A classical polarizable force field for the structure and dynamics of water and cations in clays and zeolites

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The wide use of clay minerals in industrial applications, energy and ecological engineering is partly due to their remarkable properties of retention at the mineral surface. The role of water on clay permeability and retention properties is crucial.

Molecular simulations allow a detailed picture of the fluid at its interface with the clay layers[1,2]. Unfortunately, they do not always reproduce quantitatively the experimental results, which casts a doubt on the validity of simulations interpretations[3]. In particular, the polarizability can play a significant role especially when an electric field is present at the interface, as it is the case with charged clays.

Therefore we developed a polarizable force field (PIM) based on DFT calculations. The structures of two uncharged clays (Pyrophyllite & Talc) and dry and hydrated montmorillonites with different types of counter-ions (Na^+, Cs^+, Ca^{2+} and Sr^{2+}) were simulated and compared with diffraction data. The comparison between the results obtained with PIM and the non-polarizable force field CLAYFF show improvements which encouraged us to extend PIM development to other types of clays and porous media like zeolites[4].

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