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How Does the 2-Thiophenecarboxaldehyde Behaves on the Ge(100) Surface

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High-resolution photoemission spectroscopy (HRPES) measurements were collected and density functional theory (DFT) calculations were conducted to track the coverage dependent variation of the absorption structure of 2-thiophenecarboxaldehyde (C4H3SCHO: TPCA) on the Ge(100) surface at room temperature. In an effort to identify the most probably adsorption structures on the Ge(100) surface, we deposited TPCA molecules at a low coverage and at a high coverage and compared the differences between the electronic features measured using HRPES. The HRPES data provided three possible adsorption structures of TPCA on the Ge(100) surfaces, and DFT calculations were used to determine the plausibility of the structures. HRPES analysis, corroborated by DFT calculations, indicated that an S-dative bonded structure was the most probable adsorption structure at relatively lower coverage levels, the [4+2] cycloaddition structure was the second most probable structure, and the [2+2]-C=O cycloaddition structure was the last probable structure on the Ge(100) surfaces at relatively higher coverage levels.

Keywords: HRPES, DFT calculation, 2-thiophenecarboxaldehyde, Ge(100) surface, Adsorption structure