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ENVIRONMENTAL MOLECULAR SCIENCES LABORATORY

EMSL

The Development of New User Research Capabilities in Environmental Molecular Science Workshop

August 1-2, 2006

William R. Wiley
EMSL
Environmental Molecular Sciences Laboratory

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The Development of New User Research Capabilities in Environmental Molecular Science:

Workshop Report

Held August 1-2, 2006
W.R. Wiley Environmental Molecular Sciences Laboratory
Richland, WA

Executive Summary

On August 1, and 2, 2006, 104 scientists representing 40 institutions including 24 Universities and 5 National Laboratories gathered at the W.R. Wiley Environmental Molecular Sciences Laboratory, a National scientific user facility, to outline important science challenges for the next decade and identify major capabilities needed to pursue advanced research in the environmental molecular sciences. EMSL's four science themes served as the framework for the workshop. The four science themes are 1) Biological Interactions and Interfaces, 2) Geochemistry/Biogeochemistry and Surface Science, 3) Atmospheric Aerosol Chemistry, and 4) Science of Interfacial Phenomena.

Examples of key scientific challenges that were identified in the four science themes included: What are the molecular level mechanisms by which microbes sense changes in environmental conditions? What are the mechanisms of nucleation and growth of cloud droplets and ice crystals? How do we unravel the genesis, properties, and effects of nanominerals and nanostructured materials (anthropogenic and natural) in the environment? How do we understand and control structure-function relationships of surfaces and interfaces, including those relevant to catalysis and energy production.

Examples of key investment needs outlined in the workshop to address these scientific challenges included: system dynamics and in situ capabilities for probing interfacial reactions, nanoscale structure synthesis and characterization capabilities, development of a microbial dynamics and visualization laboratory, enhanced capabilities in mass spectrometry and electron paramagnetic resonance spectroscopy, and enhanced sample synthesis and preparation capabilities. Specific examples of needed capability development of capital equipment are given in each section.

These new investments can impact a wide range of National and Department of Energy needs related to global climate change, subsurface remediation, and development of new energy technologies.

Background

The W.R. Wiley Environmental Molecular Sciences Laboratory (EMSL) was conceived by PNNL Director William R. Wiley and his leadership team some twenty years ago. An extensive set of workshops and reviews were organized involving experts in experimental and theoretical molecular sciences to define the rationale and scope of what is now the W. R. Wiley Environmental Molecular Sciences Laboratory. However, much has changed in the science and technology universe since EMSL was dedicated in 1997, and these changes in science and technology require that we re-examine our priorities and retool capabilities in the context of 21st Century challenges. It was therefore timely to organize a workshop that took both a snapshot of the environmental molecular sciences in 2006 and identified needs for user capabilities for research in environmental molecular sciences for the next decade.

Scope of the Workshop

The objectives of the workshop were to define important science challenges for the next decade, describe limitations in present approaches, and identify major tools and advances in the measurement sciences needed to pursue advanced research in the environmental molecular sciences. EMSL's four science themes served as the framework for the workshop. The four science themes are 1) Biological Interactions and Interfaces, 2) Atmospheric Aerosol Chemistry, 3) Geochemistry/Biogeochemistry and Surface Science, and 4) Science of Interfacial Phenomena. There were 104 workshop participants representing 40 institutions including 24 Universities and 5 National Laboratories.

During the workshop the insights of workshop participants were collected in written form and by taking notes during the discussions. This information was collected to assemble participants' collective views on:

1. Key scientific challenges in the area of environmental molecular sciences that should be addressed over the next ten years. *(i.e. What science challenges should EMSL capabilities be updated to address?)*

2. Important technical challenges and opportunities that if adequately addressed will provide the research tools to enable progress on the scientific challenges. *(i.e. What are the research techniques that will fuel cutting edge science and should be included in the EMSL?)*

3. Recommendations on specific capabilities where investments should be made to meet or address the technical challenges.[i]

[i] The major focus on the workshop was identification of key science and technical challenges and workshop participants were asked to prioritize topics in those areas. The listing of specific capabilities for investment helped clarify the how the technical challenges might be met, but these items were not systematically prioritized.

The workshop involved plenary sessions where experts explored both future issues in areas relevant to EMSL science themes and the frontiers of experimental methods development. Input was collected from participants both by written notes and recorded discussion comments. Four breakout groups worked to synthesize and prioritize the science issues, technological challenges and to identify, where possible, specific investment recommendations. The following sections summarize the outputs from the different breakout groups.

Although the scientific challenges are different in each area, there are several common themes in technical approach or capability needs. These will be summarized in the last section of this workshop report.

This workshop report provides essential information about scientific and potential EMSL user needs regarding equipment and facilities that will be incorporated into a Refreshment Plan for EMSL. The workshop and the report identify needs and the relevance of types and classes of capabilities for the next generation of environmental molecular science. Additional issues such as budget, scheduling, space and facilities as well as input from other workshops will be integrated into a final EMSL Refreshment Plan.

Biological Interactions and Interfaces

Understanding and optimizing the response of biological systems to interactions with their environment can have a significant impact on achieving viable solutions to several problems of national concern. For example, anaerobic microbial metabolism is of direct relevance to the Department of Energy (DOE) missions in environmental stewardship (contaminant bioremediation, microbial impacts on global warming through production and sequestration of methane and carbon dioxide), clean and secure energy (methane and H_2 from wastes as alternative energy sources), and basic science (cycling of carbon, nitrogen, metals, and radionuclides). As one example, molecular scale measurements, and the corresponding insight into biochemical processes, can lead us to new predictive computational models that will provide a solid basis for using microbes effectively and safely to mitigate the impacts of energy-production-related activities on the environment and human health.

Scientific Challenges

Biology is making a transition from a descriptive to a predictive science. This transition is being driven by exponentially increasing amounts of genomic, proteomic and metabolomic data. Fundamental to making sense of this flood of data is an appropriate computational infrastructure that can handle both the amount and complexity of biological data. This transition involves a combination of technical and scientific challenges. The science challenge of identifying molecular processes that control environmentally dependent behavior of cells will occur in the overall context of rapidly expanding creation, collection and integration of many types and scales of information.

The overall picture of the cell microenvironment and cellular response, illustrated in Figure 1, helps identify the molecular processes that control the context-dependent behavior of cells. Microorganisms must be able to sense changes in their surroundings and they must be able to respond to these changes by producing new proteins, or metabolites. This picture leads directly to the following key environmental molecular science challenges that need to be addressed.

- *What are the molecular level mechanisms by which microbes sense changes in environmental conditions?*

- *What are the molecular level responses to these changes in conditions in terms of production of specific proteins, multiprotein complexes, metalloproteins, cell surface molecules or metabolites?*

- *Where within (or possibly outside) of the organism are these specifically produced molecular complexes located and how do they catalyze the specific reactions for which they were intended?*

