



EMSL Geochemistry, Biogeochemistry and Subsurface Science–Science Theme Advisory Panel Meeting

December 8–9, 2010
Report: June 2011

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

Pacific Northwest National Laboratory
Richland, Washington 99352



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Environmental Research under Contract DE-AC05-76RL01830

Pacific Northwest National Laboratory
Richland, Washington 99352

Meeting Attendees

External Members

Gordon Brown, co-chair

Stanford University

Anne Chaka (offsite)

*National Institute of Standards and
Technology (NIST)*

David Shuh

*Lawrence Berkeley National Laboratory
(LBNL)*

Eric Roden (offsite)

University of Wisconsin

Charles Werth

University of Illinois at Urbana-Champaign

EMSL/PNNL members

Nancy Hess, co-chair

Andy Felmy

Jim Fredrickson (not attending)

Kevin Rosso

EMSL/PNNL Participants

Don Baer

Vanessa Bailey

Mark Bowden

Jay Grate

David Hoyt

Laura Kuprat

Scott Lea

Karl Mueller

Mart Oostrom

Galya Orr

Ljiljana Pasa Tolic

Charity Plata

E. Robby Robinson

Ray Teller

Theva Thevuthasan

Hongfei Wang

Steve Wiley

Michael Wilkins

Executive Summary

On December 8 and 9, 2010, the Geochemistry, Biogeochemistry, and Subsurface Science (GBSS) Science Theme Advisory Panel (STAP) convened for a more in-depth exploration of the five Science Theme focus areas developed at a similar meeting held in 2009. The goal for the fiscal year (FY) 2011 meeting was to identify potential topical areas for science campaigns, necessary experimental development needs, and scientific members for potential research teams.

After a review of the current science in each of the five focus areas, the 2010 STAP discussions successfully led to the identification of one well focused campaign idea in pore-scale modeling and five longer-term potential research campaign ideas that would likely require additional workshops to identify specific research thrusts. These five campaign areas can be grouped into two categories: 1) the application of advanced high-resolution, high mass accuracy experimental techniques to elucidate the interplay between geochemistry and microbial communities in terrestrial ecosystems and 2) coupled computation/experimental investigations of the electron transfer reactions either between mineral surfaces and outer membranes of microbial cells or between the outer and inner membranes of microbial cells.

Background

Formed as a result of a recommendation by the 2008 Biological and Environmental Research (BER)'s scientific and organization review of the Environmental Molecular Sciences Laboratory (EMSL) to increase planning and documentation associated with each of EMSL's Science Themes, the STAPs were created to identify specific scientific questions that will drive the development of new capabilities and serve to attract outstanding scientists to EMSL—both as users and potential staff members. The primary outcome of the FY10 STAP meeting was the identification of five potential focus areas for the GBSS Science Theme:

1. Linking molecular-scale processes to reactive transport
2. Biogeotransformations of organic matter in terrestrial ecosystems
3. Interplay between the structure and activities of microbial communities and geochemistry
4. Nanosensing for *in situ* characterization
5. Chemical and biological interactions at complex environmental interfaces.

Three of these themes—linking molecular-scale processes to reactive transport, biogeotransformations of organic matter in terrestrial ecosystems, and chemical and biological interactions at complex environmental interfaces—were selected for the 2010 Science Theme Call and resulted in a strong, favorable response to the call.

2010 GBSS STAP Meeting

The 2010 GBSS STAP panel membership included last year's members, although Dr. Jim Fredrickson, Professor Mary Wheeler, and Professor James Rustad were unable to participate. This year, Professor Eric Roden and Dr. Anne Chaka participated via video link. Because Dr. Andy Felmy returned to full-time research at Pacific Northwest National Laboratory (PNNL), he resigned from his EMSL roles as GBSS Science Lead and EMSL Chief Scientist. Dr. Nancy Hess took served as co-chair of the 2010 GBSS STAP. In addition, PNNL scientists Dr. Mart Oostrom, Dr. Vanessa Bailey, Dr. Michael Wilkins, Dr. Jay Grate, and Dr. Kevin Rosso gave brief talks about current research in each focus area and participated in panel discussions.

