Molecular-scale

Water/Ion Solvation

(I) What are the most-pressing science questions ($\leq$ 5 yrs) (pink)	
	Quantify differences in (uniform) surface reactivity toward water and ions and explain these trends through underlying physical (structural, electronic) surface properties.
	Water/surface interaction: How much do water layers interact with themselves vs. with the surface? How does the surface structure, composition influence this balance?
	How or what is the process for losing ion solvation to gain surface coordination?
	Elucidating water's self interactions as a function of temp and pressure.
	Electrical double layer passivates surface: How do all these redox reactions occur if surface is passivated?
	What is the form of mercury that is taken up into bacteria?
	The structure of water at interfaces and in confinement. How does that impact the understanding of chemical, biological processes in the environment.
(II) What are the long-term science questions (> 5 yrs) (green)	
	Quantify and understand how surface reactivity evolves with size and morphology (from perfect single crystal → nanoparticle).
	Mechanisms and kinetics of how hydrated ions go from solution to surface complexes.
(III) What advances in experimental probes or computation would be required? (blue)	
	Current methods for quantitatively probing mineral surfaces are generally not usable for nanoparticles, particularly at extreme small particle sizes (<10 nm). New methods may be required if traditional methods cannot be adapted.
	Tractable *ab initio* molecular dynamics.
	How many H_2O molecules will be sufficient to predict the actual water structure at the interface?
	More synchrotron time to go on "tangents" observed during experiments => more experimental details/analysis or faster detectors, ↑ beam intensity.
	Analysis software "model" generator for surface structure "starting point".
	Speciation and structure of metal ions in solution.
	Need in-situ surface characterization techniques to understand surface reactivity.

Interfaces	
(I) What are the most-pressing science questions (≤ 5 yrs) (pink)	
	Understand how surface defects affect mineral reactivity.
	Understand complex environmental interfaces including biofilm/organic/inorganic and surface coatings.
	The structures of topmost layer of a surface in proximity with molecules and particles, etc.
	Proximity effects on conducting surfaces: How does this enhance sorption processes? More experimental observations of such interactions.
	Understanding the electronic structure of surface environments, e.g., electron density differences at surfaces versus bulk. How does this affect surface processes?
	Electron transfer - how, where, why.
	pK_a's of solid-aqueous interfaces (1-2 nm, or first few layers of water).
	Structure reactivity relationships for geochemically important molecular species, e.g., surfaces and surface complexes; need experimental and theoretical information.
	Surface terminations: What really is the surface? (most likely not the substrate we think we have).
	What are the composition, structure and reactivity of poorly-ordered and ordered biogenic nanoparticles, fully hydrated and under physiological conditions?
	Electronic structure of bulk surfaces and the bulk is a function of grain size (bulk surface→nanoparticles); properties of nanoparticles compared to bulk for key bulk substrate; say PbS, Fe_3O_4, Fe_2O_3.
	Pores and defects.
	Are there simple rules that can organize the body of empirical data concerning the structure and stability of ions at surfaces?
	What is the structure of the EDL as a function of solid type, solution conditions, and T and P?
	How does the structure of the surfaces of environmental nanoparticles differ from those of large particles?
	Charge transfer processes.
	From solutions to surfaces and the other way around.
	Defects on oxides. They are there most of the time, and are nucleation centers. That's one of the differences between model surfaces and real surfaces.
	Can surface techniques such as RAXR be used to observe polynuclear species on mineral surfaces?
	Fundamental bonding/mechanisms/kinetics at interfaces (good, amorphous, nano-) and adding time resolution.