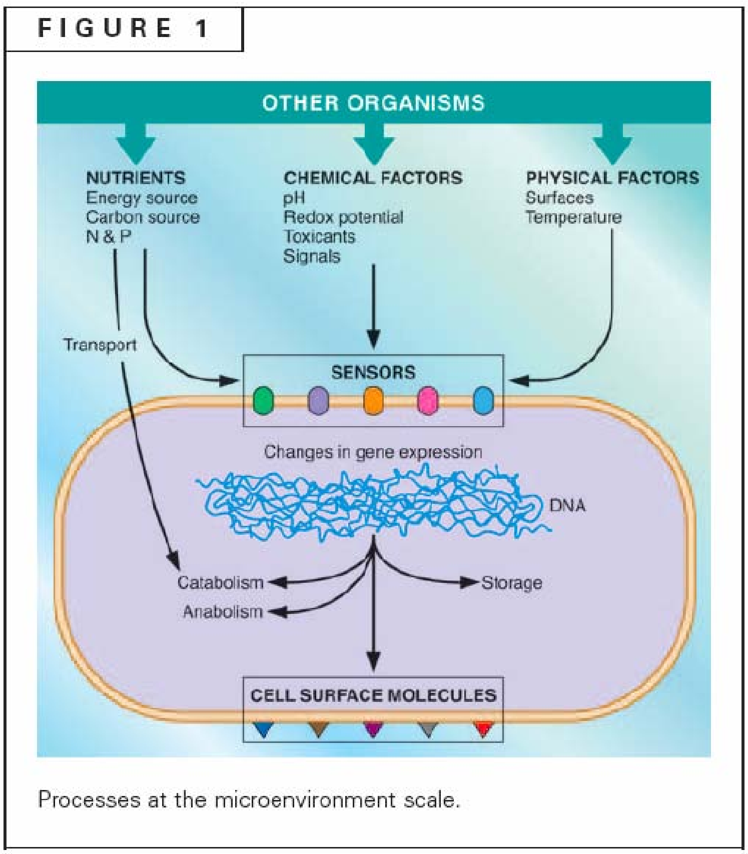
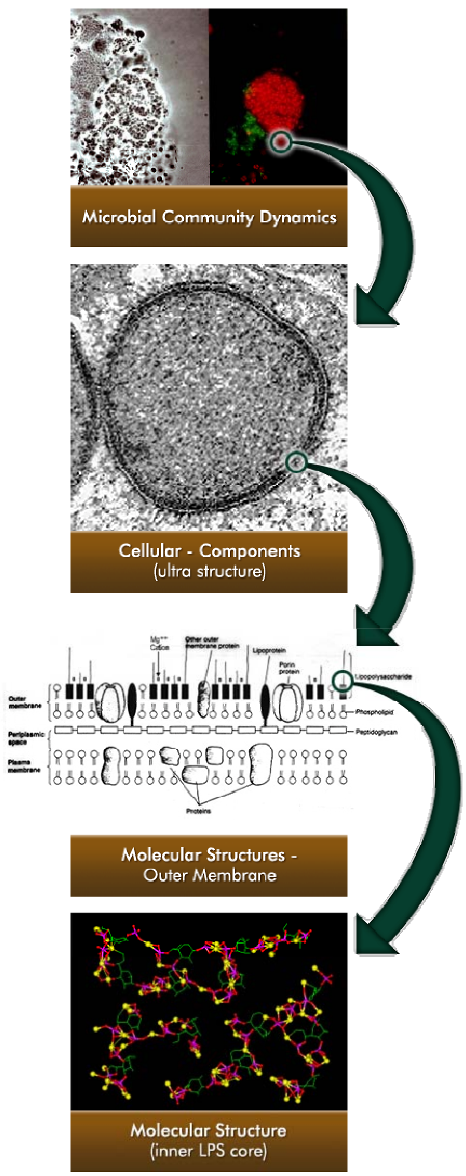


Figure 1. The microbial microenvironment and cellular responses (from presentation by Allan Konopka during this workshop, August 1, 2006).

Technical Challenges

The key technical challenges required to address these science challenges occur at different scales of measurement ranging from identifying the microbial community in which the organism exists down to the scale of nanometers in identifying the specific molecular level structures. *For maximum scientific impact EMSL must provide a range of capabilities to deal with scale dependence.* There must also be appropriate data management and analysis systems in place to both organize and understand complex, multi-scale information. The series of technical challenges and their inter-relationships are illustrated in Figure 2, and described in detail below.



(a) Image on the left is a black and white image of the microbial consortium using conventional light microscopy. In color on the right is a fluorescent in situ hybridization (FISH) image that shows ammonium oxidizing bacteria in red; the green cells are nitrite oxidizers that use nitrite produced by the ammonium oxidizers.

(b) Microbial ultrastructure of a gram-negative bacterium.

(c) Diagrammatic representation of the major components in the outer microbial membrane of a gram-negative bacterium.

(d) Molecular dynamic simulation of the inner core of the external lipopolysacchardides in the bacterium *Pseudomonas aeruginosa*

Figure 2. Scale dependence of technical challenges in the area of biological interactions and interfaces.

The first main technical challenge is at the level of the microbial community (see Figure 2a). *Capabilities should be developed to grow, identify and select individual organisms or subsets of organisms from a microbial consortium.* These facilities should be available within the EMSL and allow the ability to vary environmental conditions, observe the microbial community both spatially and temporally, and select specific members of the population for more detailed mesoscale or molecular level analysis. This capability is essential to meeting all three scientific challenges but especially challenges one and two.

A second main technical challenge is at the cellular and subcellular level (see Figure 2b,c). *Capabilities need to be developed to characterize the surfaces of living cells, determine the location of specific proteins or metalloproteins, and to subsection individual cellular structures for ex situ detailed molecular level analysis*. It was suggested that many of these capabilities could be co-located as part of an overall Microbial Cell Dynamics Laboratory for ease of user access (see below for details). This capability is critical for the last two scientific challenges.

The third main technical challenge is at the level of characterizing specific molecular level interactions that occur in biological systems. *Capabilities need to be developed to characterize specific posttranslational modifications of proteins, multiprotein complexes and metalloproteins, their 3-D structure, and where applicable their catalytic mechanisms.* The identification of catalytic mechanisms will require the ability to identify the reactant molecules in real-time along with the associated biological structures.

The information related technical challenge is the development of software systems that can facilitate the analysis of the large amount of data that can be collected and which support predictive modeling and exploit the computer resources at the EMSL. This software should exploit the sequence data that is being generated by other facilities, such as the JGI and broadly enable the understanding of complex, multicellular systems. Because interaction data is being gathered on multiple spatial and temporal scales, from the atomic to the community level, computational systems that can link these scale is essential. Data linking, integration, analysis and access are fundamental requirements for enabling the system-level approach to biology that promise to solve important problems in the next several decades.

Recommendations on Specific Investments

Numerous investment recommendations were offered during the workshop to address these technical challenges and these have been grouped into the following three areas: development of a microbial cell dynamics and visualization laboratory, enhanced capabilities in the areas of NMR/EPR/MS, and development of bioinformatics and data analysis capabilities. *The computational infrastructure needed for the next generation of biological studies was considered very important, but it was also generally agreed that* *this topic would require a separate workshop to develop specific implementation plans.* Specific recommendations in the other two areas are described below.

Development of a Microbial Cell Dynamics and Visualization Laboratory

The technical challenges related to the need to grow and characterize living cells under specific growth conditions, determine the location of specific molecular structures within the cells, and subsectioning the cells or microbes for more detailed molecular level characterization requires an integrated suite of *in situ* microbial growth and characterization capabilities. Capabilities recommended to be located in such a facility include:

- Growth chambers for culturing microbes under specific environmental conditions and with *in situ* optical and fluorescence imaging capability.
- Analysis of gene expression profiles and molecular modification of cells to facilitate visualization of gene expression patterns.
- Sample preparation capabilities for proteomics and metabolomics studies.
- Development of NMR centric chemostats or bioreactors for studying cellular systems *in situ* and in real-time.
- Extended spectral range, high speed, high power, multiphoton confocal microscope for imaging living cells.
- Laser capture microdissection and other methods for subcellular fractionation.
- Cryo TEM for cellular and subcellular imaging and analysis.
- AFM for force measurements with whole cells or to use with specific antibody tags for cell surface imaging.
- NanoSIMS for enhanced imaging and spectral resolution of cellular structures.
- Coupled confocal microscopy and NMR analysis methods.
- Surface Plasmon Resonance (SPR) microscope for probing protein-protein, protein-DNA, and protein-ligand binding.

Taken together such a cell dynamics and visualization capability would represent an invaluable resource to the scientific user community.

