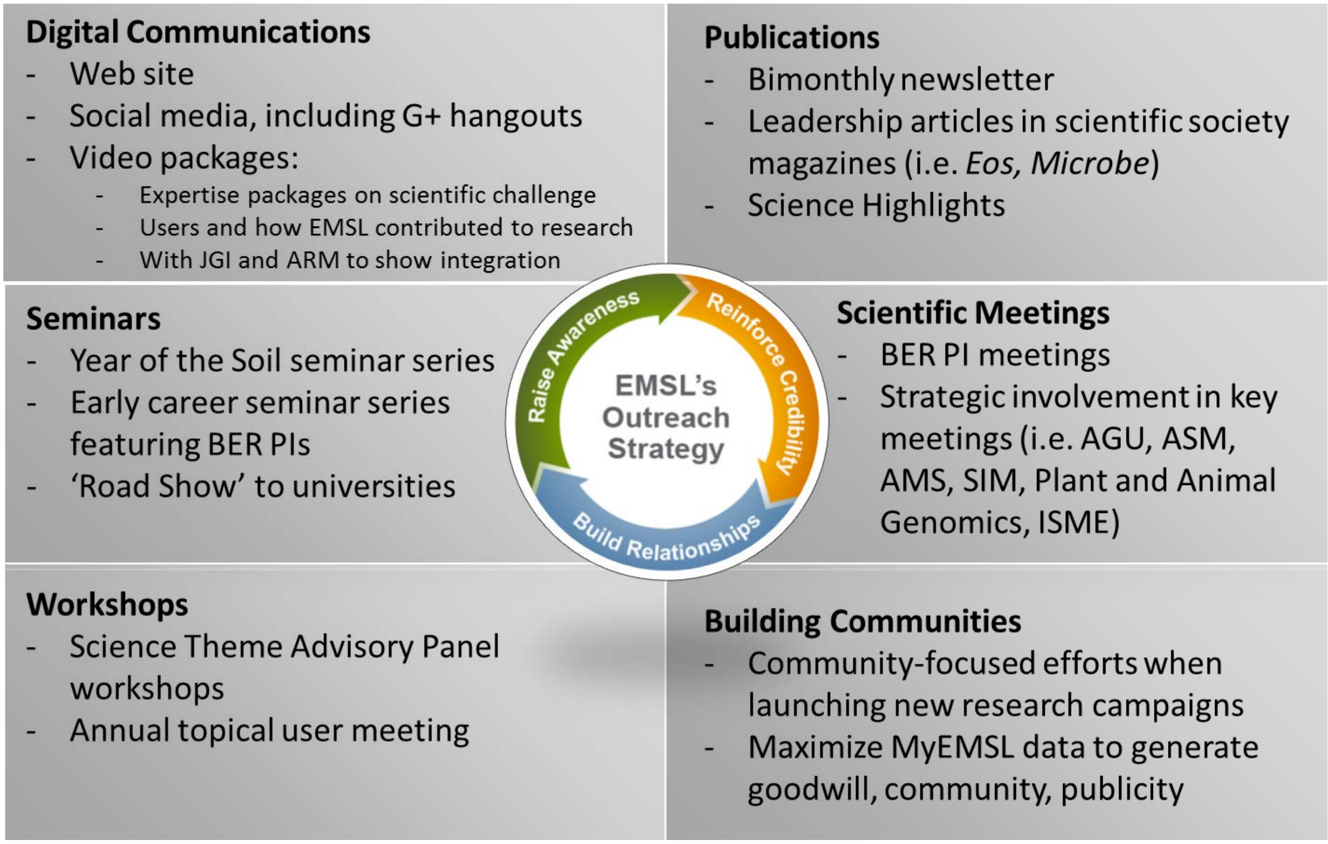
One example of our flexible approach to facilitate use and increase our leadership in the broader community nationally is the affiliation we established with the Pooled Resources for Electron Microscopy Informatics, Education and Research (PREMIER) Network. PREMIER Network is an affiliation between PNNL and 20-plus research universities (primarily in the Pacific Northwest but growing nationally and internationally) aimed at optimizing the use of electron microscopes for cutting-edge research in biology, environmental sciences, and energy storage and conversion systems (www.premiernetwork.org).

The electron microscopes in our Quiet Wing and RadEMSL are some of the most advanced and unique microscopes in the world. As part of EMSL's leadership in the PREMIER Network, a collaborative access team (CAT) project with EMSL allows PREMIER Network users to access these microscopes for short periods of time (8-24 hours). The PREMIER CAT enhances the use of these unique instruments by allowing network participants to "try" novel high-risk experiments that require little support from EMSL staff and no instrumentation other than that related to electron microscopy.

Access to the CAT allocation of EMSL's instrument time is through a short proposal that is reviewed and approved by the PREMIER Network coordinators and then assigned and managed by the EMSL Microscopy Lead. Typically network members have access to basic instrumentation at their own site and have significant preliminary data in hand. Access through the EMSL CAT is aimed at moderate-to-expert users who can make the most of the instrumentation with the least assistance. Affiliation is also intended to build awareness of the broader range of instruments available to encourage users to develop a larger scale interaction with EMSL.

Joint Calls Increases Partnerships and Collaboration

In addition to focused partnerships such as the PREMIER Network CAT, EMSL is collaborating with other user facilities to facilitate access to a broader range of resources through joint calls for proposals. For example, the JGI-EMSL Collaborative Science Initiative (JECSI) is a joint effort between EMSL and DOE's Joint Genome Institute to provide a unique opportunity to combine the power of genomics and molecular characterization in one research project. This partnering extends past offering access to each facility, but builds a single team between the researchers and the two facilities to expedite results. At a recent project meeting, one PI indicated that the communication and synergy of the JECSI program has accelerated her project results by at least two years from what would have been possible in the normal proposal route. This type of acceleration is EMSL's goal for joint programs, and calls with additional facilities are in development to continue to expedite results through an integrated multi-facility and multidisciplinary approach.



Digital Communications
- Web site
- Social media, including G+ hangouts
- Video packages:
  - Expertise packages on scientific challenge
  - Users and how EMSL contributed to research
  - With JGI and ARM to show integration

Publications
- Bimonthly newsletter
- Leadership articles in scientific society magazines (i.e. *Eos, Microbe*)
- Science Highlights

Seminars
- Year of the Soil seminar series
- Early career seminar series featuring BER PIs
- 'Road Show' to universities

Scientific Meetings
- BER PI meetings
- Strategic involvement in key meetings (i.e. AGU, ASM, AMS, SIM, Plant and Animal Genomics, ISME)

Workshops
- Science Theme Advisory Panel workshops
- Annual topical user meeting

Building Communities
- Community-focused efforts when launching new research campaigns
- Maximize MyEMSL data to generate goodwill, community, publicity

Figure 4.1. EMSL uses a variety of outreach approaches for building, growing, and engaging a user community.

