Effects of an electric field on the adsorption of water molecules on the Cd(0001) surface

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ABSTRACT: The adsorption of water molecules on the Cd(0001) surface has been systematically investigated in the absence or presence of the electric field using first principles calculations based on density functional theory. It has been determined that the adsorption is enhanced by the electric field. From the geometries and energetics, we find that the water-cadmium interaction become stronger (weaker) under a negative (positive) field in the adsorbed monomer. Otherwise, the formation of the hydrogen bonds makes it difficult for molecules in the water clusters to response the electric field. Most importantly, the stability of the water bilayers depends on the strength of the negative electric field. Instead of the H-up bilayer, the H-down bilayer is more stable when the negative field is sufficiently strong. In this case, the dipole-field interaction is the dominant interaction in the change of stability. These results are helpful in the understanding of the fundamental processes at the water-electrode interfaces.

Keywords: water adsorption; electric field; cadmium electrode;

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