Development of Enhanced Capabilities in NMR, EPR, and MS.

Several key technical challenges associated with determining multiprotein complexes, posttranslational modifications to proteins, and the catalytic mechanisms of protein function can be addressed by mass spectrometry or magnetic resonance approaches, which are current strengths within the EMSL. Specific recommendations on how these capabilities should be enhanced in the future include:

- Electron transfer and electron capture dissociation mass spectrometry methods for determining posttranslational modifications of proteins.
- Development of a high field (as high as 21 Tesla) Fourier transform ion cyclotron resonance (FTICR) mass spectrometer for whole protein analysis and enhanced sensitivity and resolution in analysis of proteome complexity.

- High-field EPR (>10 Tesla) capabilities for electron and proton transfer reactions in biological systems.
- New high sensitivity cryogenically cooled NMR probes for examining metalloproteins, multiprotein complexes, and metabolites.

Atmospheric Aerosol Chemistry

Atmospheric aerosols (solid and liquid particles suspended in air) are produced by dozens of different processes that occur on land and water surfaces, as well as in the atmosphere itself. Aerosols occur in both the troposphere and the stratosphere, but there are considerable differences in the size ranges, chemical nature, and sources of the aerosols that occur in these two atmospheric layers. Many research efforts are under way to measure, characterize and model aerosols. This is because aerosols have important consequences for global climate, ecosystem processes, and human health.

Aerosols influence the Earth's radiation budget through *direct radiative forcing* by scattering and absorption of incoming solar radiation. They also affect climate *indirectly* by acting as cloud condensation nuclei (CCN) and ice nuclei (IN). The extent of *direct or indirect radiative* forcing by aerosols (see Figure 3) is an area of significant uncertainty in global and regional climate modeling. This uncertainty is inherent considering the variation of mass, composition and optical properties of tropospheric aerosols on local to regional scales.

Indirect radiative forcing by aerosols is of largest uncertainty. The efficiency of aerosols to act as CCN and IN depends critically on the hygroscopic properties of aerosols. It's generally believed that aerosols composed of highly soluble compounds enhance cloud formation while those composed of low-solubility constituents inhibit cloud formation. In addition, the chemical composition and physical properties of aerosols evolve during their lifetime as a result of photochemical processing and heterogeneous chemical interactions. Fundamental understanding of these dynamics is prerequisite for accurate atmospheric chemistry and climate modeling. Yet, the role of aerosols, especially organic aerosols, is one of the greatest sources of uncertainty in the interpretation of climate change over the last century and in the modeling of future climate changes.

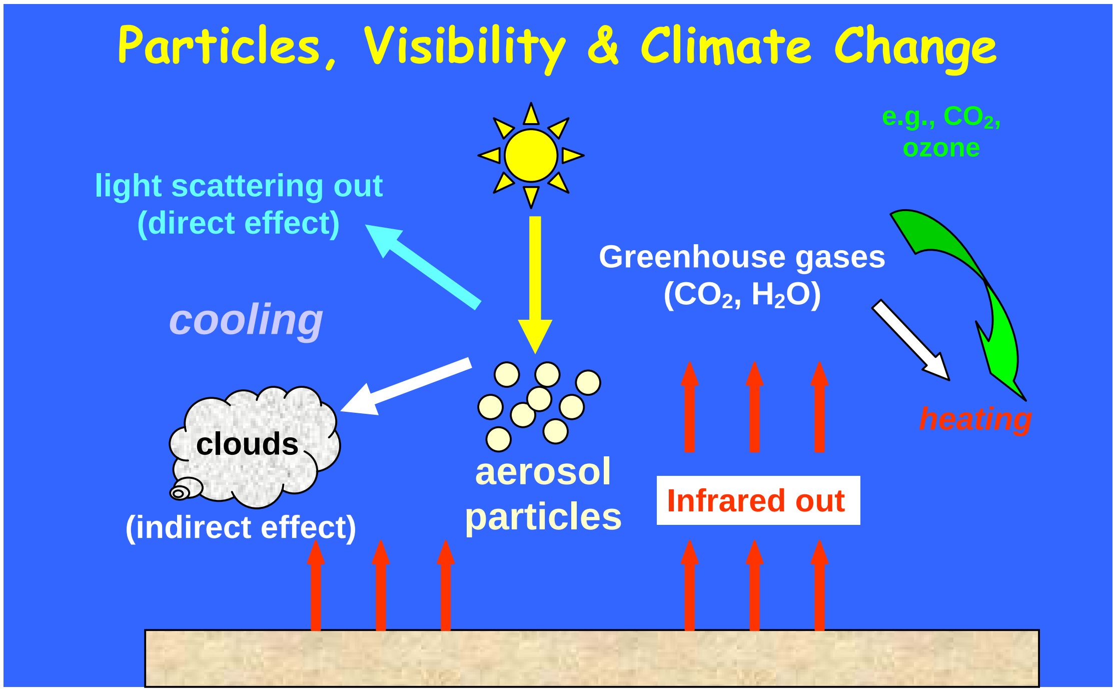


Figure 3. The impacts of aerosol formation on climate change (presentation by Barbara Finlayson-Pitts, UC Irvine, at this workshop August 1, 2006).

Scientific Challenges

The overall objective of this science theme area as articulated in the workshop was to *understand how physical properties and chemical composition of aerosols affect their interaction with radiation, water, and other gaseous species in the atmosphere and how these characteristics change during the aerosol life cycle*. As such, the key science challenges identified related to three processes in the aerosol life cycle: (1) aerosol sources, formation and growth, (2) aerosol transformation, and (3) aerosol impact on cloud formation and eventual deposition from the atmosphere.

Specific science challenges that workshop participants recommended for addressing in the EMSL user program included (Figure 4):

Aerosol Sources, Formation, and Growth: *Unravel the mechanisms of aerosol particle formation and growth.* This includes evaluating the processes leading to new particle formation, measuring the impacts of organics on aerosol particle formation and life-cycles, and deciphering the mechanisms of cloud droplet and ice crystal formation and growth in the atmosphere.

Aerosol Transformation (Evolution and Aging): *Understand the changes that occur inside and on the surfaces of aerosols during their atmospheric lifetime.* This includes unraveling the complexities of organic substances (including black carbon) in the atmospheric gas, particle, and droplet phases; their mixing and partitioning on the surface and in the bulk of the aerosols, and their evolution and transformations.

Cloud Processes, Scavenging and Deposition: *Evaluate how the changing chemical and physical properties of aerosols affect the formation and evolution of cloud droplets and ice crystals and subsequent aerosol deposition*. This includes understanding the impact of chemical and physical properties of aerosols on the formation and evolution of cloud droplets and the influence of solution non-ideality on warm cloud formation.

