

Study on interface dipole at organic/metal interfaces by ultraviolet photoelectron spectroscopy

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Introduction

An interface dipole formed at organic/metal interfaces influences their energy level alignment and carrier injection probability, hence it affects the performance of organic semiconductor devices. The origin of the interface dipole has been widely discussed recently and many possible mechanisms, e.g., Pauli repulsion and chemical interaction, have been proposed for explaining the effect [1,2]; however, the mechanism is still unclear. In this study, the interactions between metals and four types of carbazole-based molecules, of which electrical properties are similar to each other, have been investigated to clarify the relation of the delocalization of π -electrons with the dipole formation.

Experimental

All specimens used in the experiments were prepared in an ultrahigh-vacuum (UHV) system with a base pressure of 2×10^{-7} Pa at room temperature. The various kinds of metal (Ca, Mg, Ag, Cu, and Au) were deposited on Si(100) substrates and then carbazole-based molecules were deposited on them. The chemical structures of carbazole-based molecules are shown in Fig. 1. The UPS measurements were carried out in a UHV system with a base pressure of 1.6×10^{-8} Pa at the beamline 11D and 13A at the KEK Photon Factory. The photon energy was maintained constant at 65 eV.

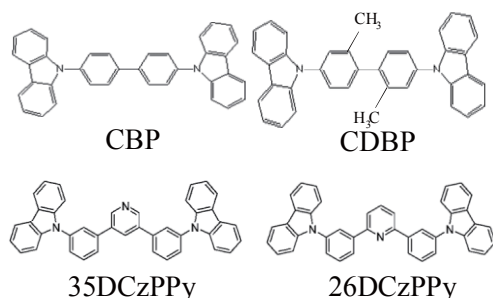


Fig.1 Chemical structure of carbazole-based molecules

Results and Discussion

Figure 2 shows the dependence of the vacuum level shift (Δ_{VL}) at organic/metal interfaces on metal work function. When the metal work function is more than 4.5 eV, Δ_{VL} is fixed at ~ 0.8 eV for CBP, CDBP and 26DCzPPy. In contrast, it turns to be ~ 1.5 eV for 35DCzPPy, of which

chemical structure is identical to 26DCzPPy except for the position of nitrogen atom in the pyridine component. From the calculation of the Mulliken charge determined by density functional theory, it can be deduced that the localization of the π -electrons depended on the position of nitrogen. Since interactions between π -orbitals of organic molecules and metals have a crucial role in their interfacial electric properties [3], the variation in the π -orbital characters must affect the hybridization of molecular orbitals at metal surfaces. Thus, we considered the vacuum shift is affected by the chemical interaction between π -orbital and metals.

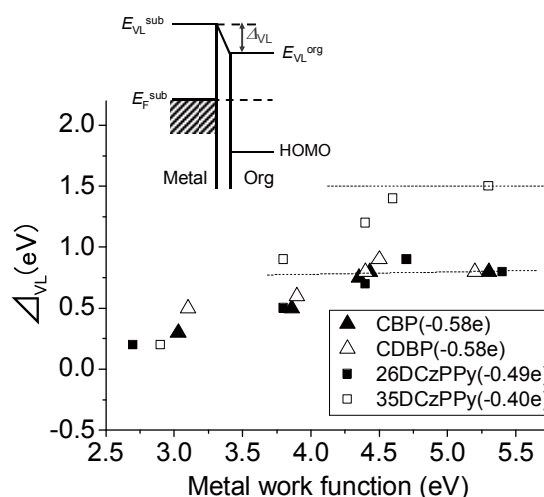


Fig. 2 Dependence of the vacuum level shift (Δ_{VL}) at organic/metal interfaces on metal work function. Numerical values suggest the Mulliken charge at nitrogen atom.

References

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