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**Coverage and Temperature Dependence of Bond Character of Thiophene on Ge(100)** S.M. JEON, S.J. JUNG, Dept. of Chem. and School of Mol. Sci. (BK21), H.-D. KIM, Beamline Research Div., Pohang Accelerator Lab (PAL), D.K. LIM, BK21, H. LEE, PAL, S. KIM, BK21, KAIST COLLABORATION, PAL COLLABORATION — We studied the adsorption and decomposition of thiophene (C4H4S) on Ge(100) using high-resolution core-level photoemission spectroscopy (HRPES) and scanning tunnelling microscopy (STM). Ge 3d, S 2p, and C 1s core level spectra show the existence of three different adsorption geometries, which are assigned to a weakly bound state, a chemisorbed bonding state ([4+2] cycloaddition reaction product), and a decomposed bonding state (desulfurization reaction product). Furthermore, we found that the ratio of the components induced by three adsorption geometries changes depending on the molecular coverage and the annealing temperature. Under 0.25 ML, the kinetically favorable weakly bound state is initially formed. As the molecular coverage is increased (over 0.25 ML), thermodynamically stable [4+2] cycloaddition reaction products are additionally produced. In addition, the temperature dependent behaviors show that the weakly bound state desorbs followed by the [4+2] cycloaddition reaction product as the molecular thiophene or may decompose to form metallocyclic compounds (C4H4Ge2) and sulfide (Ge2S). We elucidate systematically the change of the bonding states of adsorbed thiophene on Ge(100) according to the amounts of thiophene molecules and annealing temperature. Moreover, we performed density functional theory (DFT) calculations to observe the energetics of three bonding states of thiophene on Ge (100) system.

Hangil Lee
Beamline Research Division, Pohang Accelerator Laboratory (PAL),

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