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Electronic properties of pristine and potassium-doped dibenzopentacene on Au(111) studied by UPS, MAES, and first-principles calculation

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Considerable attention has been paid to elucidate the electronic properties of organic semiconductors in bulk and at interface for the basic understanding and the potential application to organic-based devices such as organic field-effect transistors, organic light emitting diodes, etc. The -conjugated hydrocarbons composed of fused benzene rings are typical organic semiconductors with high hole mobility, e.g., high-purity pentacene (C22H14) crystal reveals 35 cm2 V−1 s−1 at 290 K.1 Such a high hole mobility indicates that the band-like transport is dominant, reflecting the itinerant character of electrons in the highest-occupied molecular orbital (HOMO) derived band. Another novel interest is superconductivity in potassium-doped -conjugated hydrocarbon with high transition temperature (Tc), which was realized first by K3picene (Tc = 18 K)2 followed by Kxdibenzopentacene ($3 \le x \le 3.5$, Tc = 33 K).3 In the conference, we report following two topics investigated by ultraviolet photoemission spectroscopy (UPS), metastable atom electron spectroscopy (MAES), and first-principles calculation using the density functional theory (DFT).
I. Local electronic states of dibenzopentacene (C30H18, DBP) on Au(111). DBP is weakly bound on Au(111) as in the case of pentacene on Au(111). In the He I UPS spectrum, the HOMO-derived band shows the vibrational satellite due to the hole-vibration coupling. Furthermore, the He*(23S) MAES spectrum, which provides selective information on the topmost layer,4 shows that the deexcitation channel of He*(23S) (resonance ionization or Penning ionization) is governed by the electronic properties of adsorbed DBP.
II. Formation of Mott-Hubbard states in K-doped DBP. For K1DBP, K2DBP, and K3DBP, two gap states due to charge transfer were observed by the UPS and MAES spectra5 and are discussed on the basis of the Mott-Hubbard model.

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