

NANO HIGHLIGHT

Structure and Reactivity of Geochemical Interfaces: Molecular and Nanoscale Controls on Surface Reactivity

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Chemical processes at the metal-oxide/aqueous solution interface play a critical role in dictating the chemistry of aquatic systems and are often a dominant factor controlling contaminant transformation, transport and solid phase partitioning. Iron-(hydr)oxide phases play a particularly important role in the heterogeneous chemistry of aquatic systems due to their widespread abundance and typically small (sub-micron) particle size. The aim of the Geochemical Interfaces NIRT project is to investigate the nano- and molecular-scale factors that influence the surface reactivity of iron-oxides. We utilize a combined approach of batch scale measurements of surface reactivity (Fig. 1) and surface structure analysis (Fig. 2) coupled to high level *ab-initio* predictions of surface structure and energetics¹⁻³. Our results suggest that reactivity (and reactivity differences) can largely be explained in terms of the composition and local coordination chemistry of surface functional groups. These results, based primarily on analysis of well characterized single crystal systems, are beginning to provide a basis for understanding how particle size, morphology and chemical modification of surfaces (e.g. surface hydroxylation or reaction with common aqueous solutes) influence surface structure, and thus dictates the reactivity of iron-hydroxides in natural environments.

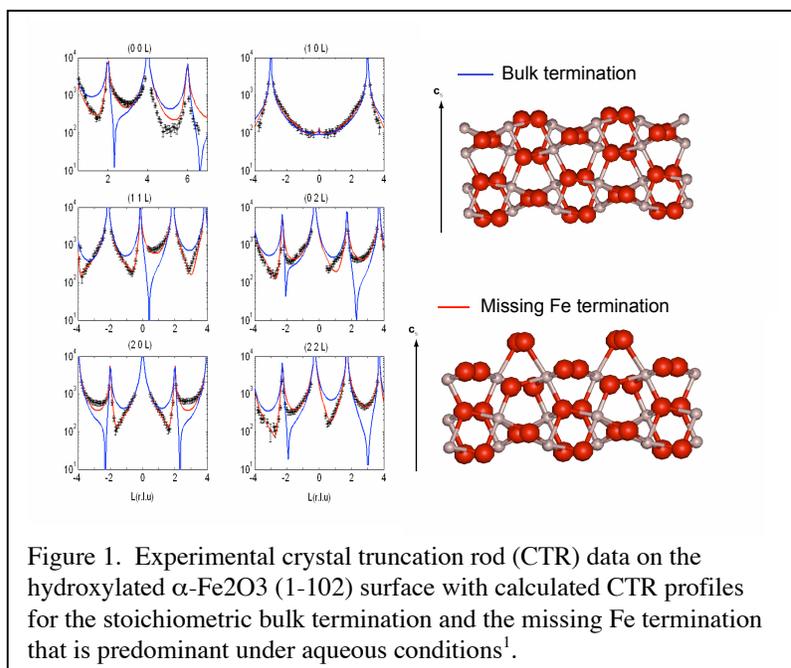
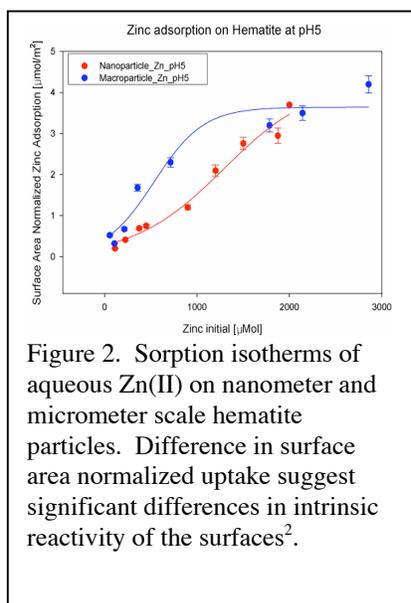


Figure 1. Experimental crystal truncation rod (CTR) data on the hydroxylated α -Fe₂O₃ (1-102) surface with calculated CTR profiles for the stoichiometric bulk termination and the missing Fe termination that is predominant under aqueous conditions¹.

References

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