Remote Utilization Increases Productivity

A unique feature of EMSL is the breadth of capabilities that can be operated by users remotely. In addition to Cascade, EMSL's supercomputer, all NMR and EPR instruments, x-ray diffractometers, and the focused ion beam scanning electron microscopes (**Figure 4.2**) can be operated from offsite. Remote activity allows users to run the instrument from any location in the world, with minimal assistance from EMSL staff to load or change out samples. Initial use typically begins with onsite operation to become familiar with the instruments before using from their home institutions. The remote access has been especially helpful for operational efficiency in that vendors can log on to diagnose and tune instruments. Staff scientists can log in from offsite when onsite users are having problems after hours or run multiple instruments at once. In addition, operating instruments in RadEMSL from user turnaround office space eliminates the time and expense of taking extensive radiological training for laboratory access.

Figure 4.2. This scanning electron microscopy image is of the protein ubiquitin mixed with a MALDI matrix from which samples for atom probe tomography were prepared. The image will help researchers choose regions for further detailed atomic-scale characterization of these proteins by atom probe tomography analysis.

In addition to operating instruments located at EMSL from offsite, we have several specially designed compact portable platforms that can operate on a lab bench, deployed onsite in the field, or installed on aircraft. These platforms, such as the aerosol mass spectrometer and single-particle laser ablation time-of-flight mass spectrometer, typically have been related to aerosol research efforts and have enabled and supported field campaigns around the world, such as GOAmazon. They have been featured in the NY Times and the DOE Pulse and results have been published in the *Proceedings of the National Academy of Sciences* [31, 32, 33].

Finally, we are working to ensure our digital information portals are providing appropriate levels of data, information, tools, and other support to conduct research. We are working on a consolidated information portal called MyEMSL, to provide "one-stop" access to data for our users, other DOE facility users (e.g. DOE JGI, DOE Systems Biology Knowledgebase, and Bioenergy Research Centers), the broader scientific community, and the public. MyEMSL includes a functional data management engine and search interface, and already has EMSL data and metadata from the PRISM proteomics database and genomics data from JGI. A test interface dramatically simplified and accelerated automatic downloads of JGI genomics data. Independent evaluations of the system have already been performed and provide the foundation for plans to expand MyEMSL to other EMSL data types, with the eventual goal of semi-automated uploading and annotation of data from all major instruments. As MyEMSL continues to develop and becomes more closely integrated with other EMSL portals, expanded mechanisms for automated data archival and delivery will become prevalent over manual data transmission paths.

10-year Goals and Metrics of Success	Key Partnerships or Other Needs
Enhance EMSL's science communication outreach via blogs, trade publication commentary and leadership pieces, and science media.	One FTE science writer to increase communication of EMSL's science to bloggers, professional societies, and science media.
Strengthen EMSL's position as an expert resource for BER scientific community.	Will involve webinars, tutorials
Establish collaborative research opportunities with other national laboratory user facilities for expedited access to multi-facility and multidisciplinary resources and accelerated results. Partner to establish fast-track access for small allocations of time outside of Calls.	Chief Science Officers at BER-aligned light sources to develop joint calls. Interlaboratory software development NUFO supported User Portal for multi-facility access.
Integrate access to EMSL into BER announcements for Annual Funding Opportunities for cohesive application process and accelerated access.	BER Program Managers to support idea of embedded EMSL access. Integrated application software/data streams.
Enhance instrument training materials for increased and effective resource utilization under existing budgets.	EMSL's management to develop, enhance, and deploy training materials for web-based access.

5.0 Critical Actions

Sections 1-4 described our overarching goals and three strategic objectives:

- Advance EMSL's scientific leadership, impact, and alignment to BER/DOE scientific missions through our science themes and leadership areas (Strategic Objective 1)
- Advance EMSL's capabilities (a combination of world-class expertise, state-of-the-art equipment, and mission-ready facilities) and accelerate their utilization for breakthrough science (Strategic Objective 2)
- Maintain an engaged and productive user community through sustained excellence in operations and management, including outreach and user experience (Strategic Objective 3).

In the sections that follow, we describe the critical actions where sustained, focused effort and resources are needed over the next three-to-five years to accomplish these objectives.

5.1 Advance EMSL's Scientific Leadership, Impact, and Alignment

Demonstrating scientific leadership is essential to creating recognition, visibility, and ultimately engagement by the scientific community. To do this, we will focus our annual proposal call in areas that fill gaps in understanding and on key questions defined by the scientific challenges described in Section 2. Selected proposals will create a cohesive portfolio of user projects that collectively and individually advance understanding.

We will invest in internal projects using the EMSL Intramural Research Program and PNNL Laboratory-Directed Research and Development funds for scientific impact. Addressing the science challenges will become the main driver for the user program, bringing together collaborative users for maximum effect.

We also expect our staff scientists to be leaders in their fields and take on leadership opportunities within their respective scientific communities. EMSL's management is committed to developing scientific leaders among our staff, and we use our annual performance planning and review processes to reinforce this expectation and reward or correct individual performance.

Measures of progress will include increased EMSL publications in top tier journals, attracting leading scientists as users and scientists, organizing and leading sessions at national meetings, organizing and participating in workshops to define future scientific directions, affirmative external peer review, strong citation analysis, and additional research programs in these leadership areas. Appendix B contains detailed implementation plans for each of the four science themes.

Because visible and recognized scientific leadership is critical to EMSL's success, we are also committed to attracting, developing, and retaining a diverse, engaged, and productive workforce. Most importantly, this leadership must deliver sustained scientific impact, and operational and management excellence. Our success ultimately relies on staff performance and leadership and on the ability of management to recruit, foster, and grow top scientific, operational, and managerial talent. To do this, we use a variety of approaches including 1) targeted hiring, 2) using our Wiley Fellowship programs to engage outside scientists as partners, and 3) mentoring our early career staff. Management develops annual hiring plans, and our current (two- to four-year) plans are included in the summary of critical actions shown in Section 5.4. Strategic hires in the next two-to-four years will target leadership in plant sciences, aerosol/earth-system chamber studies, metabolic modeling, microbial cell biology, enzymology, soil biogeochemistry, radiochemistry, multiscale simulation, and pore-scale science. Hiring priorities are updated quarterly, and advertisements are in influential scientific journals (e.g., *Science*, *Nature*) and trade publications that target outstanding candidates.

For staff at EMSL, we provide support and resources for them to fully develop their careers and create a work environment that enables highly engaged people to work with passion, to drive innovation, and to move the organization forward to higher levels of scientific productivity. Key to these actions is active participation in PNNL-sponsored, nationally recognized leadership development programs, including the Scientist and Engineer Development Program focused on building and growing early career scientists and engineers. Measures of progress will be to increase the number of: 1) strategic hires, 2) EMSL scientists who win early DOE career awards, 3) EMSL scientists who reach the rank of Laboratory Fellow (PNNL’s highest scientific rank), 4) named fellows in scientific societies, and 5) national and international awards.

5.2 Identify, Develop, and Rapidly Deploy Capabilities to the Scientific User Community

EMSL has some of the most comprehensive and unique suites of scientific capabilities in the world and is poised to catalyze even greater scientific advancements through recently established or to-be-developed technical capabilities. Working with users, science advisors, and stakeholders, we use the compelling scientific questions that need to be answered to drive our capability investments.

