

Atomistic Simulation of the Interaction of Mineral Surfaces with Water

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Atomistic simulation is a valuable tool for predicting the structure of surfaces. This poster considers some of our recent work aimed at applying the approach to mineral surfaces in contact with water. In general we use energy minimisation and molecular dynamics which are coupled with inter-atomic potentials. The use of such potentials enables the surface properties to be calculated rapidly and enables the study of complex systems. Therefore it is essential that we can derive and verify suitable parameters to describe these systems.

This is illustrated with in recent work where we combined techniques that use inter-atomic with electronic structure calculations using Density Functional Theory (DFT) to investigate the interactions of water with the surfaces of carbonate minerals. We first compared the two techniques for small model systems, namely the adsorption of a monolayer of water of the $\{10\bar{1}4\}$ surface of calcite, dolomite and magnesite. We then re-considered the potential model for the water-mineral interactions to improve agreement with the DFT calculations and enabled us to model with confidence the adsorption of water on the most significant low index surfaces and on growth steps. Finally, we performed classical molecular dynamics simulations of calcite surfaces in contact with bulk water to investigate the effect of temperature and kinetics on the calcite-water interface.

The need to simulate surfaces in contact with water is illustrated in recent work concerned with the surfaces of hematite (alpha - Fe_2O_3). It was found that the relative stability of the low index surfaces, and hence the morphology is highly dependent on whether water is present and to a lesser extent on whether the water layer consists of dissociated hydroxide ions or molecular water. This is further illustrated in work where the segregation of various iso-valent cations to the (00.1) and (0.12) surfaces of hematite where the presence of water significantly effects the segregation process.

Finally we highlight a key challenge for the future, which is not only to simulate a the interface between a mineral surface and a water layer, but also consider the interaction when the water layer contains charged species.