Iron-Oxide Surfaces and Their Reactivity to Water

The interaction of water with iron oxide surfaces underlies geochemistry, corrosion, and weathering processes, and there are numerous technologies where iron oxide reactivity plays an important role. For example, the industrial catalyst for the water-gas shift reaction (CO + H₂O ⇌ CO₂ + H₂) is based on magnetite (Fe₃O₄), and hematite (α-Fe₂O₃) is a promising photoanode for photoelectrochemical water splitting and artificial photosynthesis devices. In this talk, I will describe our recent efforts to understand the adsorption of water on iron oxides at the atomic scale, with a focus on Fe₃O₄(001), (111), and (110) surfaces, as well as the α-Fe₂O₃(012). Using a combination of experimental techniques and density functional theory based calculations, I will show that partially dissociated water dimers are common to all these surfaces. I will discuss how the different surface structures dictate the evolution of the water overlayer as the coverage increases, address what might happen in high pressure and liquid environments, and attempt to put these results into the context of what is known about water adsorption on other metal oxide surfaces.