Section 3.3 described our planned capability development efforts for the future, and we will employ workshop-based and other community-based approaches to engage the scientific community in defining science needs and capability development efforts that will be required to support the science. As new capabilities are developed, we will also have a plan in place (similar to the action plans developed for RadEMSL, the 21T FTICR mass spectrometer, and Quiet Wing described in Section 3.2) to ensure rapid use, with preplanned experiments and a pipeline of users. And, as part of the investment plan, we will divest from and sunset instruments that are no longer aligned with our strategies, or are underused by our scientific user community. In this way, existing financial and personnel resources can be reassigned to activities that are better aligned and more impactful.

As new capabilities are developed, we take the following actions to maximize their use and benefit to the scientific community and BER research priorities:

- Establish advisory committees for each capability area, as appropriate, that will assist in identifying near-term scientific opportunities that will produce high-impact science; identifying and facilitating outreach opportunities; cultivating high-impact users; and providing advice on proposal selection as appropriate.

- Review existing user projects and newly submitted proposals. Projects and proposals with clear BER alignment and potential for high-impact science will receive additional attention, staff time, and funding and priority access to key capabilities to accelerate their progress and heighten chances of success.

- Hold a special call for every new capability developed to the broad scientific community and conduct an aggressive outreach effort to heighten awareness and generate promising proposals, and to ensure sustained, active use of these new capabilities.

Measures of progress include the number of new instrument systems deployed and sunsetted, leadership in forward-looking capability/science workshops, time from deployment to publication, major invited talks (by EMSL's staff and users), review papers that highlight EMSL's preeminent capability, and inclusion/mention in National Academy or other reports and projections on science and technology directions.

5.3 Maintain an Engaged and Productive User Community

An engaged and productive scientific user community is critical to EMSL's success. Consequently we have a robust user outreach program involving established scientists and early career researchers as described in Section 4. Once attracted to the facility, establishing and building user loyalty and advocacy is paramount to our long-term success. The best mechanisms for attracting such users are to communicate scientific accomplishments and impact, while also communicating tremendous opportunities and unique capabilities EMSL provides. To do this we will:

- Distribute an electronic newsletter featuring science highlights, proposal calls and new resource availability, providing timely, relevant information to past, current, and potential users.

- Conduct annual user meetings focused on specific research topics aligned with BER's objectives and EMSL's science themes that provide an opportunity to focus the scientific user community, build new collaborations and partnerships, and increase awareness of our capabilities.

- Develop an intuitive external website to support the development of an engaged user community.

- Produce tailored literature on our scientific accomplishments and impact, along with descriptions of our capabilities to build awareness within the scientific community.

- Actively encourage our current users and scientists to promote EMSL through presentations at scientific meetings and conferences, journal publications, and discussions with their colleagues and EMSL/PNNL scientists.

- Benchmark our performance against other user facilities, and with our user community, identify best practices and continuously improve our performance. This includes the triennial communications survey of past and current users to identify the most effective and efficient communication mechanisms.

The measure of success is an increase in the number and productivity of users conducting BER-relevant research.

As the complexity of our scientific challenges and collaborations increase, so do the requirements and expectations for our information technology systems and infrastructure. These systems and infrastructure must enable seamless collaboration between distant locations with novel and flexible networking and cyber systems. Enabling scientists from multiple and disparate locations to work together productively will become the norm and our data management and data portal systems will need to facilitate near-real-time access to user data, open sharing of public information, and provide the analysis tools for translating data into knowledge and understanding.

To achieve this vision, over the next one-to-two years, we will complete and release MyEMSL to enable experimental data capture and retention, required public release of data, and collaboration and dissemination of archived data. Once those aspects of the software are in place and functioning well, we will work over the next few years to establish data sharing and collaboration capabilities with partner institutions. Measures of progress include the dissemination of information via our data portal and user feedback.

The safety and welfare of our staff, users, and the environment continues to be our highest operational priority. We leverage PNNL's worker safety and health and environmental sustainability programs to properly train EMSL's scientists and users for the work they conduct, ensure they understand their responsibilities, and support them in reducing the amount of waste they generate.

The use of PNNL's Integrated Operating System (IOPS) ensures hazards are identified, mitigated, and communicated effectively. While IOPS has consistently proven to be a "best practice" for effectively managing space-based hazards, we have identified several areas for continuous improvement, including the use of mobile technologies for better communication and increased efficiency. Using mobile technology to communicate space-based hazards and simplify assessments will improve our ability to recognize and manage complex hazards. Additionally, maturing web-based translation services delivered through smart devices holds significant promise to overcome language barriers inherent in serving a global scientific user community.

EMSL is recognized within PNNL and the community as a leader in sustainable operations. Our scientists and users are committed to creating a culture of sustainability. Examples include a staff-developed process to reuse printer paper, significant participation in the telework and alternative commute program, new controls for vacuum pumps that significantly reduce run time, and smart power controllers that dramatically reduce power consumption on equipment during idle time.

We are planning a significant change in how cooling water is supplied to our High Performance Computing Facility (HPCF). This new approach will provide higher temperature cooling water at significantly reduced cost and dramatically improve the efficiency of the HPCF, EMSL's largest electrical power consumer. Lastly, our focus on incorporating both passive and active technologies that reduce waste, energy use, or labor in facility modification operations resulted in the use of mobile casework in RadEMSL, providing significant operational flexibility at reduced cost.

Measures of progress include Days Away Restricted or Transferred (DART), Total Recordable Cases (TRC), Price-Anderson Amendments Act (PAAA), waste reduction metrics, Data Center Power Utilization Effectiveness (PUE), and staff participation metrics in PNNL sustainability programs (i.e., telework).

5.4 Critical Actions, Metrics, and Timeline

Critical Action	As Measured By	1-2 Years	2-5 Years	Steward
Accelerate EMSL's scientific leadership	Total and top-10 publications	Focused annual calls	Refreshment of focus areas through workshops	EMSL Chief Scientist
		Increase number of EMSL publications in premier journals (*Science, Nature, PNAS*) by a factor of three from an average of 10 per year to an average of 30 per year by 2019.		
	Distinguished users	Investment of EMSL intramural and PNNL resources		
	External peer review	Periodic review of science themes/grand challenges		
	New research programs	Organizing and leading sessions at national meetings, organizing and participating in workshops to define future scientific directions		
	Staff scientific leadership			
Grow, foster, and recruit top talent	Strategic hires EMSL's staff early career awards Laboratory Fellows Society fellows/awards	Strategic hires in metabolic modeling, microbial cell biology, plant physiology and biochemistry, soil chemistry, radiochemistry, earth-system chamber studies, multiscale simulation	Strategic hires in pore-scale science enzymology Refreshment of hiring plan	EMSL Director and Associate Director for Science and Technology
		Staff engagement activities		
		Leadership development programs		
Identify, develop and rapidly deploy capabilities to the scientific user community	New capabilities deployed and sunsetted Workshop leadership on new capabilities Time from deployment to publication External recognition, e.g.,	Workshops to identify new capabilities Benchmarking visits Development of new MIE requests/proposals	Bring new or expanded plant growth, aerosol chamber, metabolomics/omics, single-cell capabilities online Collaborations established on key capabilities Project/Technical success on MIE projects	Chief Technology Officer, Science Theme Leads

