SF-P018

Comparison of Coverage-Dependent Adsorption Structures of Alanine and Leucine on Ge(100): Bonding Configuration and Adsorption Stability

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The bonding configuration and adsorption stability of alanine and leucine adsorbed on Ge(100)-2×1 surface were investigated and compared using core-level photoemission spectroscopy (CLPES) and density functional theory (DFT) calculations. The bonding configuration, stability, and adsorption energies were evaluated for two different coverage levels. In both cases, the C 1s, N 1s, and O 1s core-level spectra at a low coverage (0.30 ML) indicated that the carboxyl and amine groups participated in bonding with the Ge(100) surface in an "O-H dissociated-N dative bonded structure". At high coverage levels (0.60 ML), both this structure and an "O-H dissociation bonded structure" were present. As a result, we found that alanine adsorbs more easily (lower adsorption energy) than leucine on Ge(100) surfaces due to less steric hindrance of side chain.

Keywords: Alanine, Leucine, Ge(100), Density Functional Theory (DFT) Calculation, Core-level Photoelectron Spectroscopy (CLPES), Adsorption configurations