Scientific Integration

Through Innovation

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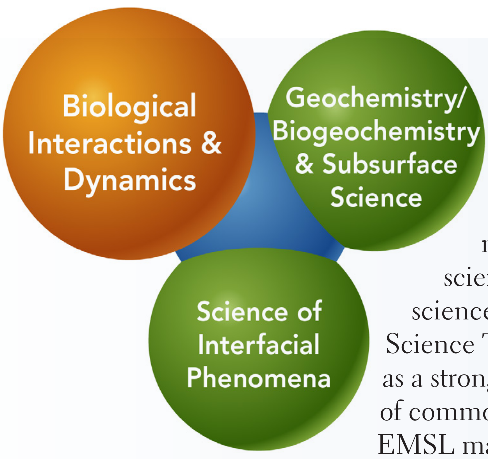
BIOLOGICAL INTERACTIONS AND DYNAMICS

Understanding and optimizing the response of biological systems to their environment can have a significant impact on achieving viable solutions to several problems of national concern. For example, a deep knowledge of anaerobic microbial metabolism can improve national efforts in environmental cleanup and site stewardship, and help provide clean and secure energy. Molecular-level measurements of biochemical processes provide foundational insights toward building predictive computational models that improve our ability to use microbes effectively and safely as an approach to mitigate the environmental and human health impacts of energy-production activities and to extend basic scientific research.

Recent advances in genome-wide sequencing of a variety of organisms and improvements in high-throughput instrumentation have contributed to a rapid transition of the biological research paradigm toward understanding biology at a systems level. As a result, biology is evolving from a descriptive to a quantitative, ultimately predictive science where the ability to collect and productively use large amounts of biological data is crucial.

Understanding how changes in gene expression patterns in cells give rise to biological outcomes is fundamental to systems biology. However, there is considerable heterogeneity in cell responses because of intrinsic variation in their composition as well as their microenvironment. Understanding the nature and sources of cellular heterogeneity is essential for building models that can predict how changes at the genetic level can alter population behavior. Understanding how different types of cells interact is also crucial for building models of complex communities. Modeling of biological systems will require new technologies and approaches to measure the composition of cellular communities and to track the temporal and spatial disposition of their components.



Science Themes focus EMSL's research direction and capability decisions. They help define and direct both the collection of user research projects accepted via EMSL's user proposal process and the development of its key capabilities made available to users, with an eye toward enhancing scientific progress in the areas of environmental molecular science most critical to DOE and the nation. Each individual Science Theme emphasizes drivers important to a field of science, and as a strong family, the themes share significant overlap and linked areas of common scientific interest. Thus, the scope of a research project in EMSL may impact all three Science Themes:

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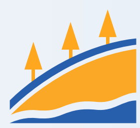
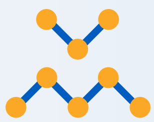
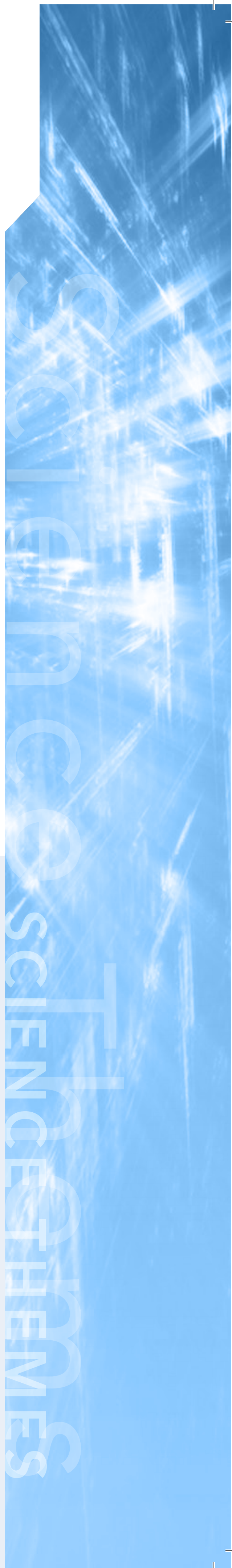


Science of Interfacial Phenomena – Developing an understanding and gaining control of atomic- and molecular-level structure-function relationships at interfaces that enable the optimization of interfacial properties, such as the control of catalytic activity and selectivity.

