Towards an improved understanding of mineral surface reactivity: Current practices and future opportunities in computational geochemistry

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Geochemical processes are frequently influenced, if not controlled, by reactions that occur at the mineral-water interface. High-resolution in situ probes (e.g. Atomic Force Microscopy and Vertical Scanning Interferometry) have dramatically shaped mechanistic interpretations of mineral dissolution and growth; however, these methods provide only indirect information about the chemical processes underlying surface reactivity. Consequently, little is known about the mechanism(s) of ion attachment and detachment, even for mineral surfaces that have been thoroughly investigated. Recognizing such limitations, experimental investigations of geochemical reactions now frequently include insights derived from molecular dynamics simulations. Unfortunately, reconciling experimental and simulation derived rates is a significant challenge in its own right, especially as reaction frequencies approach and surpass the microsecond regime. Therefore, there is a critical need to develop simulation methods that can overcome current time and length scale limitations using existing high-performance computing resources. This seminar will review the current state-of-the-art in computational studies of the mineral-water interface and introduce a new methodology for obtaining reaction rates from molecular dynamics simulations.