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PAPER

A theoretical study of the XP and NEXAFS spectra of alanine: gas phase molecule, crystal, and adsorbate at the ZnO(10$\bar{1}$0) surface

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The adsorption of alanine on the mixed-terminated ZnO(10$\bar{1}$0) surface is studied by means of quantum-chemical *ab initio* calculations. Using a finite cluster model and the adsorption geometry as obtained both by periodic CPMD and embedded cluster calculations, the C1s, N1s and O1s X-ray photoelectron spectra (XPS) and near-edge X-ray absorption fine structure (NEXAFS) spectra are calculated for single alanine molecules on ZnO(10$\bar{1}$0). These spectra are compared with the spectra calculated for alanine in the gas phase and in its crystalline form and with experimental XPS and NEXAFS data for the isolated alanine molecule and for alanine adsorbed on ZnO(10$\bar{1}$0) at multilayer and monolayer coverage. The excellent agreement between the experimental and calculated XP and NEXAFS spectra confirms the calculated adsorption geometry: A single alanine molecule is bound to ZnO(10$\bar{1}$0) in a dissociated bidentate form with the two O atoms of the acid group bound to two Zn atoms of the surface and the proton transferred to one O atom of the surface. Other possible structures, such as adsorption of alanine in one of its neutral or zwitterionic forms in which the proton of the –COOH group remains at this group or is transferred to the amino group, can be excluded since they would give rise to quite different XP spectra. In the multilayer coverage regime, on the other hand, alanine is in its crystalline form as is also shown by the analysis of the XP spectra.