The primary goal of the 2010 GBSS STAP was to identify potential research topics within each focal area that would make viable EMSL scientific campaign candidates, identify needed capabilities, and determine potential research teams. Ideally, the research topics are conceptual or technologic barriers or bottlenecks to scientific progress in a scientific field. EMSL scientific campaigns are a relative new construct based loosely on the EMSL Grand Challenges but do not extend EMSL funding to external Principal Investigators (PI). The science campaigns are research topics that require integration of multidisciplinary teams and take advantage of unique experimental capabilities and expertise at EMSL to make substantial progress toward a significant scientific challenge within the 2- to 3-year timeframe. This report includes the outcomes and initial recommendations of each Science Theme focal area discussion in terms of possible campaign ideas, new capabilities, and teams.

The meeting agenda is included in Appendix A.

Acronyms and Abbreviations

| | |
|-----------------|--|
| BER | Biological and Environmental Research |
| C | carbon |
| CO ₂ | carbon dioxide |
| EDTA | ethylenediaminetetraacetic acid |
| EMSL | Environmental Molecular Sciences Laboratory |
| EPS | extracellular polymeric substances |
| Fe | iron |
| GBSS | Geochemistry, Biogeochemistry and Subsurface Science |
| GT | gross tonnage |
| HR-MS | high-resolution mass spectrometry |
| LBNL | Lawrence Berkeley National Laboratory |
| N | nitrogen |
| NMR | nuclear magnetic resonance |
| PNNL | Pacific Northwest National Laboratory |
| S | sulfur |
| STAP | Science Theme Advisory Panel |
| TEM | transmission electron microscopy |

Contents

| | |
|---|-----|
| Meeting Attendees | iii |
| Executive Summary | v |
| Background | vii |
| Acronyms and Abbreviations..... | ix |
| 1.0 Linking Molecular Scale Processes to Reactive Transport | 1 |
| 1.1 Pore-scale modeling challenge | 1 |
| 1.2 Transport of nanoparticles and nanofluidics | 2 |
| 2.0 Biogeotransformations of Organic Matter in Terrestrial Ecosystems | 3 |
| 2.1 High-resolution mass spectroscopy of organic matter in terrestrial ecosystems..... | 4 |
| 3.0 Interplay Between the Structure and Activities of Microbial Communities and Geochemistry... | 5 |
| 3.1 Modeling of microbial community behavior..... | 5 |
| 4.0 Nanosensing for <i>In Situ</i> Characterization | 7 |
| 4.1 Nanosensors for detecting cytochrome activity | 7 |
| 5.0 Chemical and Biological Interactions at Complex Environmental Interfaces..... | 8 |
| 5.1 Electron transfer mechanisms through microbial cellular membranes | 8 |
| Appendix A : EMSL GBSS STAP Meeting Agenda..... | A.1 |

1.0 Linking Molecular Scale Processes to Reactive Transport

Advancement beyond an empirical model of observed contaminant fate and transport to reliable predictive models requires understanding and identification of the key chemical reactions that control contaminant mobility at the molecular to micro scales. Observed mineral dissolution or precipitation rates, microbial growth, and colloid transport processes in the subsurface all are influenced by the advection and diffusion of molecules. The ability to identify and adequately probe these dynamic processes at the relevant scale and to simulate these phenomena with reliable computational models is largely lacking. Current molecular-level simulation capabilities to unravel chemical transformations at the mineral-water interface as well as the dynamic aspects of such simulations are almost exclusively limited to bond breaking or bond formation with limited ability to incorporate diffusive or other transport processes. Molecular-level insights into the interplay between diffusive and advective processes that impact the formation, growth, and structure of microbial biofilms, mineral precipitation, and dissolution forms the critical basis for design of credible predictive models of contaminant fate and transport.

At the GBSS STAP meeting, two potential areas were identified where EMSL could contribute to the advancement of scientific understanding: 1) pore-scale modeling and 2) nanofluidic-nanoparticle transport research.

Developing predictive models of multiphase flow at the pore and nano scales is a challenge common to diverse science areas, but it is becoming increasingly important in subsurface research due to its importance to contaminant, nanoparticle, and colloidal transport, as well as current interest in the deep sequestration of CO₂. Currently, there are several independent research groups developing numerical simulations of multiphase flow and reactive transport at the pore-scale that use different computational approaches and assumptions. One impediment to advancements in pore-scale modeling is the lack of experimental datasets to determine the relative merits of the approaches/assumptions in different areas such as accuracy, computational speed, or scalability. This benchmarking can both highlight relative strengths of each approach and serve to accelerate progress in the field.

