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

V. Marry¹, S. Tesson¹, W. Louisfrema¹,², M. Salanne¹, B. Rotenberg¹, A. Boutin², E. Ferrage³

¹ Sorbonne Universités, UPMC Univ Paris 06, CNRS, UMR 8234, PHENIX, F-75005 Paris, France
² Ecole Normale Supérieure, PSL Research University, UPMC Univ Paris 06, CNRS, Département de Chimie, PASTEUR, 24 rue Lhomond, F-75005 Paris, France
³ Univ Poitiers, Ecole Natl Super Ingenieurs Poitiers, HydrASA, CNRS, IC2MP, UMR 7285, F-86022 Poitiers, France

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 layers¹². Unfortunately, they do not always reproduce quantitatively the experimental results, which casts a doubt on the validity of simulations interpretations³. 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⁺, Ca²⁺ and Sr²⁺) 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 zeolites⁴.