Critical Action	As Measured By	1-2 Years	2-5 Years	Steward
	review papers, reports, and projections on S&T directions, invited talks and capability lectures	Rapidly deploy new capabilities through acceleration plan (advisory groups, special calls, EMSL-led workshops at scientific meetings and other outreach activities)		
Raise awareness of EMSL and attract new users to the facility	Number of new users and submitted proposals	Execute outreach strategy, which includes newsletters, user meetings, website, highlights, benchmarking and surveys		EMSL Director
Build a collaboration infrastructure that supports forefront science	Dissemination of information via our data portal; user feedback	Complete and release MyEMSL to enable: 1) experimental data capture and retention, 2) public release of data, and 3) collaboration and dissemination of archived data	Establish data sharing and collaborations capabilities with partner institutions Submission and management of MIE projects	Chief Operating Officer
Ensure safe, secure, and sustainable operations	DART, TRC, PAAA, waste reduction metrics, Data Center PUE, and staff participation metrics in PNNL sustainability programs (i.e., telework)	Develop mobile technology-based tools Implement new approach to cooling water supply		Chief Operating Officer

6.0 Translating the Plan into Action

Implementation is the responsibility of the Director, Associate Director, Chief Officers, and internal groups responsible for planning and performance. Together, they will establish individual performance appraisals that will measure staff accountability and alignment with organizational goals. Annual metrics will track progress.

6.1 Annual Planning Process

This strategic plan is EMSL's template for achieving our vision of simultaneous excellence in all our strategic objectives. It provides the foundation for EMSL's annual planning, budget, and performance assessment processes and documents (**Figure 6.1**). EMSL employs a "plan-do-review" approach to annual planning. Each year, the EMSL management team assesses progress against our objectives and critical actions and then crafts a set of annual actions with project plans as appropriate, along with measures and targets that will guide work during the next year.

Figure 6.1. EMSL's "plan-do-review" approach to annual planning

Actions, timelines, and milestones are captured in our annual performance plans. Metrics measuring progress and our assessment plan ensure proper oversight and assurance of policies and procedures.

6.2 Making Investment Decisions

As part of the annual planning process, management identifies areas for future investment by balancing the need to invest in emerging long-term opportunities with pressing near-term needs and challenges (**Figure 6.2**). This planning effort may require sustained levels of investment over many years, or it may be more narrowly focused and change from year to year. Proposed investments are evaluated against the following:

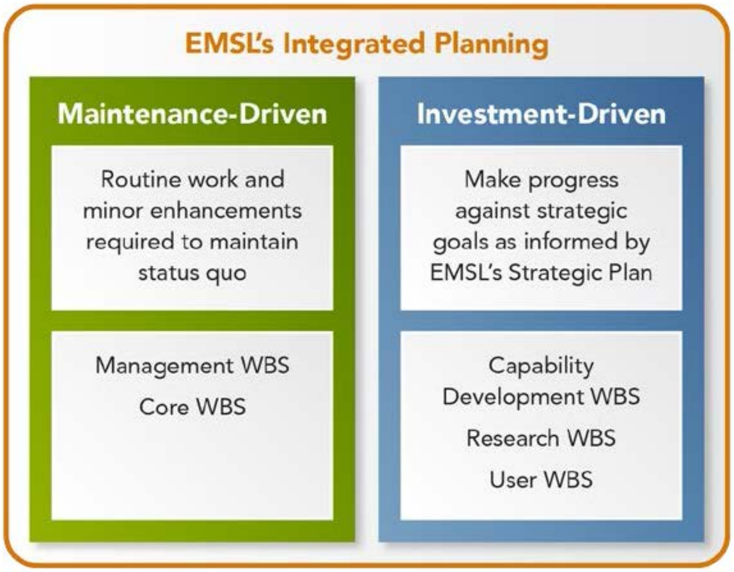


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Figure 6.2. EMSL's integrated planning balances long-term investments and near-term needs

- Alignment–Alignment with EMSL’s and BER’s mission, vision, and strategic objectives. Deciding factors include whether investments lie within the bounds established by our strategic plan, effectively address multiple goals, and do not duplicate efforts of other institutions.

- Impact and Transformation–Promote ideas that are compelling, innovative, and transformative. Deciding factors include the extent to which investments may transform a field of science, position EMSL at the forefront of an emerging field, and contribute to national research and development priorities.

- Budget and Funding–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.

- Strengthen Collaborations–Create opportunities for new, or strengthen existing, collaborations. Deciding factors include whether investments augment other BER or DOE activities, leverage other community or federal agency investments in research and infrastructure, and broaden participation in EMSL’s user program. We will also leverage industry assets and planning processes where appropriate.

- 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.

- Risk–Ensure risk is managed effectively. Deciding factors include risk mitigation approaches, risk reward ratio, and potential damage to EMSL’s and DOE’s reputation.

6.3 Performance and Assurance Management

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

Governance

Set Strategic Direction–EMSL's senior management, with input from EMSL's advisory committees, PNNL senior management and BER, sets the direction of EMSL, aligns resources with goals, approves operational and business boundaries, and monitors progress.

Management

Translate Strategy into Tactics–EMSL's management deploys resources to achieve 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.

Performance

Conduct Work–EMSL's scientists and users conduct work using processes, procedures, and tools to accomplish their objectives, while managing within established operational limits.

Assurance Processes Validate Performance

EMSL's leadership employs means such as internal audits and assessments, independent oversight, peer reviews, and benchmarking to provide reasonable assurance goals are 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 accurate and reliable data are being delivered to decision makers. Assurance is also used to verify users receive 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's management develops an annual Performance Management and Assessment Plan with an associated dashboard that evaluates and tracks performance against defined goals, objectives, and metrics across EMSL's 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 areas.

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Appendix A

Description of EMSL’s Physical Facility

Description of EMSL's Physical Facility

Since commissioning in 1997, EMSL has grown to meet the evolving mission. These strategic expansion projects have enabled EMSL to meet the growing demand in the user program, adapt to changing technology, and better align with the user community and DOE needs. Recent examples include the development of the Quiet Wing and RadEMSL.

Open in early 2012, the 9,500-square foot Quiet Wing provides a unique research environment that protects against multiple sources of interference, including acoustic noise, floor vibrations, air flow, temperature fluctuation, and electromagnetic interference. The Quiet Wing features eight quiet laboratory cells housing a unique collection of microscopy and scanning instruments, which benefit a wide range of research areas including microbiology, structural biology, atmospheric aerosol morphology and composition, subsurface science, catalysis, and fuel cell/energy storage.

In spring of 2013, RadEMSL opened to accelerate scientific discovery and deepen understanding of chemical fate and transport of radionuclides in terrestrial and subsurface ecosystems. The co-location of a radiochemistry user facility with a full suite of state-of-the-art instrumentation is unique in the United States, and one of just a few worldwide.

This facility offers the ability to make a variety of molecular measurements on radiological materials. Instruments include nuclear magnetic resonance and x-ray photoelectron spectroscopy, a variety of scanning and transmission electron microscopies, and an electron microprobe, all useful to study contaminated environmental materials, radionuclides, and chemical signatures.