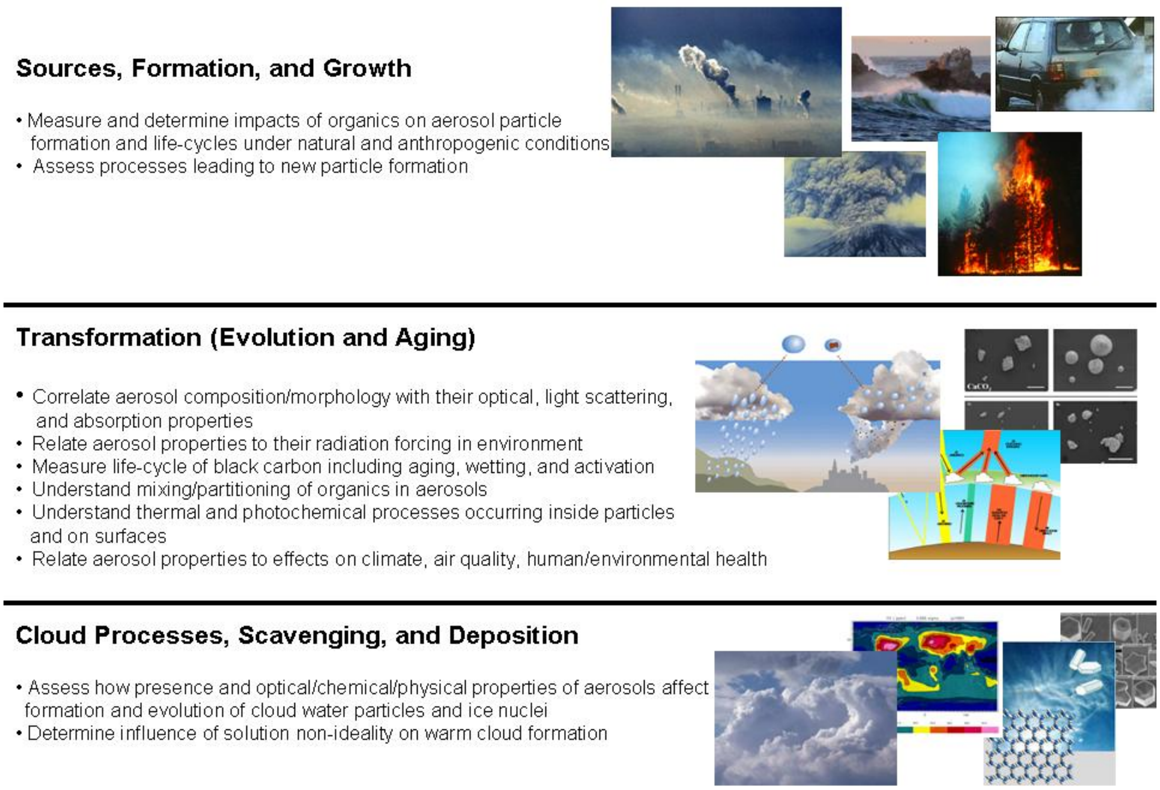


Figure 4. Scientific challenges identified in the area of atmospheric aerosol chemistry.

Technical Challenges

Workshop participants emphasized that the key technical challenges required to address these science challenges are related to characterization of chemical and physical properties of atmospheric aerosols and their evolution throughout their atmospheric life cycle. These include:

- Development of analytical techniques that operate under ambient conditions (1 atm, 0 – 100% RH, 230 – 320 K) for analysis of particles both suspended in air and collected on substrates.

- Chemical characterization of organic and inorganic aerosols and their transformations (aging, reactivity, condensation, etc.) using field deployable and laboratory techniques for both *in-situ* and *off-line* multidimensional, high-throughput analysis of atmospheric particles for both inorganic and speciated organics covering broad range of molecular weights (tens to10^4 amu) and particle sizes (~ 2 nm to 10 µm).
- Development of 3-D particle characterization techniques that provide information on heterogeneous properties of individual particles (particle morphology, bulk and surface composition, optical and hygroscopic properties, particle phases for solids and liquids, aerosol water content etc.) with respect to both inorganics and organics (not just elemental analysis) including speciated molecular information, oxidation states, etc., as a function of position in and coatings on particles.
- Development of sensitive techniques for trace isotope analysis (e.g. using carbon isotopes) of aerosol constituents to distinguish anthropogenic versus natural aerosol sources.

In the area of aerosol formation, the key technical challenges include development of improved *in-situ* chemistry probes for identification of gas-phase precursors and reaction intermediates relevant to formation of secondary organic aerosols; development of ultra-fast spectroscopic probes of non-equilibrium systems (super cooled water or water vapor) to illuminate the structure and dynamics of nucleation centers for both homogeneous and heterogeneous processes.

Other technical challenges include development of field techniques to ensure collection of representative samples (in composition, particle size, distribution, etc.) and development of large-scale data mining and analysis approaches, web based techniques for data sharing, storage and availability for scientific user community.

Recommendations on Specific Investments

Investment recommendations offered during the workshop related to the technical challenges described above included:

Advanced mass spectrometry instruments for analysis of aerosols using both in-situ and sample collection methods.

- New instrumentation for detailed real-time analysis of organic compounds in aerosols, including, but not limited to, mass spectrometry, ion and gas chromatography, and optical spectroscopic techniques.
- Particle imaging and analysis at atmospheric pressure using novel atmospheric pressure ionization techniques (DESI, DART, etc) combined with high-resolution mass spectrometry for chemical characterization of atmospheric aerosols collected on substrates and studying their transformations.
- New single-particle mass spectrometer for chemical characterization of ultra-fine (<100 nm) aerosol particles enabling simultaneous detection of particle size, shape and density.

- TOF-SIMS for submicron size single particle analysis.

Novel cutting-edge spectroscopy instruments for analysis of aerosols and their surfaces.

- XPS, SEM/EDX, TEM/EDX/EELS techniques for in-situ, real-time characterization of particle surfaces including black carbon during reactions with atmospheric oxidants and atmospherically relevant conditions (1 atm, 0 – 100% RH, 230 – 320 K, control of gas phase composition).
- Optical methods enabling real time, *in situ* and other types of analysis to be applied in a variety of ways. These should include Non-linear laser-based surface techniques (e.g., SFG, SHG) and improved capabilities for FTIR and Raman spectroscopy to study the special role that surfaces and interfaces play in atmospheric chemistry. <u>Specific applications and capabilities should include:</u>
    - temperature-controlled (down to 200 K) aerosol chambers with a suite of chemical instrumentation for real-time measurement of chemical composition and optical properties as a function of time, temperature, RH, and gas composition.
    - FTIR ellipsometry for measurements of optical constants for organics on surfaces, and
    - high spatial resolution FTIR and Raman microscopy capabilities for small area and single particle analysis.

It was also specifically noted that the development and use of many of these new capabilities will require developing the scientific expertise and personnel to operate such facilities.

Biogeochemistry and Subsurface Science

One of the most challenging and pressing issues confronting DOE and the nation is the safe and cost-effective management of environmental pollutants and the remediation of hazardous waste sites. The DOE is responsible for managing some 40 million cubic meters of contaminated soils and 1.7 trillion gallons of contaminated ground water. At Hanford alone, millions of gallons of highly radioactive and hazardous wastes in hundreds of underground tanks have leaked causing extensive contamination of the soil and groundwater. These issues are also national problems. For example, across the US, thousands of Superfund sites exist with various levels and types of contamination ranging from organics (PCBs, carbon tetrachloride, TCE), heavy metals (Hg, Cr, Pb, As), inorganics (phosphates, nitrates) to radionuclides (U, Tc, tritium, Pu, Sr, Cs, Am).

Molecular level processes, such as aqueous complexation, adsorption to different mineral phases, or microbial reduction of redox active metals, often control the transport and fate of contaminants in the environment. These processes occur in complicated subsurface environments that are chemically and physically heterogeneous. Understanding the structure, chemistry, and nano-scale geometric properties of the mineral/water and microbe/mineral interfaces are therefore key aspects of developing a mechanistic understanding of contaminant transport. As a result molecular level studies of interfacial geochemistry and biogeochemical reactions have been an active area of research for more than a decade. Unraveling these phenomena at the molecular level and determining their impact on contaminant migration and transformation in the environment is a key objective of this science theme area.

Scientific Challenges

With this general understanding of subsurface systems, workshop participants outlined three key scientific challenges in the areas of nanobiogeoscience, system complexity, and bridging spatial and temporal scales. These challenges were identified in the context of where the EMSL could have a significant scientific impact on unraveling the mechanisms behind the fate and transport of contaminants and other constituents in subsurface systems.

- *Nanobiogeoscience: Unraveling the genesis, properties, and effects of nanominerals and nanostructured materials (anthropogenic and natural) in the environment.* This scientific challenge includes understanding mechanisms of biomineralization at the molecular-level (Bacteria express nanomaterial synthesis capabilities that offer exquisite control on product properties and morphology), elucidating the structure, unique properties, reactivity, and transport of nanostructured materials in the environment.

