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Comparison of Adsorption Configurations between Phenylalanine and Tyrosine on Ge(100)

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We will investigate the bonding configurations of phenylalanine and tyrosine adsorbed on the Ge(100) surface using CLPES and DFT calculations. First, the C 1s, N 1s, and O 1s spectra obtained at 300 K revealed that both the amine and carboxyl groups of phenylalanine and tyrosine concurrently participated in adsorption on the Ge(100) surface without bond breaking using CLPES, depending on the extent of coverage. In the second place, we confirmed that the “O-H dissociated-N dative bonded structure” is the most stable structure implying kinetically favorable structure, and the “O-H dissociation bonded structure” is another stable structure manifesting thermodynamically advantageous structure using DFT calculations. This tendency turns up both phenylalanine and tyrosine, similarly. Furthermore, through the CLPES data and DFT calculation data, we discovered that the “O-H dissociated-N dative bonded structure” and the “O-H dissociation bonded structure” are preferred at 0.30 ML and 0.60 ML, respectively. Moreover, we found that the phenyl ring of phenylalanine is located in axial position to Ge(100) surface, but the phenyl ring of tyrosine is located in parallel to Ge(100) surface using DFT calculations.

Keywords: Phenylalanine, tyrosine, Bonding configuration, CLPES, SFT calculation