

ST-P002

Adsorption Configuration of Serine on Ge(100): Competition between the Hydroxymethyl and Carboxyl groups of Serine During the Adsorption Reaction

김예원, 양세나, 이한길

숙명여자대학교 화학과

We investigated the adsorption structures of serine on a Ge(100) surface by core-level photoemission spectroscopy (CLPES) in conjunction with density functional theory (DFT) calculations. 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. The core-level C 1s, N 1s, and O 1s CLPES spectra confirmed that the carboxyl oxygen competed more strongly with the hydroxymethyl oxygen during the adsorption reaction, thereby favoring formation of the “O-H dissociated-N dative bonded” and “O-H dissociation bonded” structures at 0.30 ML and 0.60 ML, respectively. The experimental results were corroborated theoretically by calculating the reaction pathways leading to the two adsorption geometries. The reaction pathways indicated that the “O-H dissociated-N dative bonded structure” is the major product of serine adsorption on Ge(100) due to comparably stable adsorption energy.

Keywords: 아미노산, 분자흡착, Ge(100), CLPES, DFT calculation