

The Evidence of Tautomerization of 2-thiazoline-2-thiol on Ge (100) Surface

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We first confirm the tautomerization of 2-thiazoline-2-thiol on Ge (100) surface using CLPES and DFT calculation. We clearly confirmed that there exist two different molecular structures (we will show in our poster) in C 1s, N 1s, and S 2p CLPES spectra. Moreover, we obtained two plausible adsorption structures using DFT calculation which are that one is s-dative bonded structure and the other is SH dissociated-N-dative bonded structure although their stabilities are different on Ge (100) surface. We will investigate this interesting result for the confirmation of tautomerization of 2-thiazoline-2-thiol molecule adsorbed on Ge (100) surface.

Keywords: Tautomerization, DFT calculation, CLPES, Ge (100) surface