Modelling the Adsorption of Bio/Organic Molecules at Montmorillonite Surface and Edge

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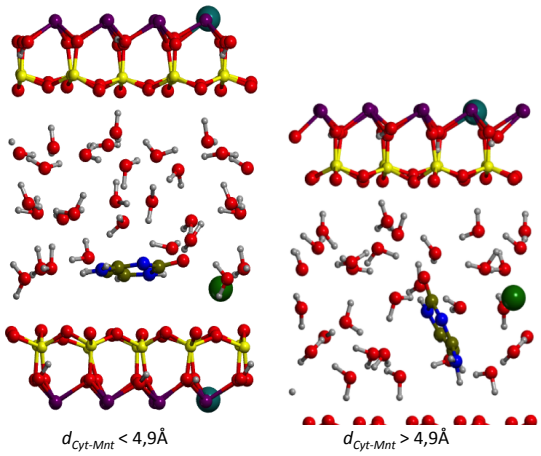
Because clay minerals are well known for their adsorption properties, they are most likely responsible for the retention and degradation of micropoluants in soils. Montmorillonite belongs to the smectite group of clays comprising tetrahedral silica layers sandwiching octahedral alumina sheets. It has been chosen as a model system to study the adsorption of biomolecules and organic molecules in clay minerals through atomistic modelling.

The study of the swelling mechanism of montmorillonite let us show the importance of tetrahedral/octahedral substitutions and interlayer alkali cations through *ab-initio* Molecular dynamics. Static calculations of biomolecules placed at the dry basal surface as well as at the edge of clay particle allow characterizing the possible molecular interactions responsible for adsorption and retention. These models are then improved by adding water and investigate the interplay between the cation, water and the molecule through short MD simulations. Similar classical MD simulations have been carried out to model on a longer time scale the adsorption/desorption mechanism of micropoluants on the clay hydrated basal surface. These results are then compared with experimental measurements allowing one to interpret more precisely the theoretical.



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.