- *Natural Complexity and Molecular Resolution: Understanding the dynamics of reactions at complex interfaces with high temporal and spatial resolution.* This scientific challenge includes characterizing mineral surface structures including natural topographic heterogeneity and defects in different geochemical environments, determining the impacts of microbes, biofilms, and organics on mineral surface reactivity, and understanding coupled processes (e.g. diffusion/electron transport, surface proximity effects) with molecular resolution (see Figure 5).

- *Bridging Scales: Bridging the gap between molecular and continuum understanding*. This scientific challenge includes relating molecular properties to macroscopic properties such as solubility, dissolution, and adsorption; as well as investigating the effects of fluid flow from the microscale (confined spaces and fractures) to the continuum level.

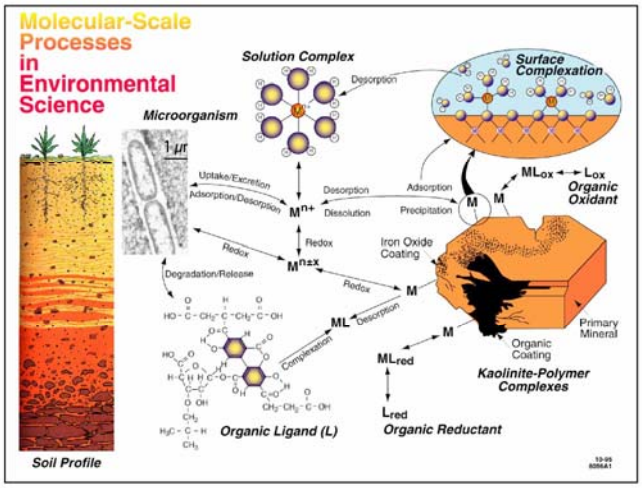


Figure 5. Molecular level complexity of biogeochemical systems (presentation by Gordon Brown, Stanford University, at this workshop August 1, 2006).

Technical Challenges

The technical challenges required to address these science challenges must therefore deal with the issues of characterizing the complexity of heterogeneous systems, evaluating coupled processes (dynamics), and linking molecular scale and macroscale reactivity (scaling).

- *Imaging of complex heterogeneous systems.* In working with complex heterogeneous materials the ability to image the system at different scales and selectively isolate fragments or parts of the system for further characterization until ultimately the molecular scale is obtained is of prime importance (see Figure 6).

- *In-situ characterization of biomineralization and mineral surface reaction dynamics.* Microbial processes, and many geochemically driven processes occur across a wide range of time scales. Furthermore, many of these processes are strongly influenced by the chemical and physical conditions of the system in its natural state. In order to evaluate such processes requires real-time, *in-situ* imaging and spectroscopic capabilities.

- *Development of techniques for microscale reactive transport studies.* The EMSL has and will continue to focus on molecular biogeochemistry. However, fluid flow and transport phenomena are also often important in the environment and in laboratory based systems in the near surface region or in confined spaces. Capabilities need to be developed in microscale reactive transport, adding chemistry on top of microfluidics, to better understand geochemical and biogeochemical reactivity as well as to help bridge the gap between molecular and continuum scales.

Recommendations on Specific Investments

Investment recommendations offered during the workshop related to these three technical challenges include:

Imaging of complex heterogeneous systems

- An aberration-corrected cryo-TEM for detailed high-resolution imaging of delicate samples such as cell structures in contact with mineral surfaces.
- Advanced capabilities in NanoSIMS for simultaneous imaging of elements/isotopes on minerals and soft surfaces at the nanoscale.
- MicroRaman/AFM/laser confocal microscope with wet cell capability for dynamic studies of living cells.

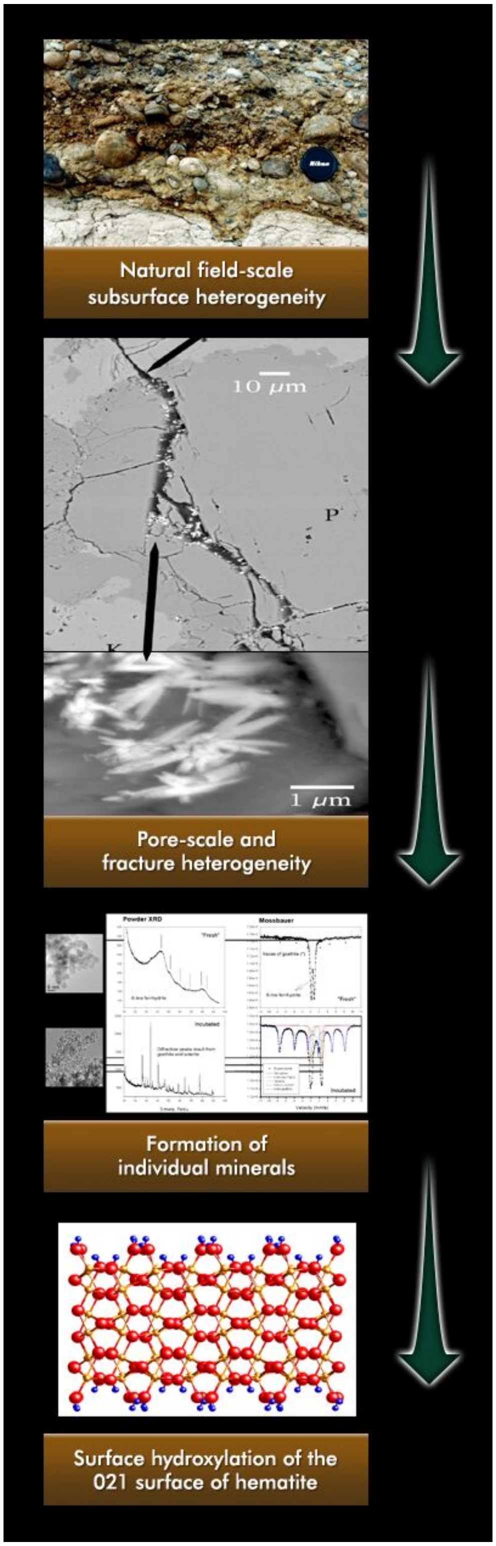
In-situ characterization of biomineralization and mineral surface reaction dynamics

- Development of Second Harmonic Generation (SHG) and Sum Frequency Generation (SFG) capabilities for probing interfacial reactions in in-situ.
- High resolution, high brightness, micro XRD for determining the mineral phases in micromineral assemblages.
- Focused ion beam (FIB) capability for partitioning and characterizing heterogeneous samples with high spatial resolution.
- Higher brightness (10x) monochromatic XPS for enhanced determination of surface phase composition and oxidation state information.

Development of techniques for microscale reactive transport studies

- Establish a Microfluidics Laboratory for studying reactive chemical transport in micron or smaller confined spaces. This facility should include capabilities for device fabrication.
- Enhanced NMR capabilities for imaging fluid flow in subsurface materials, a cryo-solids probe for analysis of low-abundance nuclei, and a MAS NMR flow-through (wet) cell.

In addition to these capabilities, there was strong support for enhanced capabilities to handle radionuclides and for the development of flexible and universal mechanisms for transferring samples between instruments under controlled atmosphere (anoxic) conditions.



(a) Soils and concretions present in the Ringold Formation (Vadose Zone) at the Hanford Site showing the intrinsically high degree of physical, spatial, and chemical heterogeneity at the field scale.

(b) Backscattered electron images of uranyl silicates within microfractures of a single granitic clast at the micron observation scale.

(c) Powder XRD and Mossbauer spectra of nanoparticulate ferrihydrite before and after microbial incubation.

