Gap state tuning at the organic/metal interface by quantum-size effects

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We have studied the interfacial electronic structure between Phthalocyanine (Pc)-based molecules and the uniform Ag films by using angle-resolved photoemission spectroscopy (ARPES). Ag films at various thicknesses were deposited and grown uniformly on the Ge(111) surface. Then Pc-based molecules such as CuPc, H_2Pc, and TTB-H_2Pc were deposited on top of the Ag film step by step up to the coverage of 10 Å, respectively. We found the emergence of gap states at the organic molecules coverage about 3 Å, and it shift in energies with the increasing thickness of the Ag films. Furthermore, we found that the energy positions of the gap states are pinned at the energy position where the quantum well state (QWS) band cross the Ge heavy hole (HH) band edge. In this energy region, the QWS band becomes very flat, and it corresponds to the abrupt change of the 2-dimensional (2D) density of state (DOS). The abrupt change of the DOS will induce and pin the gap state after the adsorption of the organic molecules. In this study, we take CuPc as a modeling system, and introduce the Newn-Anderson model [1,2] which considers the interaction between a single molecular state and the substrate band to explain the origin of the gap state and the pinning effect.

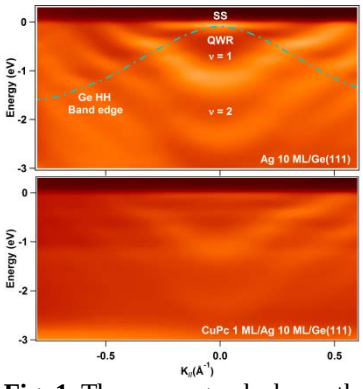

Fig. 1. The upper graph shows the 2-dimensional (2D) angle-resolved photoemission spectra for 10 monolayer (ML) Ag thin film on Ge(111). The lower graph shows the 2D spectra for CuPc 1 ML on top of 10 ML Ag thin film [3].

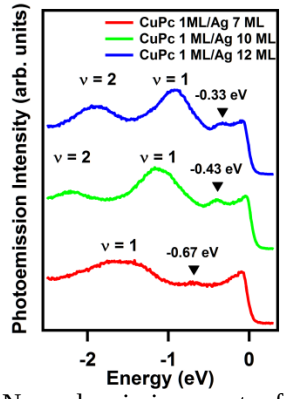

Fig. 2. Normal emission spectra for CuPc 1 ML on top of the 7, 10, and 12 ML Ag thin films. The black wedges indicate the energy positions of the gap state [3].

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