Simulation of Sr(II) Adsorption and Sr-Ba Exchange on Barite ($BaSO_4$)

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This work combines X-ray reflectivity (XR) measurements with density functional theory (DFT) and classical molecular dynamics (MD) simulations to determine the adsorption and exchange mechanisms of Sr(II) at the barite (001) surface. The overall goal of this research is to develop classical force field simulations to model the growth and dissolution of barite. At this stage, we are testing the ability of DFT and classical MD simulations to reproduce the experimental XR data. Displacements of surface sulfate ions and adsorbed H_2O molecules above the surface were consistent between the XR measurements and DFT calculations. Classical MD simulation results were somewhat less accurate. Resonant anomalous X-ray reflectivity (RAXR) measurements indicate two positions for Sr(II) at the barite (001)-water interface near -1 and +2 Å from the surface (as defined by the positions of the Ba(II) ions terminating the bulk). DFT and classical simulation were performed and resulted in similar energies for the Sr(II) in positions adsorbed 2.2 Å above the surface and exchanged with the two types of Ba(II) sites. This indicates rapid exchange is possible. Modeling of the exchange mechanism is currently underway.