(d) Molecular dynamics based prediction of the molecular-level structure and surface protonation of the hematite 021 surface.

Figure 6. Scale dependence of technical challenges in the area of biogeochemistry and subsurface science.

Science of Interfacial Phenomena:
Tailored Interfacial Structures for Dynamics, Reactivity, and Transport

Material systems with interfaces designed (tailored) and optimized to have specific properties are essential to many technologies needed to maintain a secure environment and obtain a stable energy future for the nation. Hydrogen production and storage, solid-oxide fuel cell research and development, materials for next-generation nuclear reactors, thin-film solar cells, radiation detectors and chemical sensors, the creation of a new generation of selective efficient and stable catalysts, environmental photocatalysis, and the development of solid-state lighting are all examples of technical areas that rely on improved understanding and control of molecular-level structural, dynamic, and transport properties of interfaces. As indicated in Figure 7, sensors, catalysts, photocells and other environmentally important systems usually involve solid-solid, solid-liquid, or solid-gas/vacuum interfaces of a variety of physical structures from which we need to extract chemical and functional information at the atomic or molecular scale. This science theme focuses on developing an understanding and gaining control of structure-function relationships at the atomic level that will allow, for example, the design of catalytic activity and selectivity. The science and technological issues identified highly link to those in the atmospheric, geological and biological areas.

Scientific Challenges

- *Expanding our understanding and ability to rationally design, synthesize and characterize complex surfaces, films and interfaces.* One focus of this area is enhancing our ability to deal with complex materials, complex structures and complex environments some of which are illustrated in Figure 7. These materials and the related interfaces are relevant to geochemical and biogeochemical processes and to the creation of films/materials with designed chemical, electronic, magnetic and optical properties related to sensor, detector, catalysis, and energy needs. Extension of the level of experimental and theoretical understanding available for metal and semiconductor surfaces to metal oxide, hydroxide, layered silicate and other insulating systems was a scientific challenge undertaken by EMSL at the inception. Success in addressing this challenge for relatively simple oxides provides capabilities and resources that will help fuel progress in many of the current science theme areas and leads naturally to facing the challenge of growing, characterizing and designing more complex oxides for a variety of applications.

- *Understanding or controlling structure-function relationships of surfaces and interfaces.* We are just beginning to understand the truly dynamic (time and environmental dependent) nature of surface and interface structures that will have major impacts on the nature and presence of defects and reaction sites. These dynamic effects may be more apparent for organic or biomaterials, but also apply to what has been commonly viewed as “static” inorganic surfaces and interfaces. This time and environment dependent nature adds new challenges and opportunities for understanding and controlling structure-function relationships at surfaces and interfaces of many types. These dynamic effects will influence our understanding of chemical reactivity (catalysis, photocatalysis, and bioactive materials) and have significant implications for processes involving mass and charge transport (detectors, sensors, fuel cells, photovoltaics) and may offer new approaches to control reaction processes. Water at surfaces and buried interfaces (including solid/solid and solid/liquid) are particularly important interfaces to understand and very challenging to probe experimentally.

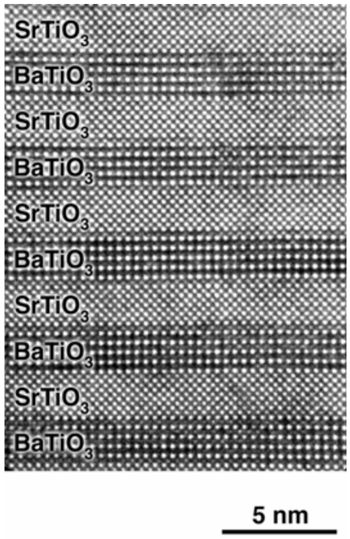
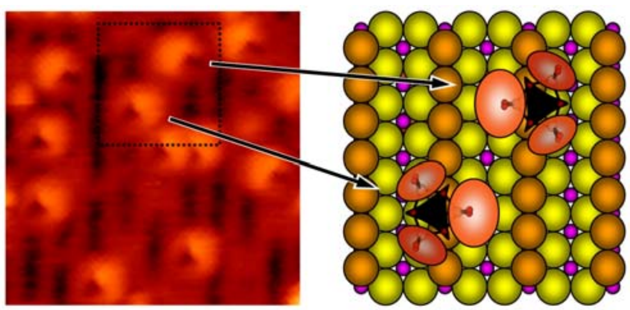
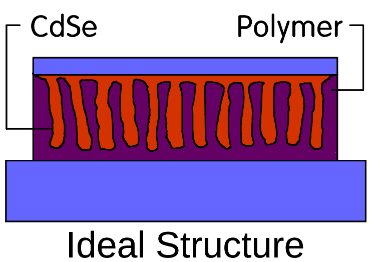


Figure 7 Examples of a variety of interfaces relevant to energy, environmental or sensor technologies

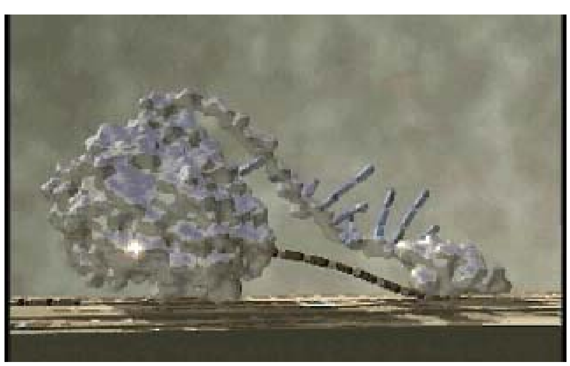
a) TEM image of multi-layer oxide structure grown by MBE. Such structures are relevant to ferroelectric materials, magnetic components or sensors and provide one example of buried solid-solid interfaces for which atomic level order (and deviation from that order) is significant. From Y. Suzuki presentation.



b) Scanning Tunneling Microscope image of catalytically nanometer sized active sites on an oxide surface. Specific reactive sites and sometimes defects play a major role in defining the chemical properties of surfaces and interfaces. From J. M. White presentation.



c) Model of future solar cell involving organic and inorganic materials and a complex geometrical structure. The ability to adequately characterize such complex mixed phase system is an important challenge. From M. Al-Jassime presentation.



d) Drawing of endoglucanase on a cellulose surface. Biological surfaces and interfaces are a challenge to fully characterize, but play a major role biomass conversion. From M. Davis presentation.

Technical Challenges

Several important general instrumental needs that involved a variety of technical challenges were identified in this area. It was clear that a wide range of different capabilities was necessary for Users to have access to the set of tools needed to make important scientific contributions. Specific areas included material synthesis, capabilities for probing single sites on surfaces, *in situ*/operado/real-time capabilities, surface and buried Interface capabilities. Participants especially noted that in a few areas US researchers do not have access to current state of the art instrumentation.

- *In situ/Operando/Real Time Probes.* The ability to measure chemical and structural characteristics of surfaces and nanostructured materials as a function of environment and time is critical for understanding the dynamical and transient behaviors of materials and interfaces relevant for a more advanced understanding of structure-property relationships. Capability developments that facilitate i*n situ* capabilities should be emphasized.

- *High Resolution and Interfacial Analysis Tools.* It is increasingly important to obtain information about the structure, composition and chemical properties of specific (single) sites and small areas. High resolution tools are also important for engineering and natural materials. The ability to probe atomic and molecular structure and composition of solid/solid (including organic/inorganic, inorganic/inorganic and organic/organic), solid/liquid, solid/gas interfaces is critically important and should include chemical imaging to the extent possible. It is increasingly important to combine spectroscopy (physical and chemical information) and microscopy (spatial information).