(II) What are the long-term science questions (> 5 yrs) (green)	
	Research in which water, CO_2, matter, and energy recycling are optimized without constraints on anthropic cycles, adding isotopes, M-speciation.
	How do the solution and surface interactions of ions of different types interact together?
	Understand ion distributions at complex interfaces.
	Surface structure under environmental conditions (hydrated, freshly cleaved, etc.), experimental and theoretical.
	Amorphous substrates; Identify composition and location => "structure", then how a non-ordered substrate is so reactive.
	Understand influence of interfacial pH at mineral-water interface on sorption and chemistry or abiotic/biotic systems.
	What is chemistry of H_2O at interfaces?
	Measure chemical structure and dynamics in situ w/high accuracy but simultaneously over a layer surface area to get geographic distribution and statistical significance, without destroying the sample.
	Develop predictive models of ion sorption as a function of surface structure based on the electronic structure of both.
	What are the mechanisms of chemical reactions at solid-water interfaces?
	How do bacteria interact with mineral surfaces at the molecular level (particularly MRB's)?
	What is the structure of water at interfaces and in confined spaces?
(III) What advances in experimental probes or computation would be required? (blue)	
	Nano-(surface) x-ray diffraction.
	Dynamics of structure; structure properties of disordered interfaces.
	New LCLS methods that allow XAFS measurements.
	Development of x-ray fluorescence STXM spectromicroscopy.
	Improvements in computational methods that allow studies of large systems.
	Focus more on defects on oxides. Many interesting or unexpected things are related to defects. Experimental tools probing defects (locally) are crutial.
	New concepts in wet cells. Introduction and measurement of biomaterials.
	Can we develop a high energy x-ray nanoprobe to get element distribution and speciation with nano-XRD and nano-XAS?
	Devices to study structures of adsorbed organic molecules, including macromolecules.
	Feedback from fundamental science studies into rational molecular (or materials) design processes, from an molecular environmental science perspective.
	Measurement of the kinetics of surface reactions on a molecular scale under environmental conditions.

Intermediate-scale	
Microscopic reaction processes	
(I) What are the most-pressing science questions (≤ 5 yrs) (pink)	
	Link between molecular and macroscale processes: How far are we from really linking the two (between model systems and real world problems).
	Effect of impurities on structure (physical and electronic) of nanoparticles.
(II) What are the long-term science questions (> 5 yrs) (green)	
	Water-rock geochemical interfaces and mineral-microbe interactions in pore scale simulations (e.g., lattice boltzmann) using molecular constraints.
	How can new ideas of surface structure and speciation be used to understand and predict rates of surface processes (e.g., nucleation, catalysis)?
	Whole "picture" system; carbon-pH-species-microbe on surface: Really mimic nature.
	Studying altered layers on silicate surfaces.
	Nature of surface complexes and the link between its structure, redox , solubility, bioaccumulation, etc.
Microbiology	
(I) What are the most-pressing science questions (≤ 5 yrs) (pink)	
	Do bugs talk and communicate with each other, or coordinate and help each other?
	Determine which microbes (I.D.) are associated with which minerals across environmental gradients: In-situ work on natural samples.
	Can we define the rates of ion adsorption/desorption?
	How do microbes modify surfaces and on what time scale?
	Measuring low concentrations typical for biological and environmental samples.
	How do microbes survive in a highly mineralizing environment?
	Is there any control of microbes on nucleation/growth of minerals?
	Which and how do biomolecules template formation of minerals?
	How can we monitor bacterial metabolic processes in real time (as is currently done with eukaryotic cells)?

(II) What are the long-term science questions (> 5 yrs) (green)	
	What controls microbe-mineral electron transfer?
	In natural systems, how are microbes interacting with surfaces (compared to "lab" systems)?
	Where do the "functional" microbes reside?
	Can we elucidate the general mechanism for bugs to do what they do across species?
	Detection of species in the whole sample to avoid excessive sample prep or sectioning which completely changes the speciation and distribution.
	Where do you actually find the nanoparticles and how do they interact with microbes in nature?
	How do recent advances in structure of water impact our understanding of water within cells (e.g., thermophiles and psychrophiles)?
	Abiotic vs. biotic adsorption of heavy metals and radiocuclies. Is it the nature of the adsorbate or substrate that determines adsorption behavior? (or both?) Why the similarity among bacteria? Are there differences with different mineral surfaces?
	Figure out how symbiosis impacts mineral dissolution and nanoparticle precipitation. Link single cell/culture experiments to field by including symbiosis of communities into labs.
(III) What advances in experimental probes or computation would be required? (blue)	
	Fast imaging techniques.
	How to determine that a texture is biosigned.
	STXM at 10 nm with cryo-device and fluorescence detection. Cryo-prep and spectroscopy (EELS) on cryo-TEM samples.
	Tandem nano-SIMS/x-ray microprobe.