1.1 Pore-scale modeling challenge

Currently, there are several independent, ongoing pore-scale modeling efforts. These groups are each using their own numerical simulation codes without the benefit of experimental data sets to evaluate the performance of each model. A possible concept is to form a consortium of pore-scale modelers to design a set of common experiments based on the microfluidic fabrication and experimental capability at EMSL with the goal of producing experimental data sets that participants would simulate with their models. Ideally, the set of experiments would be designed to test a particular aspect of the modeling that creates either large uncertainty or for which the community has developed different computational strategies. The simulated results would be compared to the experimental results, highlighting strengths and weaknesses of different numerical approaches. These results either would be presented at national meeting/workshop and/or written for publication. The next generation of experimental sets could be designed at the same venue.

EMSL Role: Current capabilities exist at EMSL to fabricate and perform pore-scale experiments. An initial workshop would be needed to design the experimental system being investigated.

Potential Partners

- Markus Hilpert (Johns Hopkins University)–Multiphase flow
- Bayeni Cardenas and Matt Balhoff (The University of Texas [UT])–UT/Sandia Energy Frontiers Research Center (EFRC); CO₂

- Scott Bradford (United States Department of Agriculture [USDA], Riverside, California)–Colloid transport
- Bill Johnson (University of Utah)–Colloid transport
- Xiqing Li (Peking University)–Colloid transport
- Tim Ginn (University of California, Davis)–Colloid transport
- Brent Lindquist (State University of New York [SUNY] at Stony Brook)
- Catherine Peters and Mike Celia (Princeton University)
- Dorthe Wildenschild (Oregon State University)–Pore-scale imaging with synchrotron and multiphase flow
- Majid Hassanizadeh (Utrecht University)–Multiphase flow
- Albert Valocchi (University of Illinois)
- Helen Nguyen (University of Illinois)
- Eugene LeBoeuf (Vanderbilt University)
- Eric Seagren (Michigan Technological University)
- Yusong Li (University of Nebraska)
- Cass Miller (The University of North Carolina [UNC] at Chapel Hill)
- Peter Kitanidis (Stanford University)
- Olaf Chirpka (University of Tübingen).

1.2 Transport of nanoparticles and nanofluidics

An extremely new and unexplored research area both experimentally and theoretically is nanofluidics and nanoparticle transport. The current interest in nanoparticles is due both to the known increased surface reactivity and the unknown nature of their impact on human health and the environment. The transport of nanoparticles is known to depend on their concentration, size, agglomeration state, surface functionalization, and charge—although it is currently held that the agglomerate size is most strongly correlated with their transportability. In addition to agglomeration, important research questions include how nanoparticles behave adjacent to hydrophilic or hydrophobic interfaces, how do they behave at air/water or fluid/fluid interfaces. The size of nanoparticles makes direct *in situ* visualization of nanoparticles difficult with existing technologies. However, there are spectroscopic techniques and new transmission electron microscopy (TEM) environmental cells that could be developed to study these phenomena.

Nanofluidics can be defined as the unique physical behavior of fluids confined in nanostructures on the order 1 to 100 nanometers (nm). The characteristic physical scaling lengths of the fluid, (e.g., Debye length, hydrodynamic radius) closely coincide with the dimensions of the nanostructure itself. Nanofluidics has implications in a variety of application areas, such as biotechnology, analytical separations, and lab-on-a-chip technologies.

