Interfacial Electronic Properties of the Rubrene/C_{60} Heterojunctions

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Organic molecules are receiving a great deal of attention because of their potential applications in large-area, flexible electronic systems, and low-cost, ease fabrication. Regarding organic electronics applications, rubrene ($C_{42}H_{28}$, 5, 6, 11, 12-tetraphenylnaphthacen) is a versatile molecular material. In addition to using it as dye or dopant in organic light-emitting devices (OLEDs) and organic photovoltaic (OPV) devices to increase the efficiency and stability of devices, a remarkable large charge carrier mobility of up to 20 cm^2/V s at room temperature for single crystals has led it to be a benchmark material for organic field effect transistors (OFETs). Recently, Pandey et al. have demonstrated a new organic dual device, rubrene/ C_{60} heterostructure, that permits efficient integration of both light- and current-generation functions. The solar power conversion efficiency reaches 3% with a 5.3 $mAcm^{-2}$ short-circuit current density and about 1 V open-circuit voltage under AM 1.5 illumination. The electroluminescence (EL) turn-on voltage is <1 V with the characteristic color of rubrene. Surprisingly, it is about half the value of the rubrene bandgap (2.2 eV), that cannot be explained using current models of charge injection into organic semiconductors. It has known that charge injection in organic devices resides at hybrid interface, thus the interfacial properties of the organic heterojunction are crucial to understanding the transport mechanism. However, the fundamental issue has not yet been investigated until now.

In this report, we have used synchrotron-radiation photoemission spectroscopy to study the interfacial properties of the rubrene/C_{60} heterojunction. The valence-band spectra have shown that the interface is free from chemical interaction. Upon rubrene deposition, the observation of a pronounced down shift in vacuum level indicates the formation of a dipole layer. With increasing rubrene coverage, the highest occupied molecular orbital of rubrene gradually moves toward higher binding energy. These results may be attributed to the alignment of the charge neutrality levels of the two organic semiconductors.

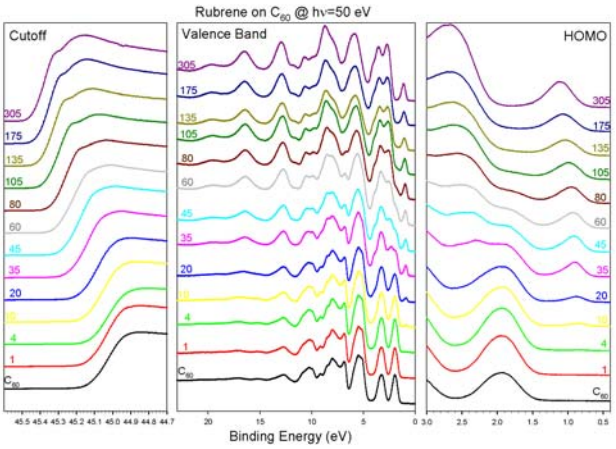

Fig. 1: Valence-band spectra recorded at a photon energy of 50 eV for rubrene adsorption on C_{60}.The right panel is a magnification of the spectra at the vicinity of the E_F and the HOMO, while the left panel presents the low-energy cutoff.

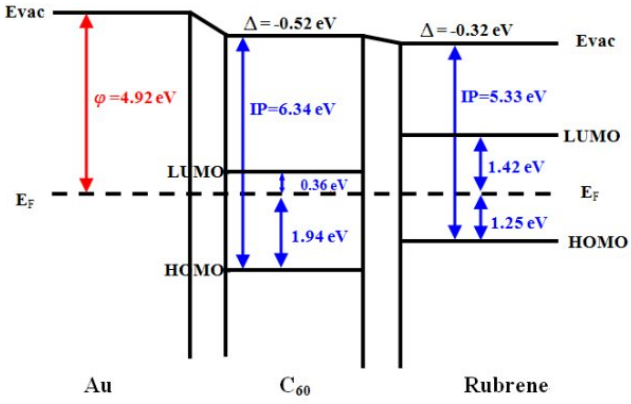

Fig. 2: Interfacial energy diagrams for rubrene on C_{60}.