Expansion plans include a high-efficiency cooling infrastructure to support high-performance computing and new facilities to support expanding research in metabolic compartmentalization and biogenic organic aerosols, and ensure the EMSL's users and scientists have sustained scientific impact.

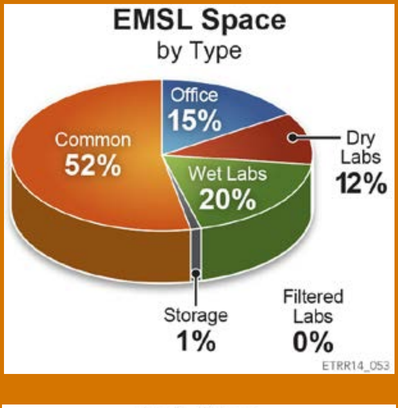
EMSL at a Glance

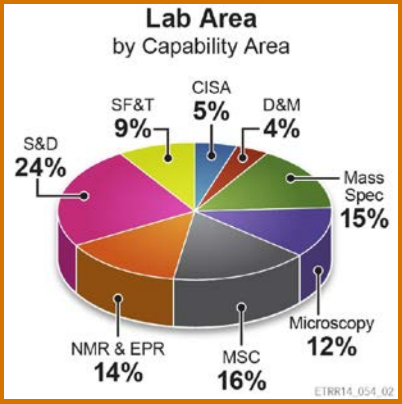
Facility Facts

Constructed: 1997
Construction Cost: $229.9 M
Original Size: 198,300 sf
Current Size: 239,000 sf

Space Details:

Lab Area: 77,500 sf
Lab Count: 84 laboratories
Office Area: 36,900 sf
Office Count: 270 offices
Storage Area: 1,300 sf
Common Area: 125,300 sf





Occupancy:

Staff Total: 382
EMSL Staff: 192
PNNL Staff: 190

Figure A.1. Schematic floor plan of RadEMSL (inset) and EMSL

Appendix B

Five-year Science Theme Implementation Plans

Five-year Science Theme Implementation Plans

Table B.1. Five-year BDD Implementation Plan Timeline

<table>
<tr><th>Critical Action</th><th>As Measured By</th><th colspan="2">1-2 Years</th><th colspan="2">3-5 Years</th></tr>
<tr><td rowspan="2">Extend EMSL’s leadership</td><td rowspan="2">EMSL-led workshops
EMSL-led symposia
AC and reviews
Invited talks
Early career and staff awards
Total and top-10 publications</td><td colspan="4">Chair symposia at national meetings (e.g. ASM, SIMB, GRCs)</td></tr>
<tr><td colspan="2">Workshop: Metabolic exchange
Workshop: Metabolic modeling grand challenge
Workshop: Plant phenomics</td><td colspan="2">Workshop: Modeling metabolism in microbes and plants</td></tr>
<tr><td rowspan="3">Capabilities for the user community</td><td rowspan="3">Peer review recognition of leadership
User demand for new capabilities</td><td colspan="2">Metabolomics
• Mass spectrometry
• NMR
• Fluxomics/informatics</td><td colspan="2" rowspan="2">21T FTICR mass spectrometer
• Top-down proteomics
• Imaging
Data interpretation and visualization tools for MS data</td></tr>
<tr><td colspan="2">Bioimaging
• Electron and light microscopy
• Mass spectrometry imaging</td></tr>
<tr><td colspan="2">Initiate metabolic modeling grand challenge
• Model system
• Generate initial metabolite abundance data</td><td colspan="2">Phase II metabolic modeling grand challenge
• Integration of transcriptomics and proteomics
• Compartmentalization</td></tr>
<tr><td rowspan="3">Hire, matrix, and mentor scientific leadership</td><td rowspan="3">Increase leadership in plant biology and microbiology</td><td>Plant science and metabolic modeling hires</td><td>Microbial cell biology hire</td><td>Enzymology hire</td><td>Hire, TBD</td></tr>
<tr><td colspan="2">Postdoctoral researchers</td><td colspan="2">Postdoctoral researchers</td></tr>
<tr><td>Intramural projects in plant biology</td><td>Intramural project in microbiology</td><td colspan="2">Intramural projects, TBD</td></tr>
<tr><td>Infrastructure needs for emerging science</td><td></td><td colspan="2">Develop science case for plant phenomics platform</td><td colspan="2">Plant phenomics platform</td></tr>
<tr><td>Collaboration across user facilities</td><td>Joint proposal calls</td><td>Develop science case/pilot proposals with structural biology user facilities</td><td>Issue call for pilot projects</td><td colspan="2">Annual joint calls</td></tr>
</table>

Table B.2. Five-year AAS Implementation Plan Timeline

<table>
<tr><th>Critical Action</th><th>As Measured By</th><th colspan="2">1-2 Years</th><th colspan="2">3-5 Years</th></tr>
<tr><td rowspan="2">Extend EMSL leadership and visibility in AAS research</td><td rowspan="2">EMSL-led workshops
EMSL-led symposia
SAC and reviews
Invited talks
Early career and staff awards
Total and top-10 publications
Peer review recognition of leadership</td><td colspan="4">Chair symposia at national meetings (e.g. AGU, AAAR, GRC)</td></tr>
<tr><td colspan="2">Workshop: Novel high-resolution mass spectrometry approaches for atmospheric organics
Workshop: Multi-modal dynamic chemical imaging of atmospheric particles
Workshop: Earth system chamber for biosphere-atmosphere-cloud-climate studies</td><td colspan="2">Organize additional workshops</td></tr>
<tr><td rowspan="3">Enhance capabilities for the user community</td><td rowspan="3">Develop and deploy new capabilities
High user demand for new capabilities</td><td colspan="2">Novel high-resolution mass spectrometry approaches for atmospheric organics</td><td colspan="2" rowspan="2">Earth system chamber for biosphere-atmosphere-cloud-climate studies</td></tr>
<tr><td colspan="2">NWChem computational chemistry applied to particle formation and growth</td></tr>
<tr><td colspan="2">High-resolution explicit model of biogenic emissions and secondary aerosol growth for evaluating earth-system model parameterizations</td><td colspan="2">Multi-modal dynamic 3D chemical imaging of atmospheric organic aerosol</td></tr>
<tr><td rowspan="3">Hire, matrix, and mentor scientific leadership</td><td rowspan="3">Increase leadership and depth in plant volatile organic emissions and aerosol science</td><td>PTRMS/CIMS hire</td><td>Plant VOC physiology/ biochemical hire</td><td>Earth system chamber hire</td><td>Hire, TBD</td></tr>
<tr><td colspan="2">Postdoctoral researchers</td><td colspan="2">Postdoctoral researchers</td></tr>
<tr><td>Intramural projects in atmospheric ecometabolomics</td><td>Intramural project in phyllosphere</td><td colspan="2">Intramural projects, TBD</td></tr>
<tr><td>Partnership with ARM and ASR</td><td>Collaborative field studies</td><td colspan="2">EMSL's leadership of a molecular-scale contribution to an ARM field campaign that informs ASR modeling activities</td><td colspan="2">Second field campaign</td></tr>
</table>