Field-scale

Contaminant geochemistry

(I) What are the most-pressing science questions (≤ 5 yrs) (pink)	
	Identifying impactful processes governing contaminant mobility (metals, etc.) on a molecular level.
	Be able to quantitatively predict contaminant release under various environmental settings. What parameter controls how much….
	Need to determine speciation of operationally defined field parameters. Examples: (Reactive Hg) acid volatile S, Cr volatile S, etc.
	Extrapolating lab-scale experiments to much longer durations (centuries and more).
(II) What are the long-term science questions (> 5 yrs) (green)	
	Linking molecular-scale observation to physically complex systems: The natural environment.
	Does nature house the materials required for the stabilization of radioactive waste?
	What are the connections and real applicable ideas to enhance solutions to macroscopic earth science problems (mines, pollution, etc.).
	How will we compile vast amounts of data for a huge number of minerals and nanominerals into databases that are accessible and usable by the broad scientific community for predictive modeling? (i.e., usable at the field scale).
	Molecular measurements back to environmentally relevant processes.
(III) What advances in experimental probes or computation would be required? (blue)	
	Experiments, measurements, analyses that bridge the gap between molecular, interfaces , etc., with contaminant mobility.
	Need to marry genomes with (micro)spectroscopy to define specific microbes within natural conditions.
	Transportation path and rate of contaminant release from nuclear waste repositories and their reaction with organic matter and other elements in the environment.
	Improvement in detection for lower concentration samples. Separation method of the reactive phase (nanophase) from natural samples.

Scale cross-cutting

(I) What are the most-pressing science questions (≤ 5 yrs) (pink)	
	Imaging the very small and very fast in a complex measurement. Time resolved dynamics of the chemistry in complex systems in situ (without killing the cells). Simultaneously measure chemical resolution with statistical significance.
	Can we convince people that these processes are dynamic Fe crystals etc.
	How can we reverse or slow-down the effects of global warming?
	What is the cheap and elegant means of cleaning water of inorganic and organic chemicals and salt?
	How can we couple molecular-scale understanding of arsenic interaction with microbiota and minerals to field scale prediction of mobility in time and space?
(II) What are the long-term science questions (> 5 yrs) (green)	
	How to quantitatively assess geochemical fluxes/processes from description of the system at the (sub)-micron scale? Overcome the diversity of life.
	How do we relate model or single crystal work to natural particles? With respect to pH_{pzc}, surface reactivity, etc.
	Think about how to categorize macro-scale/field-scale reaction pathways in terms of key molecular-scale processes. What are key variables that impact intermediate and field scale?
	Applied applications. Soil/H_2O remediation nanowires → photocells. Electron transfer → electricity.
	Link microbial oxidation of carbon to mineral reduction on the global scale or to global climate models.
(III) What advances in experimental probes or computation would be required? (blue)	
	Microbiology techniques? In-situ protein expression probes, and measurements to link theoretical redox calculations (modeling) to empirical data on microbial activity in natural settings.
	Large scale computing. Molecular simulation of intermediate-scale systems. In-scale interactions to model field scale.
	Advances in computation to make this work. Increased experiment and theory collaborations: Reverse roles?
	Tools to observe molecular structures in living materials without damage or alteration or with sensitivities not yet available.
	Linking atomic-scale processes and rates to macroscopic values/observations.