



## Site-specific, size-dependent reactivity at mineral-water interfaces

**Wednesday November 14, 2007  
Burchard Room 118, Time: 11am**

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Computation is now well established as a primary means of discovering and understanding chemical reactivity in aqueous and interfacial systems. Progress has not moved as quickly in the Earth sciences as it has in molecular biology because low-temperature Earth materials are so difficult to characterize. An important aspect of the nanomineralogy revolution is that while “small” is not necessarily different, “small” may be more precisely characterized. Recent advances in research on nanometer-sized aqueous poly(hydr)oxocations provide a particularly well defined path toward understanding surface reactivity in aqueous oxide systems. Experimental investigations on these ions form an unusually tight link with computer simulation, allowing determination of site-specific acid-base and ligand exchange reactions in aqueous systems. We find that exchange mechanisms are highly cooperative and not at all similar to mechanisms derived from the studies of octahedral substitution in aquo ions, which are often used in conceptualization of ligand exchange processes on oxide surfaces. Understanding the kinetics of water-rock interaction at the molecular level leads to the best possible understanding of the processes governing the fate and transport of contaminants in the Earth's subsurface.

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**Dr. James Rustad** received his Ph.D. from the University of Minnesota in 1992. His research interests include interfacial and mineral surface geochemistry; mineralogy; and mineral physics. His groups efforts are focused on computational chemical models of interfacial structure as well as surface charging, sorption, dissolution, and precipitation phenomena at oxide-water interfaces. Computational methods are also applied to problems in mineralogy and in aqueous and silicate melt geochemistry, including physics of hydrated minerals, ligand exchange and electron transfer reactions. Current projects include large-scale molecular dynamics modeling of surface charging, aggregation, and electron transfer reactions on colloidal iron oxide particles, and multiscale description of mineral surfaces.

**Light refreshments will be served prior to seminar**



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