Table B.3. Five-year TSE Implementation Plan Timeline

<table>
<tr><th>Critical Action</th><th>As Measured By</th><th colspan="2">1-2 Years</th><th colspan="2">3-5 Years</th></tr>
<tr><td rowspan="2">Extend EMSL’s leadership</td><td rowspan="2">EMSL-led workshops
EMSL-led symposia
SAC and reviews
Invited talks
Early career and staff awards
Total and top-10 publications</td><td colspan="4">Chair symposia at national meetings (e.g. AGU, Migration, ACS)</td></tr>
<tr><td colspan="2">Workshop: Tc chemistry challenges in environmental science and nuclear fuel cycle
Workshop: Unsaturated pore-scale biogeochemistry of thin water films</td><td colspan="2">Workshop: Belowground carbon dynamics in wetlands
Workshop: Root processes</td></tr>
<tr><td rowspan="3">Capabilities for the user community</td><td rowspan="3">Peer review recognition of leadership
User demand for new capabilities</td><td colspan="2">SOM characterization
• HRMS
• NMR
• Computational chemistry</td><td colspan="2" rowspan="2">21T FTICR mass spectrometer studies of SOM, rhizosphere
Data interpretation and visualization tools for MS data</td></tr>
<tr><td colspan="2">Spatially-resolved-multimodal rhizosphere studies
• TEM
• Confocal fluorescence microscopy
• LA-AMS</td></tr>
<tr><td colspan="2">Complete pore-scale modeling challenge
• reactive transport
• multiphase displacement</td><td colspan="2">Unsaturated pore-to-core-scale experimental capability
in-situ CXT and MRI for rhizosphere studies</td></tr>
<tr><td rowspan="3">Hire, matrix, and mentor scientific leadership</td><td rowspan="3">Increase leadership in soil chemistry and radiochemistry</td><td>Soil chemistry hire</td><td>Radiochemistry hire</td><td>Pore-scale hire</td><td>Plant hire</td></tr>
<tr><td colspan="2">Postdoctoral researchers</td><td colspan="2">Postdoctoral researchers</td></tr>
<tr><td>Intramural projects in soil chemistry</td><td>Intramural project in radiochemistry</td><td colspan="2">Intramural projects, TBD</td></tr>
<tr><td>Infrastructure needs for emerging science</td><td></td><td colspan="2">Develop science case for:
Plant/aerosol chambers</td><td colspan="2"></td></tr>
</table>

Table B.4. Five-year EMP Implementation Plan Timeline

Critical Actions	As Measured By	1-2 Years	3-5 Years
Enhance EMSL's visibility/leadership in EMP areas	EMSL-led symposia EMSL-led workshops	Organize/lead symposia for national/international meetings	
		AAAS, AVS	ACS, ECS
	Invited talks	Organize workshops	
	Staff awards	Presentations and major meetings	
		Visit targeted leading institutions/researchers	
Assemble, grow and enable critical mass to enhance scientific progress	Growth in top-10 and highly cited publications	Build teams with critical expertise (PNNL, user, projects)	
		IIC partnership	Research Campaign
		JCESR, BATT, FCSD	
	EMSL and users receive recognition for scientific impact	Develop staff expertise	
		Recruit scientific leaders as users	
		New EFRC awardees	
		Engage scientific leaders as Wiley and Visiting Fellows	
		2	2
	EMSL recognized as leader in group/team approach to molecular science	Fill expertise gaps with staff, hires, or visiting scientists	
		Electrolyte expertise	Electrochemist
		Build programs from existing projects	
	Distinguished users	BES, JCESR, BATT	
Provide cutting-edge capabilities to users	High demand for cutting-edge capabilities	Enhance visibility/use of NWChem for catalysis	Extend NWChem capability for reliable mesoscale calculations
		Continue advances in *in-situ* probes for NMR, EPR, EM, x-rays, others	
		Keep pushing frontiers of real-time measurements	
	New capabilities developed and deployed	Apply DTEM	Push toward ultrafast microscopy capability, next generation NMR
		Partner with Advanced Light Source to provide easy access to important tools and other capabilities	
		Store and deliver data in a "semantic" structure that enhances ability to integrate and transfer data to address fundamental and applied challenges	

Appendix C

Five-year Capability Development and Implementation Plan

Five-year Capability Development and Implementation Plan

Critical Action	As Measured By	1-2 Years	3-5 Years
Develop, enhance EMSL's metabolomics and single-cell analysis capabilities	Recognition of leadership (invited talks, review articles) User demand, interactions External funding	Metabolomics • Add new metabolomics instrumentation (GC QTOF MS) • Add 2 FTEs (new personnel), including statistical/computational expertise Single cell • Develop new FISH, CyTOF techniques for single-cell analysis	• Advanced spatial-metabolomics analysis capability in place, rivaling proteomics reputation • Integrated NMR/MS efforts in metabolomics • Integrated, single-cell analysis to quantify microbial community diversity
Establish EMSL as the go-to laboratory for NOM/SOM characterization	Peer recognition of leadership User demand for new capabilities DOE viewed as leader in this area Collaborative inclusion in major proposals	MS capability • Add new, dedicated environmental MS (NOM) capability • Couple with AAS MS efforts	• EMSL's MS, NMR capabilities have wide use by BER researchers for SOM/NOM • Integrated NMR/MS in SOM/NOM area • New senior staff in these areas
		NMR capability • Demonstrate NMR, EPR relevance, application	
		Microscopy capability • NanoSIMS, DTEM application • Ultrafast microscopy mapability MIE funded and underway	• NanoSIMS, DTEM in wide use by BER researchers • Ultrafast microscopy capability completion
Develop and establish new plant phenomics science/capability focus	Plant phenomics space, facility, capability infrastructure; Emergent capability recognition Unique, new user facility capability	• Establish basic plant science space and capability • Hold plant phenomics workshop(s), technical sessions, etc. • Conduct benchmarking studies of existing plant phenomics centers • Develop master plan for plant phenomics science and capabilities	• Continue to build plant science capability (staff, instrumentation) • Develop, submit, obtain approval for MIE item for signature plant phenomics capability
Develop and establish aerosol/earth-system capability	Aerosol science space, facility, capability infrastructure enhancements Emergent capability recognition for biogenic aerosol analysis Unique, new user facility capability	• Coordinate and optimize existing aerosol science capabilities • Add additional AMS capability to support additional field/lab studies • Enhance biogenic aerosol analysis capabilities • Benchmark existing aerosol/earth-system chambers and facilities • Develop master vision/plan for aerosol science and capabilities	• Establish expertise in biogenic aerosol characterization • Develop, submit, obtain approval for MIE investment in aerosol/earth-system chamber/capability
Enhance *in-situ* capabilities for energy materials	Recognition of leadership (invited talks, review articles) User demand, interactions External funding	• Develop new *in-situ* cells and techniques for catalysis, interface characterization • Full development and application of DTEM • Ultrafast microscopy capability MIE funded and underway	• Strong reputation in *in-situ* microscopy • Ultrafast microscopy mapability completion, unique applications in progress and/or published

Appendix D

Progress against EMSL 2008 and Draft 2011 Strategic Plan Objectives

Progress against EMSL 2008 and Draft 2011

Strategic Plan Objectives

This appendix provides a status of critical actions from the EMSL 2008 and draft 2011 strategic plans:

- Establish scientific leadership in EMSL's science themes
- Develop and deploy transformational scientific capabilities to the scientific user community
- Integrate computing with experiment
- Create partnerships
- Ensure scientific leadership meets challenges of the future
- Attract and engage users in EMSL's long-term strategy
- Create partnerships.