In the terrestrial ecosystem and subsurface environments, the occurrence of nanostructures reaches fractal dimensionality by envisioning the extension of nearly every micron-scale pore branching to a series of nano-pores. Mass transport in nanostructures will be impacted not only by the physical behavior of water, but also by the electrical double layer of solvated ions and charged surfaces than can completely span the width of the nanostructure and may result in chemical environments not in equilibrium with adjacent “bulk” regions. Clearly, such nanodomains can have significant impact on

the larger-scale geochemistry. Currently, much of the research in nanofluidics consists of molecular dynamic (MD) simulations, and experimental measurement is limited by the same challenges (already mentioned herein) for nanoparticle research. Experimental capabilities are being developed at Lawrence Berkeley National Laboratory (LBNL) where TEM sample environments are being designed for the study of nanoparticles. As such, LBNL could be a good partner if there is interest in pursuing this area. Sandia National Laboratories (Sandia) also has established a leadership role in this area. Of note, the efforts at LBNL and Sandia are not in the subsurface reactive transport area. Rather, they are related to medicine, electronics, etc. However, both entities could be good partners to help EMSL advance. This research area can be thought of either as focused on nanofluidics or nanoparticles, both of which have relevance to this Science Theme.

EMSL Role: Currently, EMSL is not a leader in this area, but it has some experimental capabilities and expertise that could be focused toward a viable research effort in either the nanoparticle or nanofluidics area. A good strategy would be to invite research leaders from LBNL and Sandia to visit EMSL to discuss possible niche research areas and possible collaboration.

Needed Experimental Capabilities at EMSL

1. New technologies to deposit chemically reactive or bioavailable films in micromodels for study of microbial growth at the pore scale and development of microbial communities
2. *In situ* nanofluidic/nanoparticle capabilities based on TEM imaging and scanning transmission electron microscopy (STEM) for elemental characterization
3. Extension of nuclear magnetic resonance (NMR) and other spectroscopic capabilities into nanofluidics and nanoparticles
4. Microfluidic- and intermediate-scale capabilities for radionuclides.

Potential Partners

- LBNL
- Sandia
- Dr. Michal Borkovec (University of Geneva)
- Michael Gaitan (National Institute of Standards and Technology [NIST]).

2.0 Biogeotransformations of Organic Matter in Terrestrial Ecosystems

In geochemistry, the significance of naturally occurring organic matter traditionally has been considered in its role as a potential complexant for contaminants that influence the fate and transport of contaminants in the subsurface. In the past, much of this attention has focused on naturally occurring organic matter, such as fulvic and humic acids. Anthropogenic compounds, such as ethylenediaminetetraacetic acid (EDTA), and the products of the alkaline degradation of cellulosic wastes also have been considered because these compounds often are co-disposed with radionuclides and they form stable complexes that significantly impact radionuclide fate and transport.

Recently, the role of organic matter in the terrestrial ecosystem has received heightened interest as the significance of carbon (C) and nitrogen (N) cycles in climate change is recognized as a serious environmental issue with long-term consequences for the planet. Soils store 12,000 gross tonnage (GT) of C and exchange 120 GT of C annually. In contrast, anthropogenic annual C emissions are on the order of 10 GT. Of particular interest are the natural processes that result in

the accumulation of refractory natural organic matter in soils, which, if understood, potentially could represent a significant sink for anthropogenic CO₂. However, the ability to predict how global climate change will impact the stability of soil C stores is of greater significance. Unfortunately, unraveling the biogeochemical transformations and environmental transport pathways of these compounds has proven to be a difficult challenge.

Some of the key scientific questions include:

- Can analytical methods be developed to give spatially resolved compositional information on organic matter associations with the geochemical and biogeochemical environment?
- What role do microbial communities play in stabilizing refractory organic matter?
- What are the primary environmental drivers that impact refractory organic matter stores?

2.1 High-resolution mass spectroscopy of organic matter in terrestrial ecosystems

Current models showing the flow of carbon through the terrestrial ecosystem are generally described in terms of the extractability from soil, dissolved organic matter, etc. Recently, advances in mass spectroscopy have resulted in improved mass accuracy, mass resolution, sensitivity, and sample collection times, making it possible to look at samples that were previously too small or chemically complicated. These advances opened the technology to the study of natural organic matter, resulting in the ability to understand—on a molecular level—the flow of C and N through the terrestrial ecosystem, including both plant and microbial transformers.

