

## **Density functional theory on adsorption thermodynamics of oxyanions and organic acids onto Fe-oxy(hydr)oxides**

JAMES D. KUBICKI

Department of Geological Sciences, The University of Texas at El Paso, [jdkubicki@utep.edu](mailto:jdkubicki@utep.edu), USA

Mineral surfaces present a range of adsorption sites with various reactivities. From radical sites to step corners and regular terraces, the potential energies at different sites can range over 100s of kJ. This means that high-energy defect sites are generally low-density sites that are responsible for adsorption at low concentrations and surface coverages. However, to observe surface complexes spectroscopically or with calorimetry, higher surface coverages are necessary. This discrepancy is problematic for geochemical reactions in nature where the adsorbate is in low concentrations in solution because experiments may not be detecting the geochemically-relevant species (Ainsworth et al., 1998).

This work explores various adsorption sites on ferrihydrite and goethite by calculating the adsorption energies of oxyanions (e.g., arsenate, phosphate) and organic acids (e.g., oxalic, salicylic) onto defect and regular surface sites. The range of adsorption energies and surface concentrations are discussed and the implications for matching molecular models of individual sites with spectroscopic and thermodynamic data are explored.

Ainsworth C. C., Friedrich D. M., Gassman P. L., Wang Z., and Joly A. G. (1998) Characterization of salicylate-alumina surface complexes by polarized fluorescence spectroscopy. *Geochim. Cosmochim. Acta* **62**, 595–612.