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Coverage Dependent Adsorption and Electronic Structure of Threonine on Ge (100) Surface

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The Coverage dependent attachment of multifunctional groups included in threonine molecules adsorbed to Ge (100)-2×1 surface was investigated using core-level photoemission spectroscopy (CLPES) and density functional theory (DFT) calculations. The core-level spectra at a low coverage indicated that the both carboxyl and amine groups participated in the bonding with the Ge (100) surface by "O-H dissociated and N-dative bonded structure". However, at high coverage level, additional adsorption geometry of "O-H dissociation bonded structure" appeared possibly to minimize the steric hindrance between adsorbed molecules. Moreover, the C 1s, N 1s, and O 1s core level spectra confirmed that the carboxyl oxygen is more competitive against the hydroxymethyl oxygen in the adsorption reaction. The adsorption energies calculated using DFT methods suggested that four of six adsorption structures were plausible. These structures were the "O-H dissociated-N dative bonded structure", the "O-H dissociation bonded structure", the "Om-H dissociated-N dative bonded structure", and the "Om-H dissociation bonded structure" (where Om indicates the hydroxymethyl oxygen). These structures are equally likely, according to the adsorption energies alone. Conclusively, we investigate in threonine on Ge (100) surface system that the "O-H dissociated-N dative bonded structure" and the "O-H dissociation bonded structure" are preferred at low coverage and high coverage.

Keywords: Threonine, Ge(100) surface, CLPES, DFT calculation, Adsorption Structure