Structure of the iron-oxide - aqueous solution interface: surface x-ray diffraction and density functional theory studies.

T.P. TRAINOR[1] , P.J. ENG[2], A.M. CHAKA[3], C.S. LO[1,3], K.S. TANWAR[1], S. GHOSE[2], AND S.C. PETITTO[1]

[1] Dept. of Chemistry and Biochemistry, University of Alaska Fairbanks, Fairbanks AK, USA; fftpt@uaf.edu.
[2] Consortium for Advanced Radiation Sources, The University of Chicago.
[3] National Insititutes of Standards and Technology, Gaithersburg, MD, USA.

Establishing results on mineral-water interface structure, and structural modifications that result from changes in aqueous composition, are critical to furthering the development of a structure based understanding of aqueous geochemical interface systems and improving both conceptual and quantitative models of geochemical chemical pathways. However, detailed analysis of aqueous geochemical interfaces has been limited by the difficulty of studying heterogeneous systems, particularly under realistic environmental conditions [1]. Here, we will present some of our recent work focused on determining the structure of low index faces of hematite using synchrotron based surface x-ray diffraction [2,3]. Specifically, we will discuss the influence of water on the resulting surface structures, the surface modification of hematite due to reaction with aqueous Fe(II), and the resulting changes in surface reactivity with respect to aqueous Pb(II) adsorption. The experimental models will be compared with the results of periodic density functional theory and ab initio thermodynamic calculations to provide a detailed interpretation of the energetics of the systems under investigation.

References

[1] T.P. Trainor, P.J. Eng, A.S. Templeton (2006) *J. Electron. Spectr. Relat. Phenom* **150,** 66-85.
[2] T.P. Trainor et al. (2004) *Surf. Sci* **573,** 204-224.
[3] K. Tanwar et al. (2006) *Submitted*.