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Dissociative adsorption of water molecules on uncharged surfaces of indium(111) and gallium

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Abstract

A possible mechanism of dissociative adsorption (DA) of water on the (111) surface of indium and liquid gallium is investigated within a cluster model for metal using a density functional method (B3LYP). The adsorption interaction of H and O atoms and OH group with these metals is studied. The free energy of DA of H2 and O2 molecules is calculated. An analysis of DA is performed both for the case of the metal/vacuum interface and with allowance made for solvation effects within a continuum approach. According to quantum-chemical calculations, DA of water on the In(111) surface is more thermodynamically probable than on gallium. In the case of indium, DA with the participation of a water dimer may have a smaller activation energy compared with DA of monomer H2Oads. The data obtained are used to interpret the experimentally observed nonmonotonous dependence of the work function for indium and gallium on the partial pressure of water vapor. The hypothesis about the origin of the absorption band in electroreflectance spectra for the gallium/aqueous solution interface as a result of the electron transfer from an adsorbed water molecule into the metal's conduction band is confirmed.

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Keywords

Cluster model of metal, Dissociative adsorption, Gallium, In(111), Quantum-chemical calculation, Water molecules