D.1 Critical Action: Establish Scientific Leadership in EMSL's Science Themes

Metric: Total and top-10 publications and SAC ad hoc reviews

4-year outcome: SAC ad hoc review of each science theme (one per year)

Steward: Chief Scientist

Status for SAC ad hoc review of each Science Theme (one per year): Completed. EMSL provides a status update of the science themes to the SAC each year. Updates include reports of STAP meetings, user highlights, publications with a percent appearing in top-10 journals, and planned changes or goals.

The following activities helped advance the goals for each science theme.

1) BID (BDD)–EMSL developed a collaborative science program with JGI that would allow researchers to combine the power of genomics and molecular characterization in one proposed research project. This joint opportunity was announced in EMSL's FY 2013 Call for Proposals.
2) GBSS (TSE)–In 2010, the GBSS STAP identified a pore-scale modeling challenge that would improve our ability to predict and modify pollutant transport or transformation in the subsurface. In 2011, 40 participants from 14 institutions representing both experimental and modeling communities discussed research challenges that impede progress in the development of predictive models. Two major research areas were identified where fundamental experimental data sets are needed to advance modeling and simulation. A new paradigm for how experimental data generated at EMSL could be shared with the modeling community to greatly facilitate model development and validation was endorsed. This led to the pore-scale modeling research campaign in 2012. Based on information from this campaign, all

current models required significant modification to accurately simulate and predict experimental results. Several publications are already in press, including Oostrom et al. *Computational Geochemistry,* 2014.

3) Science of Interfacial Phenomena (SIP) (EMP)–Focusing the annual call topics led to increased user projects directed toward developing new understanding that enables the optimization of interfacial properties, such as the control of catalytic activity and longevity. To support these projects, a suite of *in-situ* and real-time methods to collect high-resolution structural and chemical information were developed, as well as combined spectroscopy and microscopy for 3-dimensional analysis of structures, including buried interfaces. Fulfilling both the 2008 plan and the 2011 drafted strategic plan, EMSL completed and deployed a NanoSIMS, OA-MBE, and chemical TEM. The TEMs provide *in-situ* real-time measurement with gas and liquid stages. A gas heating state is being developed with Hummingbird, and a unique gas handling system has been used heavily by the user community. This unique system delivers up to 10 different gases to the sample of *in-situ* experiments and was prominent in the multi-lab effort led by Haimei Zheng from LBNL to examine real-time changes in the atomic structure of nanoparticles to improve bimetallic catalysts for fuel and chemical industries. *Nano Letters*, 2014, 14(6): 3203-3207. DOI: 10.1021/nl500553a.
4) AAC (AAS)–In 2008, the committee felt the Atmospheric Aerosol Chemistry (AAC) Science Theme was not strong enough to stand alone and recommended it be captured under the SIP until EMSL brought in leadership and a user community was more fully developed. Since that recommendation, EMSL has partnered with PNNL's Atmospheric and Global Change Division to stand up the new AAS Science Theme.

Status for Assess Aerosol Science Theme: Completed. Beginning in FY 2009, the AAC Science Theme was subsumed under SIP, and annual calls for proposals included focused aerosol topics to begin building the user community. In 2013, with the hire of Alex Guenther and increased collaboration with PNNL's ARM user facility and Atmospheric Sciences and Global Change division, the AAS Science Theme was announced. Submitted proposals with aerosol-relevant research have doubled since FY 2011.

Status for Deep Dive New Science Theme Area: On hold. EMSL led a deep dive to identify biology research that would advance BER mission areas and bring in additional leadership in our BDD Science Theme. Although PNNL put the deep dive on hold in order to refocus the PNNL-level strategy for biology, it forced us to take a critical look at biology in EMSL and FCSD. As a result, we hired Scott Baker as Science Theme Lead to develop our current strategy and leadership area in biology.

D.2 Critical Action: Develop and Deploy Transformational Scientific Capabilities to the Scientific User Community

Metric: New capabilities

4-year outcome: 21T FTICR mass spectrometer (CD0 in FY 2009)

Steward: Chief Technology Officer

4-year status for 21T FTICR mass spectrometer (CD0 in FY 2009): Completed. Approval and project funding were received in late 2010, and construction is underway. As of August 2014, the 21T FTICR mass spectrometer reached 21T and testing is expected to begin in mid-August.

1-2-year status to make decision on NanoSIMS: Completed. EMSL was the first user facility in the world to make a NanoSIMS available to users. Funded by the American Recovery and Reinvestment Act of 2009, and available for users in FY 2012, the NanoSIMS can be used for enhanced imaging of cellular structures; simultaneous imaging of elements/isotopes on minerals and soft surfaces at the nanoscale; and imaging elements and isotopes of aerosols, nanoparticles, and organic and inorganic surfaces.

1-2-year status for second recapitalization workshop: Revised and in process. In lieu of a large workshop like the 2006 Recapitalization Workshop, EMSL decided to address and couple its science and capability needs in the form of STAP workshops. Advantages include smaller, more focused working groups, more specific and directed recommendations, and lower costs and logistics. Following the completion of the four science theme workshops in mid-August 2014, recommendations from these and prior STAPs will be used to develop renewed capability plans to be reflected in EMSL’s new strategic plan.

1-2-year status for SFG/SHG: Completed. To be able to synthesize more complex controlled oxide layers and films, Lead Scientist Hongfei Wang developed two sum frequency/second harmonic generation systems. Research problems can involve areas such as liquid surfaces, catalytic, nanomaterial surfaces, geo/biogeo-surfaces, porous surfaces, and membranes. The power and application of these spectrometers have been showcased in the *Journal of Physical Chemistry C* and the *Journal of Chemical Physics*.

Steward: Science Lead for Biology

1-2-year status for build and deploy STORM: **Completed.** In support of the CISA capability, EMSL developed STORM (stochastic optical reconstruction microscope) in 2009. Also known as PALM (photo-activated localization microscopy), STORM is a fully automated super-resolution fluorescence microscope that images the intact cell with nanometer resolution. It incorporates single-molecule fluorescence techniques to reconstruct super-resolution images using software that automatically acquires and analyzes data in real time.

4-year status for build and deploy SMERF capability: Completed. Renamed SMERF to CISA (Cell Isolation and Systems Analysis) and deployed in 2009. The capability includes techniques for isolating cells from complex cell populations or environmental samples for further omics and imaging analyses.

Instruments include sequencers, mass and flow cytometry, laser capture microdissection, cell culture and bioreactors, confocal, single-molecule, and super-resolution fluorescence microscopes. A comprehensive data management system to link experimental conditions to the compositional analysis of cells and community development is underway. The integration system for proteomics and transcriptomics data is already available, but full system development was postponed pending MyEMSL design/construction.