EMSL Role: Since its inception, EMSL has made significant investments in high-resolution mass spectrometry (HR-MS) methods and recently expanded its throughput and sensitivity via American Recovery and Reinvestment Act (ARRA) funding. Some of those investments have been directed toward building unique sampling front ends for HR-MS that permit spatially resolved analysis of biological tissue and microbial films, as well as desorption electrospray ionization (DESI) techniques for the study of atmospheric organic aerosols. These methods could readily be applied to determining the *in situ* structure and composition of natural organic matter on mineral surfaces. In addition, EMSL has been investing in NMR instrumentation capable of providing enhanced structural information on organic matter assemblages. For both of these techniques, meaningful interpretation of the vast amounts of compositional information generated by HR-MS approaches likely will generate a secondary need for advanced data analysis and informatics techniques. The nano secondary ion mass spectrometry (nanoSIMS) capability, planned for installation in 2012, also will be a valuable addition to this effort. A workshop with BER Terrestrial EcoSystem investigators as target community may be an appropriate next step to continue to refine specific challenges in this research area.

Needed Experimental Capabilities at EMSL

1. Spatially resolved analysis of soil aggregates and soil cores with minimal preparation of the soil and without relying on extraction of the organic matter.
2. Techniques to evaluate quantitatively the amount of C present in each fraction identified by high-resolution mass spectroscopy.
3. Ability to discriminate between or label native organic matter, a target substrate, and microbial C.
4. Micromodels that more accurately represent soil aggregate architecture.

Potential Partners

- Current Biological and Environmental Research (BER) supported thermal emission spectrometer (TES) researchers
- Stan Wulschelger (Oak Ridge National Laboratory [ORNL])
- Ben Bond-Lamberty (Joint Global Change Research Institute [JGCRI])
- Joshua Schimel (University of California, Santa Barbara [UCSB])
- Mary Firestone (LBNL)
- Margaret Torn (LBNL)
- J.P. Croue (King Abdullah University of Science and Technology [KAUST])
- Baoshan Xing (University of Massachusetts Amherst [UMass Amherst]).

3.0 Interplay Between the Structure and Activities of Microbial Communities and Geochemistry

One of the foundational principles of bioremediation is that microbial community activities impact subsurface geochemistry, and microbial communities can be manipulated in ways that alter contaminant fate and transport. In fact, the impact of microbes on geochemical systems is difficult to predict from laboratory studies of monocultures because microbes exist in complex microbial community arrangements in natural systems and biofilms. Also, as it is only possible to identify a fraction of the natural microbial community even using advanced genomic techniques, it is difficult to fully assess the microbial community structure and function of natural systems. Recently, bioremediation field studies have demonstrated using proteomics and transcriptomics data that an intact microbial community structure can undergo long-term change when stimulated with a nutrient substrate to produce a change in geochemical conditions, such as redox.

Continuing fundamental questions include:

- How do functionally different microbes, such as iron- (Fe) versus sulfur (S)-reducing bacteria, co-exist in the subsurface?
- Does the subsurface geochemistry influence Fe and S distribution, especially with respect to detection of insoluble mineral phases that can serve as electron acceptors?
- How do we relate the chemical environments within microbial communities to external geochemical gradients?
- Can overall microbial community function also be related to the observable geochemistry?

3.1 Modeling of microbial community behavior

There is much speculation as to what drives the stability of microbial communities—not just at the species level, but at the functional level. Some of these relationships are extremely important to understand in trying to manipulate native communities to enhance remediation of contaminants.

Example questions include:

- What is the interaction and interdependencies between Fe- and S-reducing bacteria?
- Do microbial communities return to the same community structure following stimulation and how long does that take?
- Does perturbation of the microbial community also result in lasting geochemical changes in the subsurface?
- Can computer models of microbial communities and geochemistry be developed that can simulate what is seen experimentally in the lab and the field?

EMSL Role: EMSL has a world-class proteomics facility that already has attracted scientific users concerned with the changing protein and metabolite concentration in microbial communities. In addition, EMSL has invested in microbial cell isolation, cell-sorting technology, and transcriptomics capabilities, while PNNL has sponsored the Microbial Communities Initiative, a Laboratory-directed research project. The ability to fully integrate genomics, transcriptomics, proteomics, and metabolomics data is a major challenge. However, this integration also is necessary and under development within proteomics-based human health studies at PNNL. EMSL's microfluidics platforms have been used to study microbial growth under different chemical and flow conditions. Advanced imaging capabilities, such as the cryo-TEM, focused ion beam (FIB)/scanning electron microscope (SEM), and helium ion microscope (HIM), can help identify and determine microbial-mineral associations. EMSL currently has multiple users in this research area. It may be worth having a mini-workshop with these users to ascertain any common challenges that could be approached as a research team.

