Hydrated Montmorillonite interlayer properties and adsorption of DNA nucleobases studied through static and MD *ab-initio* simulations

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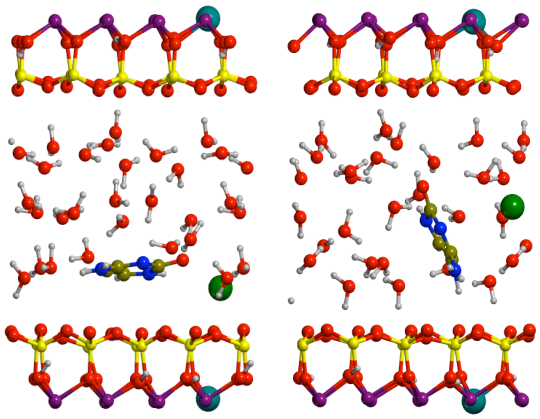
Montmorillonite belongs to the smectite group of clays comprising tetrahedral silica layers sandwiching octahedral alumina sheets. Alkali cation solvation and adsorption properties have been studied via periodic DFT plane wave calculations through the analyses of electronic density/electrostatic potential and via *ab-initio* MD.

In addition, in relation with prebiotic chemistry, structural behaviours of a nucleobase in the hydrated Na^+-montmorillonite clay interlayer have been investigated through short constrained simulations that allowed us to identify stable configurations. Longer simulations, carried out for the observed stable configurations are analysed in terms of the conformation of the nucleobase within the interlayer as well as its interaction with the surface the cation and water molecules. Simulation with larger systems ultimately investigated will be presented.



Ref:
J. Phys.Chem. C., 2013, 117, 26179–26189; Phys. Chem. Chem. Phys., 2012, 14, 945-954; Phys. Chem. Chem. Phys., 2010, 12, 688-697; J. Phys.Chem. C., 2009, 113, 13741–13749.