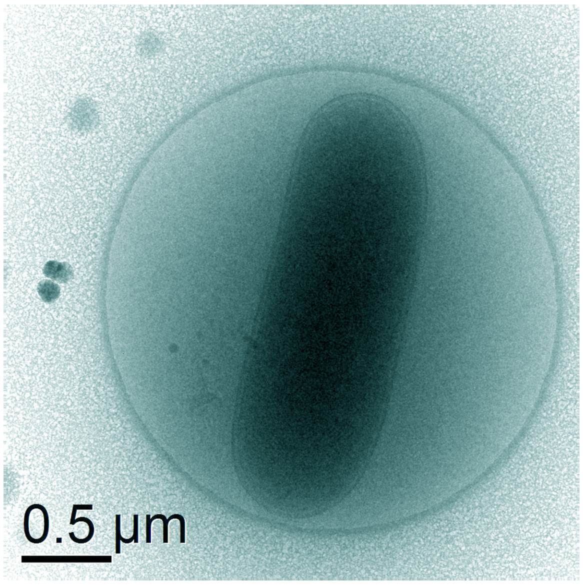




To facilitate the development of biology as an increasingly quantitative science, we encourage user research that focuses on the following key topical areas:

- The dynamics of cellular composition as well as the localization and assembly of, for example, multiprotein complexes
- Protein modifications and how they impact cell regulatory networks
- Molecular mechanisms that define and control the interactions between and within prokaryotic and eukaryotic cell communities
- Understanding mechanisms of phenotypic heterogeneity in cell populations and the relative roles of genetic versus environmental factors.
- Characterizing and linking inter- and intra-cellular regulatory networks from the cell to the population level, especially those that control the response of cells to their environment.

Work in these topical areas can utilize current EMSL capabilities and ideally extend these capabilities into new technical areas. For example, a full understanding of the structure, function, and dynamics of multi-protein complexes and a detailed metabolite profiling of many cells will require extending current EMSL capabilities in high-throughput mass spectrometry and NMR. Work is also currently underway to enhance EMSL capabilities in the analysis of cellular heterogeneity and cellular interactions through new technologies, including microbial flow cytometry and multimodal and multispectral microscopy, as well as surface nonlinear spectroscopy.



Cryo-transmission electron microscope image of *Shewanella oneidensis* MR-1.

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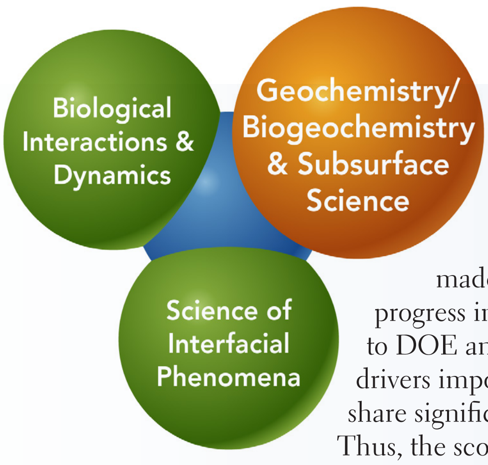
GEOCHEMISTRY/BIOGEOCHEMISTRY AND SUBSURFACE SCIENCE

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 natural environment. These processes occur in chemically and physically heterogeneous subsurface environments. Understanding the structure, chemistry, and nanoscale geometric properties of mineral-water and microbe-mineral interfaces is critical to a mechanistic understanding of subsurface reactivity and 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 to determine their impact on contaminant migration and transformation is a key objective of this science theme.

Research in this science theme addresses some of the most challenging issues confronting the nation, including the safe and cost-effective management of environmental pollutants, the safe disposal of energy production by-products, nuclear waste, and greenhouse gases. Solutions to these issues are critical both for deploying new energy technologies for the nation and for maintaining a sustainable natural environment.



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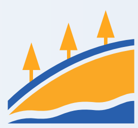

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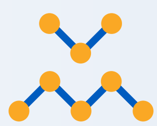

SCIENCE THEMES

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

- Linking molecular-scale processes to reactive transport: This topic area is focused on molecular to microscale processes principally related to how advection or diffusion at the microscale impacts mineral dissolution rates, cell growth and biofilm formation, and particle aggregation and transport.
- Defining the interplay between geochemistry and the structure and activities of microbial communities: There is a need to understand how microbial community structures vary in space and time and how such changes relate to changes in geochemical conditions and microbial interactions with earth materials and environmental contaminants, including radionuclides.
- Biogeotransformations of organic contaminants and natural organic matter: This topical area focuses on the transformations and transport of refractory organic compounds in the environment. Research centers on both the release of anthropogenic organic compounds into the subsurface environment, including sequestration of greenhouse gases, as well as the study of fate and transport of natural, refractory organics.
- Nano-sensing for *in situ* characterization: This topic area is focused on both the development of nanoprobes to ascertain chemical conditions in geochemical or microbial microenvironments and their applicability to sensing field-scale conditions.
- Chemical and biological interactions at complex interfaces: This topic area includes interactions that may lead to contaminant sequestration at the microbe-mineral interface, determination of reaction rates in natural geochemical systems, and metal/ligand exchange dynamics at interfaces. An overall emphasis is placed on moving the current predictive capabilities from equilibrium-based assumptions to a more reaction rate approach based upon the underlying molecular phenomena.

