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Coarse-grained simulation of chemo-mechanical coupling in swelling clay

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Clay minerals are one of the most important constituents of soils, sediments, and sedimentary rocks. The aggregation of clay nanoparticles, in particular, strongly influences porosity and permeability and is highly sensitive to both short- (hydrogen bonding, ion solvation) and long-range (charge screening) geochemical interactions. Simulation predictions of clay aggregation and swelling, to date, have relied almost exclusively on coarse-grained simulation techniques that rely on effective inter-particle potential models. Most such models are based on the Derjaguin-Landau-Verwey-Overbeek (DLVO) theory of long-range colloidal interactions and they neglect the short-range interactions that stabilize the crystalline hydrates (1-, 2-, and 3-layer hydrates). All-atom molecular dynamics (MD) simulations have the potential to help inform existing models but have focused almost exclusively on the crystalline hydrates.

Here, we present a new coarse-grained model parameterized based on all-atom simulations predictions of free energy of interaction of a pair of sodium clay nano-particles as a function of inter-particle distance and salinity[1]. We use this coarse-grained model to examine the chemo-mechanical coupling in assemblages of thousands of clay nanoparticles.

[1] Shen & Bourg (2021), *Journal of Colloid and Interface Science* 584, 610-621.

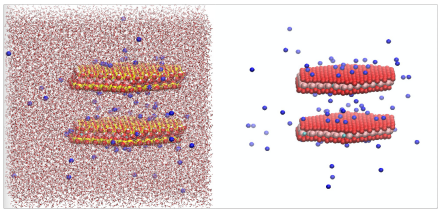

Figure 1. Comparison between all-atom model (left) and coarse-grained model (right)