2008 Stanford EMSI Meeting
Research Directions Discussion Outcomes:

I) Mineralogy:

Understanding relationships between particle size and reactivity for key minerals and key elementary reaction processes.

Understanding the reactivity of mineral surfaces in terms of its dependence on the surface electronic structure, and in turn, its dependence on atomic structure and crystallographic orientation of crystal faces.

Understanding the role of structural (e.g., vacancies, dislocations, order/disorder, etc.), morphological (e.g., roughness, pores, channels, etc.), and compositional (substitutional or interstitial impurities) defects for controlling mineral surface reactivity.

Understanding how the list of molecular-scale processes occurring at mineral surfaces that are important at larger scales is down-selected, or subsumed and reset by the addition of organic or microbial coatings on mineral grains.

II) Water:

Understanding water's self interactions as a function of temperature and pressure, and relating these properties to mechanisms of ion solvation, water exchange rates, and chemical reactivity of solutes.

Understanding of how the water macroscopic and microscopic properties are modified upon confinement in pores or membranes.

III) Mineral-Water Interfaces:

Understanding the structure of water at mineral surfaces and the structure of mineral surfaces in contact with water, with atomic resolution, and how this structure dictates the chemical behavior of near-surface water and near-surface atoms in the mineral lattice.

Understanding mechanisms and dynamics of ion (protons, metals, radionuclides, organics) solvation and adsorption to mineral surfaces, and whether or not relationships between ion ligation in bulk water with ion ligation by surface atoms in surface complexes can be found and exploited.

Understanding mechanisms and dynamics of interfacial electron transfer processes that underlie redox transformation of mineral surfaces and/or redox-active metal sorbates; includes processes characteristic to semiconducting minerals such as charge transport in surfaces and proximity effects.

Understanding how to detect or deduce molecular-scale processes that transmit importance furthest up the length scale domains into the scale of macroscopic measurement; upscaling length and time-scales from molecular through micro-/pore-scales to macroscales, and understanding the role of natural complexity on going from lab to field settings; development of predictive power on the century time-scale and beyond for field sites.

IV) Geomicrobiology / Microbe-Mineral Interfaces:

Understanding bacteria-bacteria interaction, competition and communication of relevance to community development and function in real subsurface environments, and its response to changes in geochemical variables; requires development of improved methods to detect 'who's there' in situ and monitoring of metabolic processes in real-time.

Understanding mechanisms, dynamics and function of biomineralization; includes understanding mechanisms and dynamics of metal/ion adsorption onto cells, monitoring of metabolic processes in real-time, and understanding the effects of biological substrates for catalyzing and directing mineral nucleation and growth.

Understanding mechanisms and dynamics matter and electron exchange across direct and indirect microbe / mineral interfaces for purposes of attachment, nutrient acquisition, and respiration.

V) Tool Development:

General experimental improvements include:

- Spatial resolution and detection limits necessary for study of nanoparticles and nanoparticle surfaces; local probes of defect distribution and defect structure.
- Time resolution necessary for study of surface processes from seconds to femtoseconds, and enabling of ultra fast imaging for surface dynamics.
- More availability of synchrotron radiation beam time; includes more discretionary time to pursue discovery science and development of necessary software tools that automate data analysis for more efficient use of available time.
- More adaptation of vacuum-based surface analytical techniques to accommodate higher-pressure conditions; includes continued development of all kinds of in situ techniques.
- In situ protein expression probes.
- Tools to identify and study biomolecules in living materals.

- Combining genomics with microspectroscopy for identifying ‘who’s there’.

Specific instruments include:

- STXM at 10 nm with cryo-device and fluorescence detection.
- Cryo-prep and EELS for cryo-TEM.
- Tandem nano-SIMS/x-ray microprobe.
- Nano/surface X-ray diffraction.
- Dedicated LCLS instrument for interfacial chemistry studies
- New LCLS methods that allow XAFS measurements.
- X-ray nanoprobe with nano-XRD and nano-XAS.

General computational improvements include:

- Computationally streamlined ab initio molecular dynamics that maintains a level of rigor appropriate for the science question.
- Large-scale computing hardware with highly scalable algorithms and modeling software for molecular modeling and reactive transport simulations.