

Correlating mineral-water interface structure to particle interactions and emergent phenomena

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Colloidal interactions, coupled with hydrodynamics in many cases, are critical to understand man-made processes (e.g., nuclear waste treatment), in addition to natural processes (e.g., fate of pollutants in gaseous/aqueous phases). While the classical Derjaguin-Landau-Verwey-Overbeek (DLVO) theory has been a cornerstone of colloidal science, it clearly lacks details associated with geochemistry and chemical physics at molecular scales. We will show a simple scheme to couple the mineral-water interface structure to colloidal interactions, and discuss its implication to energetics and dynamics in the assembly of mineral nanocrystals. We will also briefly overview current activities in IDREAM (Interfacial Dynamics in Radioactive Environments and Materials), an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences to achieve the scale correlation, which is very critical to obtain fundamental understanding of emergent phenomena such as rheology.