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Pentacene on Au(111) and Cu(111) studied by UPS, MAES, and first-principles calculation

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The electronic properties of organic semiconductors in bulk and at interface play an essential role in characteristic charge transport in soft matter, and eventually result in performance in organic-based devices such as organic field-effect transistors, organic thin film solar cells, organic light-emitting diodes, and single molecular junctions.¹ Pentacene (C₂₂H₁₄) is regarded as a prototype in the π -conjugated organic molecules due to high field-effect hole mobility in the crystal phase. 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 at pentacene-Au(111) and Cu(111) interfaces in the static (or equilibrium) condition. Pentacene is weakly bound on Au(111), while it chemisorbs on Cu(111) forming an induced state just below the Fermi level. The He(23S) MAES spectrum, which provides selective information on the topmost layer,² shows that the deexcitation channel of He(23S) (resonance ionization or Penning ionization) is governed by the electronic properties of adsorbed pentacene.

II. Local electronic states at pentacene-Au interface under bias voltage. A bottom-contact FET structure was used for the UPS and MAES measurements. Our data indicate that the transport properties of pentacene film on Au are strongly affected by the organic-metal interface (especially hole-injecting Schottky contact).³

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Primary author: Prof. AKIMOTO, Katsuhiko (University of Tsukuba)

Co-authors: Prof. SHUDO, Ken-ichi (Yokohama National University); Prof. AOKI, Masaru (The University of Tokyo); Prof. MASUDA, Shigeru (The University of Tokyo); Dr KOITAYA, Takanori (The University of Tokyo); Mr KAJIMOTO, Takashi (The University of Tokyo); Mr ITO, Yujiro (The University of Tokyo)

Presenter: Prof. MASUDA, Shigeru (The University of Tokyo)

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