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Structure of Hydrated α-Fe_2O_3 (0001) and (1$\bar{1}$02)[1] CYNTHIA LO, National Institute of Standards and Technology, Chemical Science and Technology Laboratory, ANNE CHAKA, National Institute of Standards and Technology, Chemical Science and Technology Laboratory, THOMAS TRAINOR, University of Alaska Fairbanks, Department of Chemistry and Biochemistry — The structure and reactivity of α-Fe_2O_3 depends on several factors, including the composition of the bulk material, crystallographic orientation, and local coordination of the surface atoms. As an example, the adsorption and dissociation of water on α-Fe_2O_3 and other metal oxide surfaces is not well understood, since the oxide surface has largely been characterized under ultrahigh vacuum or clean conditions. However, interactions at the solid-liquid and solid-solid interface play major roles in environmental processes, including contaminant sequestration, mobility, and bioavailability. In this work, we present density functional theory results on the structure of clean and hydrated α-Fe_2O_3 (0001) and (1$\bar{1}$02), and show the changes in surface structure upon heterolytic water dissociation and water physisorption.

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