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LETTER TO THE EDITOR

First-principles study of CO adsorption on ZnO surfaces

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Abstract

Using density-functional theory we have calculated the equilibrium geometries and binding energies of a CO monolayer adsorbed on the nonpolar $(10\bar{1}0)$ and the polar (0001)-Zn and $(000\bar{1})$-O surfaces of ZnO. Different adsorption sites and CO orientations were considered, and for the polar surfaces the influence of a hydrogen coverage upon CO adsorption was studied. For the clean surfaces we find that CO exclusively binds to Zn ions with a binding energy of 0.24 and 0.37 eV for the nonpolar $(10\bar{1}0)$ and the polar (0001)-Zn surface, respectively. A purely repulsive interaction of CO with surface oxygen ions is obtained. On the other hand, if the polar surfaces are hydrogen saturated, we predict a weak chemisorption of CO to the OH-terminated $(000\bar{1})$ surface with a binding energy of 0.20 eV but no CO adsorption for the ZnH-terminated (0001) face.