# 56f Surface Structure and Reactivity of Clean and Hydrated A-$Fe_2O_3$

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The structure and reactivity of metal oxides such as α-$Fe_2O_3$ depends on several factors, including the composition of the bulk material, crystallographic orientation, and local coordination of the surface atoms. In particular, interactions at the solid-liquid interface play major roles in catalysis, chemical sensors, and environmental processes such as contaminant sequestration and remediation. Unfortunately, these oxide surfaces have largely been characterized experimentally and theoretically only under UHV conditions. Therefore, it is important to understand the adsorption and dissociation of water on the α-$Fe_2O_3$ surface. We have computed, using density functional theory and *ab initio* thermodynamics, the structure and Gibbs free energy of several terminations of clean and hydrated α-$Fe_2O_3$ (0001) and (1-102). We have found that in each case, the most stable termination in the presence of water is not the bulk stoichiometric termination. For example, α-$Fe_2O_3$ (0001) is Fe-terminated when clean, but O-terminated when hydrated, and hydrated α-$Fe_2O_3$ (1-102) is missing the first layer of Fe atoms. These results have been confirmed with experimental crystal truncation rod x-ray diffraction data. Finally, we discuss implications for metal ion adsorption to these surfaces.