

Molecular structure of interlayer water governs dispersion force adhesion of clay particles

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The clay swelling is one of the most fascinating and complex phenomena in soil geochemistry, which governs the reactivity and permeability of clay-rich soils. However, we still do not understand the forces acting between clay particles in varying hydration states that regulate their assembly and chemistry.

Here we present the study of clay plates interactions across the varying number of water layers. We assessed the confinement effect on the collective dynamics of water molecules (hydrogen bonding, dipolar relaxation times, dielectric properties) using the molecular simulations and first-principle plane-wave DFT calculations.

In the bulk aqueous system, we observe the wait-and-switch mechanism to determine the timescale of dielectric relaxation. The dielectric relaxation for water in the clay interlayer is more complex and depends more on the structure imposed by the surface than the hydrogen bond dynamics.

Because the water dielectric properties vary among the different clay hydration states, the Hamaker constant, needed to predict the van der Waals interactions, is a function of separation.

What is more, the Hamaker constant for plates separated by three layers is dominated by the zero-frequency component (Keesom and Debye dispersion) rather than by high-frequency one (London dispersion) – which is a rarely observed vdw-interaction regime.

The findings are important for our understanding of the interactions in compacted clay systems, clay suspensions stability and ion/contaminant transport in clay confined spaces.