Atomistic modelling of pollutant adsorption at mineral - water interfaces

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The aim of this presentation is to highlight recent work using atom-based simulation methods to model the adsorption of different classes of pollutant at mineral-water interfaces.

One of the key challenges is to obtain a reliable description of the structure and composition of the mineral interfaces. Our approach uses a combination of DFT including van der Waals interactions, along with potential model based methods. The former, when combined with lattice dynamics can be used to evaluate the free energies of adsorption at mineral surfaces, as well as generate IR and Raman spectroscopic data, which can be compared directly with experiment. The potential based approaches using molecular dynamics and Monte Carlo techniques are applied to give a more reliable description of the dynamics at the mineral-water interface, as well as a more efficient route to explore different structures and configurations of the surfaces in contact with water.

Three different topics will be examined. Firstly, the adsorption of CO_2 and water on several surfaces of hydroxide minerals including brucite, where we demonstrate that the effect of the surface structure and composition can be modified by the composition of the gas phase species. Secondly, we describe the adsorption of organo-compounds on clay minerals, where our results indicate that the adsorption of these contaminats, which is surface-site as well as counter-ion-site sensitive, significantly disrupts the structure of the mineral-water interface and thus the surface retention capacity.The final example is that of metal cations, where the role of surface structure and composition is illustrated on both alkaline earth and iron hydroxide terminated surfaces.