

Interfacial Electronic Properties of K-doped CuPc: C₆₀ Heterojunctions

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In this report we have used synchrotron-radiation photoemission to study the interfacial properties of K-doped CuPc: C₆₀ heterointerfaces, which were obtained via C₆₀ on K_{1.5}CuPc and CuPc on K₃C₆₀. A strong energy shift of the vacuum level occurred in both cases and indicates the formation of an interfacial dipole layer. At the C₆₀/K_{1.5}CuPc interface, the K diffuses into the C₆₀ layer and transfers charge into the lowest unoccupied molecular orbital (LUMO) of C₆₀. Both the creation of gap states and an enhancement of the energy level difference between the highest occupied molecular orbital (HOMO) of CuPc and the LUMO of C₆₀ may further improve device performance. In the opposite sequence, CuPc is physisorbed on K₃C₆₀. No K could be found in the CuPc overlayer. For cases with a lack of gap states in the donor side, expanding the photon harvesting should not occur. Furthermore, since the LUMO of C₆₀ is close to that of CuPc, it could be disadvantageous to the formation of photoexcitons at the donor/acceptor interface.

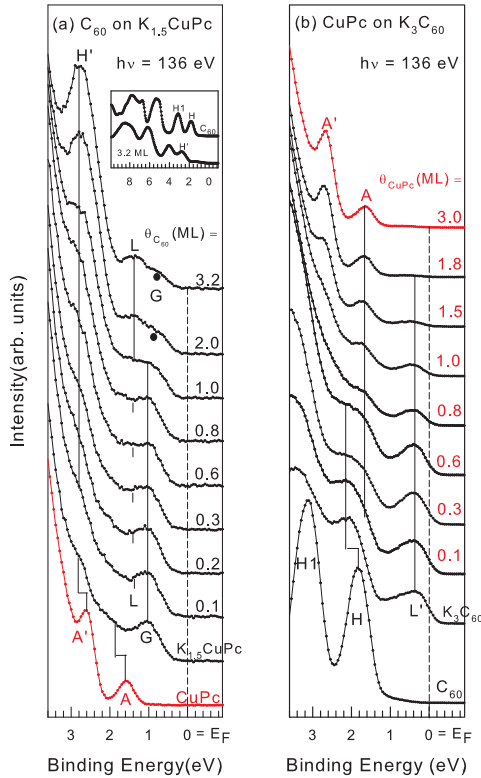


Fig. 1: Valence-band spectra in the vicinity of the HOMO, recorded at a photon energy of 136 eV for (a) C₆₀ on K_{1.5}CuPc and (b) CuPc on K₃C₆₀. The inset on the

left panel is the valence-band spectra in a wide range for 3.2-ML coverage and pristine C₆₀.

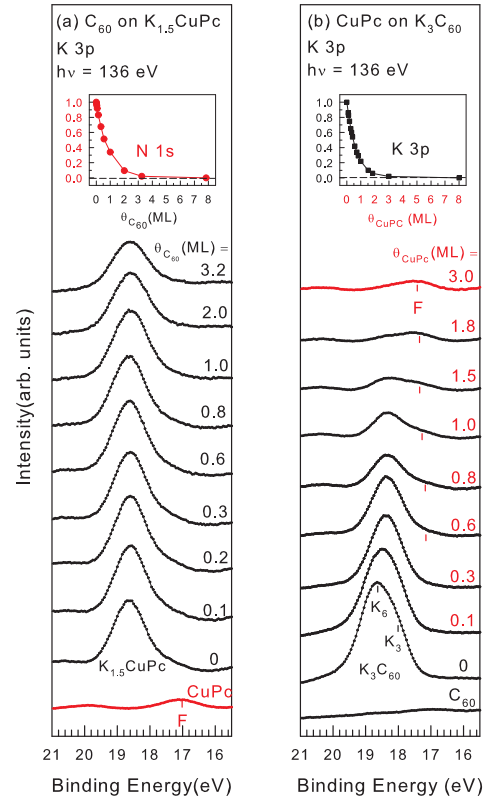


Fig. 2: Evolution of K 3p core-level spectra, recorded at a photon energy of 136 eV for (a) C₆₀ on K_{1.5}CuPc and (b) CuPc on K₃C₆₀. The insets show the variation of the relative intensity for the substrate-related core-level signal as functions of adsorbate coverage.

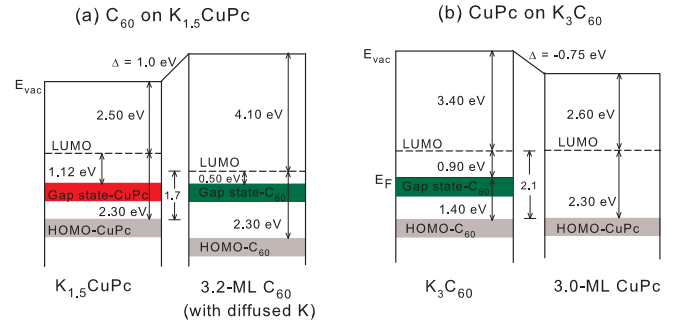


Fig. 3: Interfacial energy diagrams for (a) C₆₀ on K_{1.5}CuPc and (b) CuPc on K₃C₆₀.