Recent improvements in ClayFF and future challenges for classical molecular simulations of nano-confined water in minerals

ANDREY G. KALINICHEV[1,2]

[1] Laboratoire SUBATECH (UMR-6457), Institut Mines-Télécom Atlantique, 44307 Nantes, France

[2] International Laboratory for Supercomputer Atomistic Modelling and Multi-Scale Analysis, National Research University Higher School of Economics, Moscow, Russia (kalinich@subatech.in2p3.fr)

Molecular simulations of water and aqueous solutions in mineral nano-pores, interlayers and interfaces, have always been very challenging due to the complex crystal structure and atomic composition of their solid mineral substrates that are usually known only with significant uncertainty. Molecular level understanding of the structure and properties water in contact with clays and clay-related phases, metal (oxy-)hydroxides, layered double hydroxides, cementitious materials, zeolites, etc., is strongly affected by significant degree of structural and compositional disorder of the interfaces. ClayFF (Cygan et al., 2004) was originally developed as an *ad hoc* response to the obvious need for a robust and flexible force field for classical molecular simulations of such systems. However, despite its unexpected success, multiple shortcomings have also become evident with time.

This talk will provide a brief overview of several recent attempts to overcome these shortcomings and to improve ClayFF performance, focusing on the most recent MD simulations that probe molecular properties of water in several clay-related and cement-related materials and compare them with available experimental data.

Cygan, R.T., Liang, J.J., Kalinichev, A.G., 2004. Molecular models of hydroxide, oxyhydroxide, and clay phases and the development of a general force field. *J. Phys. Chem. B* **108**, 1255-1266.