Needed Experimental Capabilities at EMSL

1. The development of omics/geochemical analytical techniques that parallel lab and field capabilities.
2. Computer models that integrate microbial community dynamics with changes in geochemistry.
3. Incorporation of proteomic tools to correlate micro-environments and molecular processes.

Potential Partners

EMSL/PNNL scientists involved in BER-funded Scientific Focus Areas (SFA) (e.g., Rifle and Hanford Site)

Jillian Banfield (University of California, Berkeley)

Sherry Cady (Portland State University)

Angela Belcher (Massachusetts Institute of Technology)

Bruce Rittmann (Arizona State University)

Frank Loeffler (University of Tennessee)

Bruce Fouke (University of Illinois)

Kevin Finneran (Clemson University)

Craig Criddle (Stanford University)

Lisa Alvarez-Cohen (University of California, Berkeley)

Jim Davis (U.S. Geological Survey [USGS])

Andreas Kappler (University of Tübingen).

4.0 Nanosensing for *In Situ* Characterization

In recent years, the variety of technologies to measure the chemical state of remote environments has increased dramatically. Entirely new strategies have evolved based on molecular species and nanoparticles using optical technologies, radio and microwave frequencies, and on-chip electrical detection. Some of these technologies can be implemented in the laboratory setting, but there is great need to develop field-deployable sensors as well. In the case of geochemical and biogeochemical systems, use of such specially designed nanoparticles offers the possibility of probing the unique chemical properties of microenvironments both in laboratory and field systems. For example, embedding molecules or nanoparticles in films that serve as molecular probes can result in high spatial resolution. Can such devices sense solutes or bacteria in small water volumes, or do large amounts of water need to be pumped through filters or sorptive media to concentrate samples for detection at low concentrations? Also, can sensors be deployed and monitored *in situ* to measure the migration of contaminants or geochemistry in the subsurface?

4.1 Nanosensors for detecting cytochrome activity

One of the most geochemically relevant functions microbial cells perform is altering the redox potential of the geochemical environment that they inhabit. Electron transfer reactions between redox active substrates and the microbial cell are central to these functions. Much is known about these mechanisms from genomic, protein structure, and computational chemistry perspectives. However, there are no sensors to indicate the activation or activity of individual cytochromes on the surface of cellular membranes or electron shuttles in extracellular polymeric substances (EPS) that surround individual microbes. The objective would be to obtain an understanding of single-cell respiration and electron shuttling within the EPS and outer cellular membrane.

Secondary questions include:

- Are unique cytochromes expressed for specific substrates or are cytochromes generic for multiple substrates?
- Do all microbes benefit from electron shuttles in EPS?
- What is the role of other chemical entities in the EPS for electron transfer between cytochrome and the mineral surface?

EMSL Role: Micro/nano sensing is a rapidly expanding area of research—one that EMSL is well positioned to contribute to with its diverse and unique research tools. Single-cell spectroscopic capabilities exist at EMSL. Can fluorescence lifetime imaging microscopy (FLIM) or fluorescence resonance energy transfer (FRET) imaging experimentation with clones or fluorescent tags be used? Can micromodels be used to understanding the role of EPS? Can proteomic tools be used to correlate micro-environments and molecular processes? It would be useful to bring research leaders to EMSL to develop potential research areas.

Needed Experimental Capabilities at EMSL

1. This effort will require spatially resolved, high-resolution mass spectrometry or NMR capabilities that measure proteome and can be tied to techniques that measure electron transfer to mineral surfaces.

Potential Partners

Past participants of EMSL's Biogeochemistry Grand Challenge:

- Daad Saffarini (University of Wisconsin)
- Gill Geesey (Montana State University)
- Tom DiChristina (Georgia Tech)
- Mike Hochella (Virginia Tech)
- Ken Neelson (University of Southern California)
- Brian Lower (Ohio State University)
- Alfred Spormann (Stanford University)
- Yi Lu (University of Illinois).