Research in the area of biogeochemistry and subsurface science is well established at EMSL and will be expanded by creating advanced capabilities to determine the chemical form of contaminants, including radionuclides, in complex subsurface materials; developing a fundamental understanding of dynamic interfacial processes and their impact on observed reactivity; and improving the linkage of fundamental studies of molecular geochemistry/biogeochemistry to field-scale transport processes.

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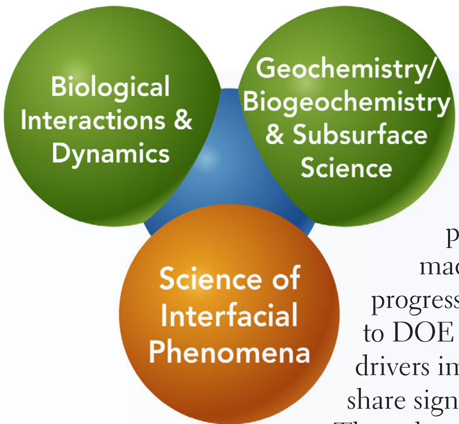
SCIENCE OF INTERFACIAL PHENOMENA

Fundamental understanding of the physical and chemical properties of interfaces in natural and engineered materials is a critical component of environmental and energy-related research, understanding and controlling global warming, and the development of technologies important to the mission of DOE and society. The importance of interfaces has been highlighted in DOE science workshops on topics that include geosciences, solid-state lighting, solar energy, and advanced nuclear energy systems.

Tailored or designed surfaces and interfaces are important as model systems for detailed study of processes that occur on natural heterogeneous materials present in atmospheric or subsurface environments and for developing materials with new properties for energy production, catalysis, and numerous other applications.

The behaviors of complex heterogeneous materials in the environment (such as aerosol photochemistry or contaminant migration) will never be fully understood without model systems that allow specific aspects of that complexity to be examined in detail. Likewise, material systems with interfaces optimized with specific properties are essential for developing technologies needed for a stable environment and a secure energy future. Understanding complex interfaces requires methods to characterize naturally complex materials and minerals found in the environment and to understand increasingly complex materials designed and synthesized for a desired functionality. These science issues complement and naturally intersect those of the biological and geoscience science themes.



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Two of the significant scientific challenges related to advancing interfacial science are: (1) developing (and verifying) predictive models for interfacial processes with energy and environmental implications and (2) advancing the understanding of structure-function relationships in complex multi-component interfacial systems. The Science of Interfacial Phenomena science theme is focused on research activities that address these two scientific challenges in specific areas with high environmental or energy impact, such as:

- Nucleation and growth in multiphase and multicomponent systems (e.g., aerosols, materials synthesis, carbon sequestration, and geochemical processes)
- Phase separation and transformation (e.g., dissolution, precipitation, deliquescence, efflorescence, and ice formation)
- Charge and mass transport processes at interfaces that influence chemical transformations and energy production or storage as relevant to catalysis and photocatalysis, photovoltaics and solid-state lighting, aerosol interactions in the environment, and fuel cells and batteries
- Rational synthesis of materials and interfaces optimized for energy production, energy storage, sensing, catalysis, solid-state lighting, and bio-compatibility.

Fields and technologies that will be impacted by the improved understanding and control of molecular-level structural, dynamic, and transport properties of interfaces include the following:

- New generations of selective catalysts
- Solid-oxide fuel cells and energy storage
- Thin-film solar cells
- Solid-state lighting
- Hydrogen production and storage
- Models of the impact of aerosol chemistry on global warming and atmospheric contamination
- Prediction and mediation of contaminant migration in groundwater
- Carbon sequestration
- Chemical sensors and radiation detectors
- Materials for next-generation nuclear reactors
- Biomaterials for medical devices and drug delivery.

Research capabilities and expertise at EMSL enable the design and characterization of a variety of material systems with specialized atomic, electronic, and ionic transport and interfacial properties. EMSL's unique blend of capabilities and staff expertise makes it a premier laboratory for the study of oxide materials and mineral surfaces.

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