CISA's transcriptomics instrumentation was crucial in supporting the isoprene research campaign, providing the data for a transcriptomics-based model that accurately predicts how much isoprene the bacterium *Bacillus subtilis* will produce when stressed or nourished. This insight is helping advance synthetic biology approaches to use bacteria as a clean, renewable fuel source, and demonstrated that transcriptomics measurements alone can provide the necessary information to understand what cellular states are conducive to making isoprene. *PLOS ONE* 8(6):e66104. DOI:10.1371/journal.pone.0066104

Steward: AD Enabling Technologies

4-year status for develop and implement next generation NWChem strategy: Completed. The next generation of NWChem was released in 2011 as open-source software under Educational Community License 2.0. New theoretical methodologies and algorithms capable of utilizing existing and emerging parallel architectures are continuously updated to enable petascale simulations. Development of petascale implementation of the CCSD(T) method earned a spot as a Gordon-Bell award finalist at the 2009 Supercomputing conference. NWChem has demonstrated the ability to scale various methodologies across up to 210,000 cores. The 2014 User Meeting included a focus to create a bridge between users interested in atomistic modeling of atmospheric processes and NWChem. The goal was to familiarize participants with general NWChem input structure and execution models on Cascade, in particular effectively use petascale computing platforms to tackle large problem sizes and expedite results.

D.3 Critical Action: Integrate Computing with Experiment

Steward: User Support Specialist

Metric: Proposals and publications with integrated capabilities

4-year outcome: Call for proposals that focus on integration

Status: **Completed.** Beginning with the FY 2008 call for proposals, calls announced a preference for proposals that couple experiments with theory, modeling, or simulation. In addition, we added a dashboard metric for tracking utilization of experimental and computational resources to identify projects that were lagging in expected use. In FY 2011 the AD for Molecular Science Computing reviewed each proposal submitted to identify those that could benefit from adding a computing component. To further support the integrated approach, special attention is paid during the resource allocation reviews to ensure adequate staff support is provided to proposals submitted by experimentalists with computing and data analysis needs.

D.4 Critical Action: Create Partnerships

Metric: Approved Memorandum of Agreement (MOA) and travel budget.

Steward: EMSL Director

2-4-year outcome: MOA with NHFML

Status: **Revised.** A formal MOA was never established with the National High Field Magnetic Laboratory, although informal collaborations occurred to develop the HRMAC project that will deliver the 21T FTICR mass spectrometer. These included the 2009 scoping workshop that we jointly organized, resulting in the funding for the 21T systems, instrument transfers, and participation on their Science Advisory Panel.

1-2-year outcome: Travel funding from NIH for users

2-4-year outcome: Co-funding of next Grand Challenge

Status: **Cancelled.** As part of the reevaluation of EMSL's science themes, the focus of our BDD Science Theme turned toward BER-relevant research areas.

D.5 Critical Action: Ensure Scientific Leadership Meets Challenges of the Future

Metric: New senior hires, awards and recognition, first authorship

Steward: Associate Directors

1-2-year outcome: Hire SFG/SHG Lead

Status: **Completed.** Hongfei Wang was hired in 2009 as a Science Lead for spectroscopy. In recognition of his leadership, he was elected Fellow in the American Physical Society in 2012 for his seminal contributions to the development of surface non-linear vibrational spectroscopy and to understanding molecular interaction and structure at interfaces.

1-2-year outcome: Hire TEM Lead

Status: **Completed.** Bernd Kabius, an expert in aberration-corrected TEM development and oxide interface analysis, was hired in 2010. Kabius was part of the team in Germany that developed the *first* aberration-corrected system for TEM and to first apply aberration correction to study materials science problems (Haider, et al. 1998 *Nature* 392:768). In addition, Nigel Browning was hired to work jointly with FCSD and EMSL. Browning's research focuses on the development of new methods in electron microscopy for high-spatial, temporal and spectroscopic resolution analysis of engineering and biological structures. Browning had been project leader for DTEM at LLNL and was a full professor in the Department of Molecular and Cellular Biology at University of California (UC Davis). At UC Davis, he worked on the development of DTEM to study live biological structures, and he is partnering with EMSL to develop a DTEM through a Scientific Partner Proposal.

2-4-year outcome: Hire NMR Lead

Status: **Completed.** Karl Mueller was hired in 2010 as Lead Scientist for Magnetic Resonance. His research focuses on utilizing high-resolution solid-state NMR in studies of reactive surface area in the environment, reactive sites for catalytic systems, ion structure and transport in battery materials, and radionuclide transport and sequestration under extreme geochemical conditions. He serves as lead and member of several multidisciplinary research teams including the Center for Environmental Kinetics Analysis (participant, Penn State, National Science Foundation, EMSL) and the JCESR (PI, PNNL, DOE Energy Hub).

D.6 Critical Action: Attract and Engage Users in EMSL's Long-Term Strategy

Metric: Distinguished users

Steward: EMSL Director

1-2-year outcome: Appoint six Wiley Fellows; **2-4-year outcome** Appoint six Wiley Fellows

Status: **Completed.** Since FY 2008, 18 Wiley Research Fellows have been selected for contributions to the success of EMSL as a user facility, supporting the user program beyond their own research projects.

1-2-year outcome: Award two Wiley Visiting Scientists: **2-4-year outcome:** Award two Wiley Visiting Scientists

Status: **Completed.** In 2009, EMSL selected three users, including Walter Ermler (University of Texas at San Antonio), Ian Farnan (University of Cambridge), and Alex Shluger (University of College London). Both Ermler and Shluger collaborated to integrate new *ab-initio* codes and spin-orbit operators into NWChem, while Farnan worked to develop the next stage of radiological magic-angle spinning NMR capabilities. Since then, EMSL has selected an additional six visiting scientists and continues seeking new researchers to collaborate on our strategic directions.

D.7 Critical Action: Build a Research Infrastructure that Meets Emerging Scientific Needs

Metric: Complete construction projects.

Steward: Chief Operations Officer

1-2-year outcome: RadEMSL

Status: **Completed.** Portions of RadEMSL were activated in FY 2012 and remaining construction was completed in FY 2013. Required exhaust stack testing and validation delayed the original schedule. Operational readiness was granted in FY 2013.

1-2-year outcome: Quiet Wing

Status: **Completed.** Construction was complete in FY 2011, exceeding the original specifications and the first electron microscope was installed in the same month. Remaining instruments were installed and accepted for research by February 2012.

2-4-year outcome: South Electrical Plant

Status: **Completed.** The project was originally planned for completion in late FY 2011. But changes in supercomputer needs resulted in revising the original scope of the centralized plant. The smaller power plant was completed in FY 2013 (Q2) and was the first step in improving our data center efficiency by providing a dedicated computing power source close to the data center and significantly reducing transmission line loss. This will contribute in part to reducing our data center PUE from approximately 2.8 PUEs to below the federal guideline of 1.4 PUEs (1.0 equaling perfect efficiency) by 2015.

2-4-year outcome: Data Center Expansion

Status: **Completed.** This project was anticipated to support HPCS4, EMSL's next generation supercomputer. However, new system designs are denser and require less floor space, eliminating the need for expansion.