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Coverage Dependent Adsorption Configuration of Phenylalanine on Ge(100)

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The Adsorption structures of phenylalanine on Ge(100) surface have been investigated as a function of coverage using high-resolution photoemission spectroscopy (HRPES) and density functional (DFT) calculation. To converge these experimental and theoretical conclusion, we systematically performed HRCLPES measurements and DFT calculation for various coverage in the adsorption structures of phenylalanine molecules on the Ge(100) surface. In this study, we found two different adsorption structure as a function of coverage in phenylalanine on Ge(100), monitoring three core level spectra (Ge 3d, C 1s, N 1s, and O 1s) using HRPES Through analysis of the binding energies, we confirmed that O-H dissociated and N dative-bonded structure emerges at low coverage (0.10 ML), which is the same to the result of glycine and alanine on Ge(100) system, whereas O-H dissociation structure also appears at higher coverage. Moreover, we observed the shape of phenyl group being included in phenylalanine is changed from flat to tilting structure at final state using DFT calculation. Through the spectral analysis for phenylalanine, we will demonstrate variation of coverage dependent structural change for phenylalanine on Ge(100) surface using experimental (HRPES) and theoretical studies (DFT calculation).