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Colloidal interactions: bridging the gap from atomistic-scale descriptions to the mesoscale Primitive Model and introducing the Explicit Solvent Primitive Model approach ROLAND PELLENQ, CNRS/MIT, ¡MSE¿2, MIT, 77 Massachusetts Avenue, Cambridge, US, BENOIT CARRIER, MATTHIEU VANDAMME, Laboratoire Navier (ENPC/IFSTTAR/CNRS), Marne-la-Valle, France, HENRI VAN DAMME, CNRS/MIT, ¡MSE¿2, MIT, 77 Massachusetts Avenue, Cambridge, US, CNRS/MIT, ¡MSE¿2 TEAM, LABORATOIRE NAVIER TEAM — We investigated the interactions responsible for the cohesion of colloidal materials such as clays, cement... The swelling/cohesive properties of these (lamellar) materials depend both on the nature of the (interlayer) cations and on the surface charge of the layers. The overall goal of this work is determining the right level of modelling complexity required to capture the cohesive behaviour of charged materials immersed in an electrolyte. In addition to the analytical mean-field DLVO theory, we used various numerical modelling approaches of increasing complexity from the so-called Primitive Model to full-atomistic description. In particular, we introduced the Explicit Solvent Primitive Model (ESPM), in which ions are modelled as charged hard spheres and solvent molecules as soft spheres with embedded point dipoles. We showed that taking explicitly into account the solvent in such a Primitive Model description, significantly impacts the cohesion. Ionic correlation interactions are always present between charged objects immersed in an electrolyte and always play an important role, even in the case of system carrying a low surface charge balanced by monovalent counter-ions.

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