

VIII-AA Study of Electronic Structure of Organic Thin film and Organic/Inorganic Interface

Organic semiconductors have gained increasing interest because of their potential use in various optoelectronic devices. In order to understand electronic processes at interface in the organic devices, many surface sensitive techniques such as high-resolution ultraviolet photoemission spectroscopy (UPS) have been performed for organic thin films, because origins of the energy position and the bandwidth of ultraviolet photoelectron spectra are keys to understand interface properties, such as the energy level alignment at the interface and molecule-molecule and/or molecule-substrate interaction. The energy-band structure is a fundamental basis for the understanding of electronic and optical properties of solids. The intermolecular band dispersion for the organic thin film is observed using angle-resolved UPS using synchrotron radiation, since the width of band dispersion depends on the intermolecular interaction.

VIII-AA-1 Intermolecular Energy-Band Dispersion in PTCDA Multilayers

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The electronic structure of a well-oriented perylene-3,4,9,10-tetracarboxylic acid-dianhydride multilayer prepared on MoS₂ single crystal surface were studied by angle-resolved ultraviolet photoemission spectroscopy using synchrotron radiation. From the photon energy dependence of normal emission spectra, we observed an intermolecular energy-band dispersion of about 0.2 eV for the highest occupied molecular orbital (HOMO) band of single π character. The observed energy-band dispersion showed a cosine curve, which originates from the intermolecular π - π interaction. Analyses using the tight-binding model gave that the transfer integral of about 0.05 eV for the π - π interaction, the effective mass of HOMO hole $m_h^* = 5.28m_0$, and the hole mobility $\mu_h > 3.8 \text{ cm}^2/\text{V s}$. This is the first observation of the intermolecular energy-band dispersion of a conventional single-component organic semiconductor only with the weak intermolecular van der Waals interaction.

VIII-AA-2 Very Narrow Photoemission Bandwidth of the Highest Occupied State in a Copper-Phthalocyanine Monolayer

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We observed a very narrow bandwidth of the highest occupied molecular orbital (HOMO) state in ultraviolet photoemission spectra (UPS) of copper-phthalocyanine monolayer deposited on graphite. The HOMO band in UPS consists of three components which may originate from the vibrational coupling. The full width at half maximum of each component was found to be $\sim 150 \text{ meV}$ at 295 K. This HOMO-bandwidth leads to an estimation that the lifetime of the HOMO hole should be at least longer than 2.2 fs, which may be dominated by the electron transfer rate from the substrate to the molecule.

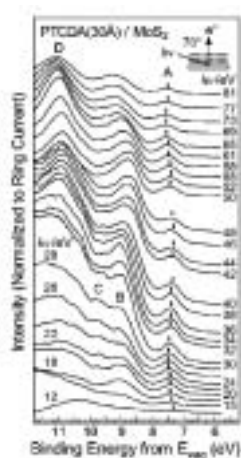


Figure 1. Photon energy ($h\nu$) dependence of SR-ARUPS spectra along the surface normal for the 30-Å-thick PTCDA multilayer ($\sim 8 \text{ ML}$) prepared on the MoS₂ surface. The binding energy (E_B) scale refers to the vacuum level (E_{vac}).