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A theoretical approach of the ethanol adsorption on Au(100), Au(110) and Au(111) surfaces (Article)

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Abstract

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The adsorption of ethanol on Au(100), Au(110) and Au(111) surfaces was studied using electronic structure calculations under the scheme of the density functional theory (DFT) with van der Waals corrections, vdW-DF2 and PBE functionals, using numerical atomic orbitals (NAO) basis set implemented in the SIESTA code and plane-waves basis set in the CASTEP code. The lowest physisorption energies using the plane-wave basis set in neutral media were observed at the TOP position in all the surfaces, with values in between –53.35 kJ.mol^{-1} and –61.80 kJ.mol^{-1}. Structurally, the method based on linear combination of atomic orbitals (LCAO) using NAO as basis set gives the best result respect to the ideal bulk. However, the relaxation of the slab is better defined by the plane-wave scheme. Band structure has shown no change in the sp-like bands and the 5d occupied bands with and without the ethanol molecule adsorbed. However, a slight variation was obtained in the unoccupied bands due to the interaction with the lone pair of electrons from the oxygen (non-bonding orbitals). © 2019 Elsevier B.V.

Author keywords

Adsorption | Band structure | Density functional theory | Ethanol | Gold | Surface science

Indexed keywords

Engineering controlled terms: Adsorption | Band structure | Chemical bonds | Elastic waves | Electronic structure | Ethanol | Gold | Quantum chemistry | Van der Waals forces | Wave propagation

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