Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Structure of Iron Oxide Water Interface: a combined CTR and DFT study SANJIT GHOSE, PETER ENG, University of chicago, CYNTHIA LO, NIST, Gaithersburg, KUNALJIT TANWAR, THOMAS TRAINOR, University of Alaska Fairbanks, GLENN WAYCHUNAS, LBNL, Berkeley — Chemical reactions at the mineral and water interface play an important role in many natural and technological processes, from controlling the fate and transport of environmental contaminants, and biological availability and geochemical cycling of iron to the electronic device fabrications. The interface structure and composition of a mineral, dictates the chemical interactions that take place between the mineral and its environment, and also play a pivotal role in nanoparticle growth process. Therefore, we have conducted a systematic investigation of the solid-solution interface structure of two of the most common and stable phases of iron oxides systems: hematite (α-Fe_2O_3) (1-102) and goethite (α-FeOOH) (100) – using the crystal truncation rod (CTR) diffraction technique. The distribution and form of surface hydroxyl groups at the interface are described using combined CTR and *ab initio* density functional theory (DFT) calculations. Goethite (100) interface structure is determined to be a relaxed double hydroxyl termination with the presence of two semi-ordered water layers exposing two types of hydroxyl groups at the surface and the hematite (1-102) interface structures show vacancies in the near surface metal occupancies and different distributions of surface hydroxyl groups.

Sanjit Ghose
University of chicago

Date submitted: 20 Nov 2006

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