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Combined Surface Science and Density Functional Theory Approach towards Water Ordered Structures Formation on Magnetite

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Abstract:

The interaction of water with iron oxide surfaces is relevant for several processes of practical interests. Three different adsorbed water species were distinguished on Fe-terminated Fe₃O₄ multilayer films using thermal desorption spectroscopy (TDS), and ultraviolet photoelectron spectroscopy (UPS) measured under adsorption-desorption equilibrium conditions [1]. By means of density functional theory (DFT) calculations, the first species (γ -water) were confirmed to correspond to dissociative water adsorption with the resulting hydroxyl (OH) groups of water on the surface iron (Fe) sites and the H-atoms adsorbed onto surface oxygen (O) sites. The DFT result for the γ -water structure is consistent with the two OH-stretch lines observed by infrared-reflection-adsorption-spectroscopy (IRAS) [2], and the UPS study [1]. The DFT calculations confirm the subsequent formation of mixed molecular- and dissociated-water structures (β -water) formed by H-bonded molecular water to the surface OH-groups on surface-Fe, and the H on the surface-O sites, respectively, as suggested by the IRAS [2] and LEED experiments [2]. The DFT results reveal that formation of the γ -water overlayer structure results from the diffusion of the mobile H-atoms from the initially molecular adsorbed water on iron sites followed by formation of a transition structure with the H-atom adsorbed the nearest-neighboring oxygen sites, diffusing over the surface to adsorb on-top onto the next O-sites.

[1] W. Weiss and W. Ranke, Prog. Surf. Sci. 70, 1 (2002).

[2] U. Leist, W. Ranke and K. Al-Shamery, Phys. Chem. Chem. Phys. 5, 2435 (2003).