

Laboratoire Physicochimie des Electrolytes, Colloïdes, et Sciences Analytiques
UMR 7195 UPMC/CNRS/ESPCI

SEMINAIRE

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The effects of organic molecules on cation-clay interactions in aqueous environment

Understanding and prediction of many natural and anthropogenic environmental processes ultimately depend on a fundamental understanding of the chemistry occurring at the mineral-fluid interfaces. Clay-related minerals and natural organic matter (NOM) are ubiquitous in the environment, and metal-NOM complexation induces strong correlations between the NOM concentration in the aqueous phase and the capacity of clay particles to bind metals, thus affecting their speciation, solubility and toxicity in the environment. Despite significant geochemical, environmental and technological interest, the molecular-level mechanisms and dynamics of the physical and chemical processes involving both clay and NOM are not yet well understood.

In this talk I will briefly introduce CLAYFF as a general force field suitable for the molecular simulations of hydrated multicomponent mineral systems and analyze three different molecular dynamics simulations of metal-NOM complexation in aqueous solutions. Their comparison with available experimental data allows us to quantitatively assess possible effects of model- and system size-dependence in such molecular simulations. Despite some obvious variations in the computed results that depend on the size of the simulated system and on the parameters of the force field models used, all three simulations are quite robust and consistent. For Ca^{2+} ions they show approximately 35-50% association with the carboxylic groups of NOM at near-neutral pH and point to a strong preference for the stability of bidentate-coordinated contact ion pair complexes. The degree of NOM supramolecular aggregation in solution and its potential mechanisms in the presence of Na^+ , Cs^+ , Mg^{2+} , and Ca^{2+} ions are also assessed on a semi-quantitative level from larger-scale MD simulations. Easy association of metal cations with negatively charged NOM functional groups and negatively charged clay surfaces makes cationic bridging the most probable mechanism of NOM association with clays in natural environments.

Mercredi 2 février 2011 à 14h30

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