5.0 Chemical and Biological Interactions at Complex Environmental Interfaces

Many of the important geochemical reactions, such as adsorption reactions, mineral dissolution/precipitation, and electron transfer reactions across the mineral-microbe interface, occur at interfaces. With new experimental developments that allow molecular-level resolution and increased coupling with computational molecular models, it now is possible to understand these interfacial processes at unprecedented levels of resolution.

Possible developmental questions include:

- Is it possible to resolve and distinguish between $\text{Fe}^{2+}/\text{Fe}^{3+}$ sites on a mineral surface experimentally?
- Is this atomic resolution visible using TEM or scanning probe microscopy (SPM)?
- Is it possible to observe individual electron transfer reactions using spectroscopy or other techniques in the appropriate timeframe?

5.1 Electron transfer mechanisms through microbial cellular membranes

The Biogeochemistry Grand Challenge revealed a great deal about electron transfer mechanisms in microbial cells and the electron transfer in Fe-oxides, but there still is much to be understood about the interfacial electron transfer reactions between the outer cell membrane cytochromes and Fe-minerals and the transfer of electrons between the microbial inner and outer membranes. Likely, the rate-limiting step is the interfacial electron transfer reactions between the outer cell membrane cytochromes and the Fe-minerals.

EMSL Role: Single-cell spectroscopic capabilities exist at EMSL. Can fluorescent tags be developed for cytochrome activity? Are there second harmonic generation (SHG)/sum-frequency generation (SFG) tools to validate predictions of protein orientation on mineral surfaces? A possible path forward is to re-engage the Biogeochemistry Grand Challenge participants and new community members in a follow-on workshop or seminar series to identify current challenges and approaches.

Needed Experimental Capabilities at EMSL

1. Facilitated access to Chinook or dedicated computational cluster.
2. More realistic computational models of electron transfer reactions between outer membrane cytochromes and mineral surfaces, taking into account the presence of EPS.
3. The ability to measure individual electron transfer events both extracellular in EPS and intracellular between outer and inner cellular membranes.
4. Modeling expertise in cytochrome electron transfer.

Potential Partners

Past participants of EMSL's Biogeochemistry Grand Challenge:

- Daad Saffarini (University of Wisconsin)
- Gill Geesey (Montana State University)
- Tom DiChristina (Georgia Tech)
- Mike Hochella (Virginia Tech)
- Ken Neilson (University of Southern California)
- Brian Lower (Ohio State University)
- Alfred Spormann (Stanford University)
- Frank Loeffler (University of Tennessee)
- Caroline Ajo-Franklin (LBNL).

**Appendix A:
EMSL GBSS STAP Meeting Agenda**

Appendix A

EMSL GBSS STAP Meeting
December 8-9, 2010

AGENDA

December 8
ETB Spokane River Room

- 7:30 am **Badging - ETB**
- 8:00 am **Welcome and Plans for the Day**
- Introductions
- 8:20 am **EMSL's Science Campaign Strategy and EMSL 2.0** – Don Baer/Steve Wiley
- Science Campaigns and EMSL 2.0
- 8:45 am **Format for Group Discussion of Topical Areas and Goals** – Nancy Hess
- Science example
 - Attainable, impactful science challenge
 - Needed capabilities
 - Ideal user teams
- 9:00 am **Topical Area 1: Linking Molecular Scale Processes to Reactive Transport**
- Science Presentation – Mart Oostrom, ETD
- 11:00 am **Topical Area 2: Interplay Between Geochemistry and the Structure Activities of Microbial Communities**
- Science Presentation – Mike Wilkins, FCSD
- 1:00 pm **Topical Area 3: Biogeotransformations of Organic Contaminants and natural Organic Matter**
- Science Presentation – Vanessa Bailey, FCSD
- 3:00 pm **Topical Area 4: Nano-sensing for in situ Characterization**
- Science Presentation – Jay Grate, FCSD
- 5:00 pm **Wrap-up**
- 6:00 pm **Posters and Dinner at Anthony's**

**December 9
ETB Spokane River Room**

8:00 am Topical Area 5: Chemical and Biological Interactions at Complex Environmental Interfaces

- Science Presentation – Kevin Rosso, FCSD

10:00 am Summary and Recommendations

- Identify 1 or 2 Science Campaign targets
- Identify 3-4 Science Theme focus areas
- Identify needed experimental, computational capabilities

2:00 pm End

Optional – Tour of new EMSL capabilities