- *Sample synthesis and preparation are enabling capabilities for much important science and technology*. Important aspects in this area include the synthesis of complex (composition and morphology) oxide interfaces, films and surfaces as well as developing methods to observe and control growth processes real time (including in solution). The ability to prepare and handle samples to retain desired properties is a special and increasingly important challenge. The integration of precision calorimetric tools with nanostructure synthesis can provide the experimental basis for testing in detail theoretical model accuracy.

- *High throughput capabilities.* In some areas (including catalysis), high throughput synthesis and analysis are important enabling capabilities that have a qualitative impact on the level of science that can be accomplished.

It is apparent that an increasing number of tools need to be applied to adequately characterize many new materials. A specific challenge to a user facility is associated with letting people know what is available and supplying the information and expertise needed to apply the tools to specific problems or materials. Among the general challenges many of the above methods introduce is the ability to process and manage large amounts of data. Transparent ability to store, share and mine large amounts of data is a general issue important in many areas of science.

Another important issue that was specifically noted in the workshop was in the area of developing a new level of verified theory especially relevant for interfaces and nanostructures. Although fundamental theoretical tools have developed such that theory can contribute to understanding molecular structures with increasing numbers of atoms and complexity, it remains difficult and important to validate theory applied to nanostructures and interfaces by comparison with critical experiments. Although it is possible to verify calculated structures, kinetic and energetics provide a more critical tests or accuracy. The objective is to achieve the ability to calculate energetics with the accuracy needed for chemical predictions.

Recommendations for Specific Investments

A wide range of recommendations for specific instruments or capabilities were made during the workshop. The items identified have been are grouped by the technology challenge areas where they apply. Some instrumental recommendations apply to more than one area.

In situ/Operando/Real Time Probes

- Chemically focused high resolution TEM to structure and single site behaviors of catalysis and structures on geochemical surfaces
- Optical methods (SHG, SFG, Raman) real time analysis of particles and interfaces and ultrafast spectroscopy and microscopy laser and detection systems for dynamical studies
- NMR/EPR with appropriate environmental controls and sample capabilities for real time in situ structure and chemistry measurements
- Ultrafast spectroscopy and microscopy laser and detection systems for dynamical studies

High Spatial Resolution and Interfacial Analysis Tools

- NanoSIMS for imaging of elements and isotopes and soft materials at the nanoscale and TOF-SIMS for molecular analysis of organic and inorganic surfaces
- FIB/SEM for three dimensional analysis and selection of specific sample areas TEM analysis
- Variable temperature UHV (cryo-shielded) STM/AFM surface analysis system for study of single site chemistry
- X-ray photoelectron capabilities including high spatial resolution, rapid data acquisition (x10 faster than current) and cryo-XPS for surface and interface analysis including solid-solution interfaces

- Near-Field Scanning Optical Microscopy and single molecule and tip enhanced optical microscopy (will require development to enhance usability) for single site and molecule measurement

Sample synthesis and preparation

- A new generation OPA MBE (with in situ structural characterization) will enable growth of complex materials and the ability to "scale-up" production.
- Anaerobic sample handling capabilities and advance sample preparation methods (FIB and advanced ion milling) to enhance ability to prepare and analyze samples without preparation or atmospheric alteration.
- The ability to synthesize complex structures, channels, and components relevant to micro-fluidic and sensor work is needed.
- Preparation of novel catalyst using soft-landing of mass-selected ions.

High throughput capabilities

- Purchase or develop advanced multiple sample catalysis testing capability for rapid property analysis
- Develop or purchase rapid testing capabilities (e.g. micro XRD) to enhance sample throughput

Cross Cutting Themes and Recommendations

Many of the suggested investments that were offered during the workshop overlapped the different science theme areas. This was natural and expected since many capabilities in environmental molecular science broadly underpin different science challenge areas from subsurface fate and transport to development of new energy systems. This section highlights several of these general areas and points out some of the interrelationships to help further refine the true science impacts of different investment recommendations related to technical challenges and specific instrument suggestions.

System Dynamics and In Situ Capabilities. Capabilities for studying dynamic properties and systems *in situ* was also a cross cutting theme of all four science theme areas. The dynamic properties of living cells have been addressed in the development of a microbial dynamics and visualization laboratory. New technologies allow an increasing range of capabilities to be applied or adapted for *in situ* and real-time measurements.

Candidates specifically mentioned at the workshop include:

- Operando TEM equipped with an environmental cell optimized for high resolution microscopy and chemical measurements.
- Development of Second Harmonic Generation (SHG) and Sum Frequency Generation (SFG) capabilities for probing interfacial reactions in in-situ.
- Development of a low temperature (down to 200K) stabilized growth chamber that is equipped with ultrafast optical probes, FTIR, and XPS for examining the growth and reactions of aerosol particles *in-situ*.

- Ultrafast spectroscopy and microscopy laser and detection systems for dynamical studies.
- Development of special purpose NMR probes for environmentally controlled studies.
- High-resolution mass spectrometry for *in situ* chemical analysis of catalyst surfaces and particle imaging using novel atmospheric pressure surface ionization techniques (DESI, DART, etc.).
- Metabolomics dedicated LC/NMR, LC/MS/NMR system for complementary mass spectrometry and NMR identification/quantification of metabolites in complex mixtures.

Multiscale Structure Synthesis and High Resolution Characterization Capabilities. Many fundamentally and practically important processes occur at specific sites or involve biological or material structures nanometers in size. The need for synthesis and characterization capabilities in this area cross cut all four science themes from determining microbial cellular structures, to aerosol particle characterization, to subsurface systems. Some synthesis capabilities are especially relevant in the interfacial sciences area but enable many types of research in other areas especially in the area of microfluidics.

Workshop participants suggested many capabilities that should be considered for inclusion in this area including:

- NanoSIMS for enhanced imaging and spectral resolution of cellular structures, aerosol particles, nanoparticles in the subsurface and Submicron size, high-energy ion beam capability for single particle analysis (TOF-SIMS).
- Focus ion beam (FIB) capability for partitioning and characterizing heterogeneous samples.
- High resolution, high brightness, micro XRD for determining the mineral phases in micromineral assemblages.
- Higher Brightness (10x) monochromatic XPS for enhanced determination of surface phase composition and cryo-XPS for surface and interface analysis including solid-solution interfaces.
- Near-Field Scanning Optical Microscopy and single molecule and tip enhanced optical microscopy (will require development to enhance usability) for single site and molecule measurements.
- Variable temperature UHV (cryo-shielded) STM/AFM surface analysis system for study of single site chemistry.
- Capabilities for highly specific preparation of novel catalysts using soft-landing of mass-selected ions.
- A new generation OPA MBE (with in situ structural characterization) will enable growth complex materials and the ability to “scale-up” production.
- Development of a Microfluidics Laboratory that includes device fabrication capabilities. The ability to synthesize complex structures, channels, and components impacts the interfacial sciences area (sensor development), biogeochemistry (flow in confined spaces and fractures) and in the biological sciences area (analytical separations). Microfluidics capabilities have been rapidly expanding throughout the world over the past two decades. The EMSL needs to take advantage of these capabilities.

Microbial Dynamics and Visualization Laboratory. This was one of the key new technical developments recommended for the biological interactions and interfaces areas but many of the capabilities also overlap with biogeochemistry and interfacial science areas.

Needed capabilities in such a facility include:

- MicroRaman/AFM/Laser Confocal Microscope with wet cell capability for dynamic studies of living cells.

- Growth chambers for culturing microbes under specific environmental conditions and with *in situ* optical and fluorescence imaging capability.
- Development of NMR centric chemostats or bioreactors for studying cellular systems *in situ* and in real-time.
- Extended spectral range, high speed, high power, multiphoton confocal microscope for imaging living cells.
- Laser capture microdissection and other methods for subcellular fractionation.
- Cryo TEM for cellular and subcellular imaging and analysis.
- AFM for force measurements with whole cells or to use with specific antibody tags for cell surface imaging.
- Coupled confocal microscopy and NMR analysis methods.
- Surface Plasmon Resonance (SPR) microscope for probing protein-protein, protein-DNA, and protein-ligand binding.

