Clay-swelling inhibition effects by SiO2 nanoparticles: a molecular dynamics study

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Silica nanoparticles (NPs) have attracted extensive interest due to their stability, cost and functional properties. Particularly, for Oil recovery applications, an interest phenomena is how these NPs can affect or be affected by the interaction with clays found in oil reservoirs. Using molecular dynamics calculations, we simulated the clay swelling effects under the presence of hydroxylated and functionalized silica nanoparticles adbsorbed onto Montmorillonite (MMT) surfaces The systems have been modeled considering clay layers filled by brine (NaCl + CaCl2) and brine+NPs. The type and the ion concentration can significantly affect the swelling phenomena. For a given salt concentration, when the NP is only dispersed, an expansion is observed. In contrast, a compression between the clay layers occurs with the NP adsorption on the MMT surface (Fig.1a). Our MD results suggest the formation of electrical double layers (EDL) in both NP and MMT surfaces (Fig.1b). When the NP is not adsorbed, there is repulsion between the EDLs, which leads to the swelling in the MMT. For the NP adsorbed, due to overlap between the EDLs, there is an increasing in the ions accumulation on the MMT surface, resulting in an attractive potential and a compression of the layers.

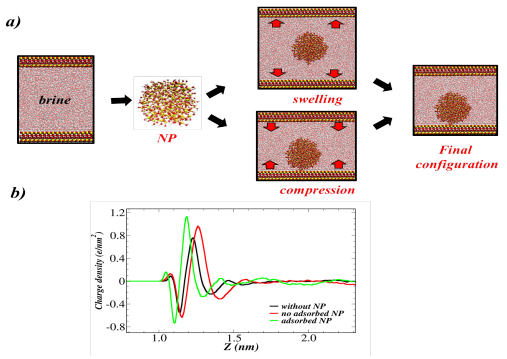

Figure 1: a) Mechanism of swelling clay with and without inclusion of nanoparticle; b) Electric double layer see in Charge density profile in the NP (Hydroxylated NP) presence.