Density Functional Theory Calculations of Oxyanions on Ferrihydrite Nanoparticles

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Ferrihydrite is a critical substrate for adsorption of oxyanion species in the environment. The nanoparticulate nature of ferrihydrite is inherent to its formation, and hence it has been called a "nano-mineral". The nano-scale size and unusual composition of ferrihydrite has made structural determination of this phase problematic. Michel et al.[1] have proposed an atomic structure for ferrihydrite, but this model has been controversial. Recent work has shown that the Michel et al.[1] model structure may be reasonably accurate despite some deficiencies. An alternative model has been proposed by Manceau[2].

This work utilizes density functional theory (DFT) calculations to model both the structure of ferrihydrite nanoparticles based on the Michel et al.[1] model as refined in Hiemstra[3] and the modified akdalaite model of Manceau[2]. Adsorption energies of carbonate, phosphate, sulfate, chromate, arsenite and arsenate are calculated. Periodic projector-augmented planewave calculations were performed with the Vienna Ab-initio Simulation Package (VASP) on an approximately 1.7 nm diameter Michel nanoparticle ($Fe_{38}O_{112}H_{110}$). After energy minimization of the surface H and O atoms. The model will be used to assess the possible configurations of adsorbed oxyanions on the model nanoparticles.

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3. Hiemstra T. (2013) *Geochimica et Cosmochimica Acta*, 105, 316-325.