Enhanced Capabilities in Mass Spectrometry and EPR. The EMSL has been one of the world's leaders in the development and application of mass spectrometry and NMR to issues in the environmental molecular sciences. These capabilities are viewed to be just as important if not more important in the future. Therefore, it is strongly recommended that the EMSL maintain strong investments in those areas. In particular, good opportunities exist to advance the EMSL capabilities in mass spectrometry and EPR. These should be pursued if possible as described below. In the case of NMR, the EMSL has one of the largest, if not the largest, suite of NMR instruments in the world including a wide bore 900MHz capability. These capabilities should be upgraded as appropriate by investing in selected unique probes (cryogenic etc.). Although there was no clear consensus at the workshop that the time was right for large investments in significant new instrumentation a need for development of special purpose probes for environmentally controlled (*in situ*) measurements was noted, as listed above.

The recommended investments in mass spectrometry and EPR include:

- Electron transfer and electron capture dissociation mass spectrometry methods for determining posttranslational modifications of proteins.
- Development of a high field (as high as 21 Tesla) Fourier transform ion cyclotron resonance (FTICR) mass spectrometer for whole protein analysis and enhanced sensitivity and resolution in analysis of proteome complexity.
- Development of high-resolution mass spectrometer for accurate determination of binding energies for biomolecules.
- High-field EPR (>10 Tesla) capabilities for electron and proton transfer reactions in biological systems.
- Metabolomics dedicated LC/NMR/MS system for complementary mass spectrometry and NMR identification of metabolites in complex mixtures.
- Development of high-resolution mass spectrometry for accurate determination of binding energies for biomolecules.

Information infrastructure and storage. The ability to transfer, store, integrate, process and mine data from a variety of sources was a comment need identified by most breakout groups. This is an important, but universal, challenge in many areas of science and for many institutions. It is clear that EMSL needs to be near the forefront in this area, but there are both scientific and technical challenges and a universal solution is not likely to be possible in the near future.

Appendix: Comments from Reviewers

It is very important for the future of the EMSL that future decisions on the recapitalization of the facility be made with as broad a range of views from the scientific community as possible. Therefore, copies of this draft workshop were sent to invited participants who were unable to attend the workshop owing to schedule conflicts and others with expertise in the science theme areas who agreed to review the report. This section contains a brief summary of the specific recommendations received. The comments are summarized/paraphrased with a view toward their possible impact on EMSL recapitalization. These recommendations are being integrated into the development of the EMSL Refreshment plan in both short term tactical investments and longer term investment strategies.

Summary of Specific Recommendations

- Expand the scientific challenges considered by the EMSL to include issues associated with biofuels. Specifically, the sustainability of continuous cropping of biomass where the soil carbon can be reduced and nutrient cycling and soil structure altered. Capabilities in the EMSL might be well qualified to help understanding these issues.
- The EMSL is ideally poised for building and maintaining a state-of-the-art smog chamber to support DOE's needs in aerosol research. Such a chamber would be extremely useful to the DOE research community in addressing many of the objectives of the atmospheric science program.
- There is a need for more instrumentation in the biogeochemistry area that addresses the 10's to 100's of nanometers scale. Suggestions for such investments might include a UV resonance Raman Spectrometer and a Quartz Crystal Microbalance with Dissipation monitoring and Optical Waveguide Light Spectroscopy.
- Access to an EMSL Aerosol Mobile Laboratory designed to make basic measurements (an aerosol MS, PTR-MS, …) would be a terrific bonus to those of us concerned with indirect aerosol affects in real environments.
- I did not see a discussion of the compact X-Ray source presented at the workshop. It's the sort of capability that really belongs in a National Lab. There should be major value in having one's own 24 hour access to such a source, even if the brightness is somewhat lower than available at dedicated major synchrotrons.
- There maybe the potential to integrate biology into the atmospheric chemistry program. We have recently done some analysis that showed that indeed there are bacterial populations in cloud water and that they are potentially metabolically active.

Agenda

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EMSL
Environmental Molecular Sciences Laboratory

A NATIONAL USER FACILITY FOR THE SCIENTIFIC COMMUNITY

The Development of New User Research Capabilities in Environmental Molecular Science

August 1-2, 2006
Richland, WA
EMSL Auditorium

Tuesday, August 1, 2006

TIME	TOPIC	SPEAKER
7:00-7:30	Registration	
7:30-7:45	Introduction and Welcome to EMSL	Allison Campbell - EMSL
7:45-7:55	Perspective from the Office of Biological and Environmental Research	Mike Kuperberg/Paul Bayer - Office of Biological & Environmental Research
7:55-8:20	Introduction and Expected Outcomes	Andrew Felmy - EMSL
8:20-8:50	Stanford EMSI - Current and Future Research Efforts	Gordon Brown - Stanford University
8:50-9:20	Electron Transfer at the Microbe-Mineral Interface	John Zachara - PNNL/FSD
9:20-9:40	Discussions	
9:40-10:10	Research Needs Related to the Center for Environmental Kinetics Analysis	James Kubicki - Penn State
10:10-10:40	Catalysis at Pacific Northwest National Laboratory	Mike White - University of Texas
10:40-11:10	Photovoltaics from the Laboratory to the Marketplace	Mowafak Al-Jassim - NREL
11:10-11:40	Challenges in Atmospheric Chemistry and Why We Should Care	Barbara Finlayson-Pitts - UC Irvine
11:40-12:10	NSF Workshop on Sustainability and Chemistry	Vicki Grassian - University of Iowa
12:10-1:30	Working Lunch	Morning presentations will be reviewed and discussed
1:30-2:00	EMSL Biology Grand Challenge	Dave Koppenaal - PNNL/Chief Research Office
2:00-2:30	How do Ecological Principles Limit and Inform the Molecular Analysis of Microbial Communities?	Allan Konopka - Purdue University
2:30-3:00	2005 DOE Biomass Energy Workshop	Mark Davis - NREL

3:00-3:20	Discussions	
3:20-3:45	Ideas Received from the Workshop Announcement and Group Instructions	Andrew Felmy - EMSL
3:45-5:00	Participant Discussions of Science Theme Challenges and Investment Ideas - Post Ideas on White Boards - Tour Facility	All
6:00-8:00	Dinner at Terra Blanca	Out of Town Guests or By Special Invitation

Wednesday, August 2, 2006

TIME	TOPIC	SPEAKER
7:30-8:00	Late Registration and Assignment Check-In	
8:00-8:30	Mass Spectrometry & Proteomics	Dick Smith - PNNL/FSD
8:30-9:00	National High Magnetic Field Laboratory at Florida State University	Alan Marshall - Florida State
9:00-9:30	Compact X-ray Sources	Steve Heald - PNNL/APS
9:30-10:00	Complex Oxide Heteroepitaxy	Yuri Suzuki - UC Berkeley
10:00-10:15	Discussions	
10:15-10:45	Ultrafast Laser Spectroscopy for Materials and Interface Research: A Unique Tool for Probing Dynamics	Jin Zhang - UC Santa Cruz
10:45-11:15	MRFM and Quantum Science: from Apollo-Style Science and Engineering to Federative Innovation and Enterprise	John Sidles - University of Washington
11:15-12:30	Working Lunch	Morning presentations will be reviewed and discussed in preparation for afternoon breakout session
12:30-1:00	Report on Day 1 Discussions; Charge to Breakout Groups	Andrew Felmy - EMSL
1:00-4:00	Breakout Group Discussions on Investment Options in Context of Science Challenges - Investment Prioritization	
4:00-5:30	Reports of Breakout Groups	
5:30	Adjourn	

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