

Structure and stability of mineral interfaces

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The aim of this presentation is to describe some recent applications of atomistic simulation studies for extending the range of applications to mineral interfaces. Two main themes will be addressed. The first is to describe our recent work on using Path Integral Molecular Dynamics. The approach is to provide quantum treatment of nuclear motion and particularly improve the description of proton motion. As a way of disentangling the electronic from nuclear motions we begin by presenting preliminary results for a number of mineral water interfaces using PIMD in the DL_POLY [1] code and employing interatomic potentials.

The second area is the application of both potential-based and DFT simulations towards modelling increasingly complex mineral interfaces. Two areas where we have investigating ways of improving the mineral surface description are (i) the simulation of polar surfaces and (ii) the interaction of nanoparticles with mineral surfaces.

A number of strategies in which the mineral can remove a surface dipole will be discussed and illustrated with several examples including the layered mineral: lizardite, where each layer is comprised of a silica sheet linked to brucite.

Finally, modelling the nanoparticle-surface interaction will be discussed. The release of nanoparticles into the environment could cause adverse ecological problems, and thus the transport of nanoparticles in the environment and the interaction of nanoparticles with the geosorbents are of concern. There are currently few studies that have addressed the interactions of nanoparticles with soil minerals, although numerous reports already showed that soil minerals such as clays can have strong interactions with organic contaminants. Here we will report our current work on these interactions. One example where all techniques can be applied is the interaction and transport of fullerene and its interaction with clay surfaces. Our results indicate that adsorption of fullerene on soil clay minerals could significantly influence its transport in the environment.

[1] Smith & Forester (1996) *J. Mol Graph* **14**, 136–141.

Mine water geochemistry and biogeochemical modeling

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In mine tailings sites, where sulfide minerals are in contact with atmospheric humidity and meteoritic water, oxidation of sulfides generate acidity leading to mobilization of metals and metalloids through the soil to surface and underground waters. The resulting acid mine drainage can impair dramatic environmental problems (i.e. toxicity of arsenic III, etc.). In the old gold mine of Chéni (France), large physical, chemical and microbiological datasets are available: mineralogical compositions of the tailings [1], long-term survey of drainage waters chemistry [2] and microbiological characterizations [3]. The pH/Eh of sampled waters through the tailing column (unsaturated and saturated zones) is in the range of 2.9–7.6 and 0–700mV respectively. Analysis of these data permitted to identify the key processes of mine water behavior. Numerical simulations, using the geochemical software PHREEQC [4], were performed aiming to identify the key mechanisms and understand those coupling processes.

First analysis of geochemistry show different redox potentials for each element (Fe, As, O₂, N, S). Such redox disequilibrium, known in natural waters [5] is rarely take into account in modeling. In our work, redox decoupling of the thermodynamical database is used to model redox behavior of mine water.

Biological oxidation of arsenic was identified as an active and sustained process in such systems. Experimental results of biological As oxidation was used to develop a thermokinetic model coupling geochemistry and biologic activity [6] and reproducing the pH-dependant activity of bacterial population.

Finally, we elaborate a mixed biogeochemical model to reproduce the behavior of an acid mine drainage, which takes into account major processes including bacterial activities, precipitation of Fe-containing minerals (Schwertmannite, ferrihydrite, jarosite) and surface complexation.

[1] Roussel (1998) *PhD thesis*, Univ. Limoges. [2] Bodéan *et al.* (2004) *Appl. Geochem.* **19**, 1785–1800. [3] Battaglia (2002) *J. Appl. Micro.* **93**, 656–667. [4] Parkhurst et Appelo (1999) USGS Rep. **99**, 4529. [5] Lindberg & Runnels (1984) *Science* **225**, 925–927. [6] Jin & Bethke (2005) *Geoch. Cosm. Acta* **69**, 1133–1143.