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Coarse-grained simulation prediction of microstructure and mechanics in clay-water mixtures

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Clay minerals are one of the primary 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 (CG) simulation techniques that rely on effective inter-particle potential models. Most such models are based on the Derjaguin-Landau-Verwey-Overbeek (DLVO) model of colloidal interactions. Unfortunately, this model neglects key short-range interactions that stabilize clay assemblages. 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 CG model of clay-water mixtures parameterized based on our recent all-atom molecular dynamics (MD) simulations predictions of the free energy of interaction of a pair of sodium clay nanoparticles as a function of inter-particle distance and salinity [1]. We use our new CG model to examine the microstructure of clay-water mixtures as a function of clay volume fraction, shear rate, and salinity. We also predict the well-known chemo-mechanical coupling (i.e., impact of salinity on swelling pressure) in assemblages of thousands of clay nanoparticles. Our results reveal key details of the interactions between charged colloids in liquid water and help bridge the gap between microscale characteristics and macroscale properties of clay-water systems.

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

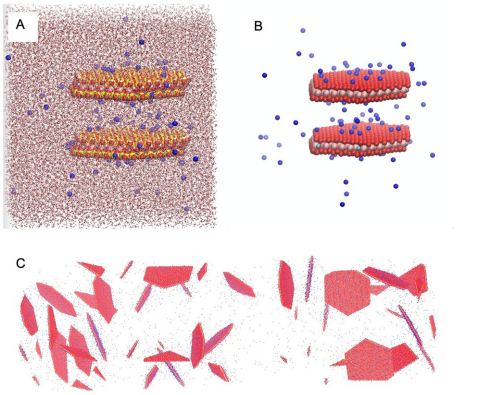

Figure 1. (A) All-atom MD simulation of two clay nanoparticles in liquid water. (B) Coarse-grained model of two clay nanoparticles in implicit water. (C) Coarse-grained model with multiple 25 nm diameter clay particles (system size is 50 × 50 × 300 nm).