Molecular Dynamics of Interfacial Water and Cations Associated with Clay Minerals

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Abstract
Clay mineral interfaces, including interlayer and external surfaces, play an essential role in many geochemical processes. Adsorption, dissolution, precipitation, nucleation, and growth mechanisms, in particular, are controlled by the interplay of structure, thermodynamics, kinetics, and transport at clay mineral-water interfaces. Molecular details of these geochemical processes are especially important in evaluating the fate of radionuclide waste in the environment. Such details are typically beyond the sensitivity of experimental and analytical methods and therefore require accurate models and simulations. Also, the basal surfaces and interlayers of clay minerals offer structurally constrained interfacial environments to better evaluate the local molecular chemistry. We have developed and used classical and quantum methods to examine the complex behavior of clay mineral-water interfaces and dynamics of interlayer species. Bulk structures, swelling behavior, diffusion, and adsorption processes are evaluated and compared to experimental and spectroscopic findings.

Bio
Jeffery Greathouse is a Principal Member of the Technical Staff at Sandia. He obtained B.S. degrees in chemistry and mathematics from Southwestern University and a Ph.D. in physical chemistry from the University of California, Davis. After postdoctoral research in the Department of Soil Science at the University of California, Berkeley and Lawrence Berkeley National Laboratory, he taught chemistry in academia before joining Sandia in 2004. His research involves molecular modeling of adsorption and interfacial processes with applications to the geosciences and materials science.

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