

Oxyanions interaction with oxyhydroxides mineral surfaces

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Oxyanion adsorption on mineral surfaces is shown to affect the distribution of contaminants in the environments significantly. The co-sorption of oxyanions (phosphate / arsenate) and heavy metals on oxyhydroxides geosorbents is of particular interest as it may interfere with natural catalysis and sorption capacity of a number of minerals. Although, decreased sorption may arise from either the competition for surface binding sites or the formation of stable non-adsorbing cation-oxyanion complexes in solution, the enhanced sorption may be attributed to the reduced electrostatic screening and the formation of surface precipitates/complexes. A number of binding models for the two types of contaminants have been proposed, and the mechanism of phosphate adsorption is still debated with the existence of both monodentate and bidentate surface complexes of phosphate ions being suggested.

In all processes involving contaminants at mineral interfaces, the molecular level interactions between adsorbants and adsorbates are key factors controlling their fate. We present therefore our recent work using a combination of quantum and potential based methods. We have evaluated the surface composition of selected Fe-rich and Ce-rich minerals to gain atom-level insights into the factors controlling the interaction of oxyanions and oxyhydroxides geosorbents.