SW-P001

A Study of Mg Capping Inside p-tert-butylcalix[4]arene Adsorbed on a Ge(100) Surface

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The electronic and adsorption structures of Mg and p-tert-butylcalix[4]arene (p-TBCA) adsorbed onto a Ge(100) surface under a variety of sample conditions were characterized using high-resolution photoemission spectroscopy (HRPES) and their corresponding DFT calculation results. Interestingly, after 0.10 ML p-TBCA molecules had been adsorbed onto a Ge(100) surface, subsequent adsorption of a small amount of metallic Mg (~0.10 ML) resulted in the formation of a capped structure inside the pre-adsorbed p-TBCA molecules. The adsorption structures resulting from further deposition of Mg (~0.50 ML) onto the Ge(100) surface were monitored based on the surface charge state and Mg 2s core level spectrum. Work function measurements clearly indicated the electronic structures of the Mg and p-TBCA adsorbed onto the Ge(100) surface. Moreover, we confirmed that three different adsorption structures are experimentally favorable at room temperature through DFT calculation results.

Keywords: Mg capping, p-tert-butylcalix[4]arene, HRPES, DFT calculation, Molecular adsorption, Ge(100)