

Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Structure, Reactivity, and Lead Sorption of Hydrated Alumina and Hematite Surfaces SARA MASON, ANNE CHAKA, NIST — It is well known that polarity and structure of oxide surfaces have significant impacts on reactivity. Experimental and theoretical studies at solid-aqueous interfaces have revealed that hydrated oxide surface morphology can vary significantly from surfaces under high vacuum conditions. We apply a combination of density functional theory simulations and *ab initio* thermodynamics to hydrated structures of α -Al₂O₃ and α -Fe₂O₃ surfaces. While geometrically isostructural in the bulk, these two oxides have sharp contrasts in electronic structure and can have thermodynamically stable surface terminations which differ in both the number and type of exposed functional groups. We use the environmentally relevant interaction of Pb(II) with the hydrated surfaces to explore relationships between reactivity and both surface structure and identity.

Sara Mason
NIST

Date submitted: 27 Nov 2007

Electronic form version 1.4