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Electronic structure of bathocuproine on metal studied by ultraviolet photoemission spectroscopy

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Introduction

Bathocuproine (BCP), whose bandgap energy is 3.5eV with the deep level of highest occupied molecular orbital (HOMO), is regarded as a key material for obtaining the highly efficient organic solar cell. The chemical structure of the BCP is shown in Fig. 1. By inserting BCP layer between a fullerene (n-type semiconductor) and a metal electrode with the thickness of several nanometers, the electrical conductivity of the organic solar cell and its power conversion efficiency were improved [1,2]. The mechanisms, however, for the improvement in the electrical properties at the interface between BCP and metal electrode is not well understood yet. In this work, we studied the electronic structure at the interface between BCP and several kinds of metals by ultraviolet photoemission spectroscopy (UPS).

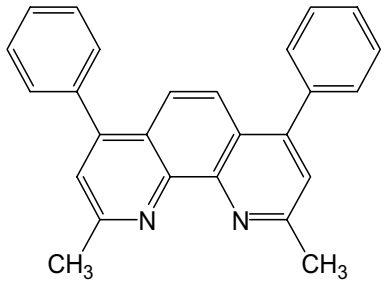

Fig.1 Chemical structure of Bathocuproine (BCP)

Experimental

The UPS measurements (hν=21.2eV) were carried out at the beam line 11C in KEK Photon Factory. Au, Ag, Al, In, Mg, and Ca were used as the electrode materials. The electrode metals were deposited on Si(100) wafers. BCP was deposited on the metal surface at room temperature with the deposition rate of 0.6nm/min. The base pressure in the UPS chamber was 1.2×10^{-10} Torr, and the pressure during deposition was 2.7×10^{-9} Torr. The thickness of the deposited layer was measured to be 4, 8, 16, 32, 50, 100Å by quartz vibrator.

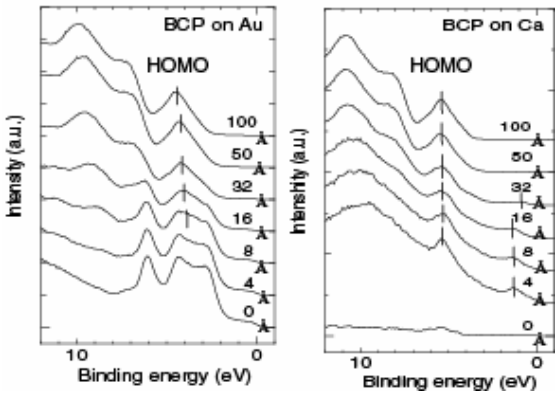

Fig. 2 UPS spectra of BCP deposited on Au (a) and Ca (b) with various thickness of BCP

Results and Discussion

Figs. 2(a) and (b) show the UPS spectra of BCP on Au (a) and Ca (b) based on the Fermi level of the metal. The spectral shape corresponding to the bulk state of BCP was observed for the BCP thickness more than 50Å in both cases. The HOMO level of BCP was indicated by an arrow in these figures. There is no peak other than the Au and BCP related peaks in the UPS spectra of BCP/Au, however, a new peak was observed at around 1.5eV in the UPS spectra of BCP/Ca for the BCP thickness between 4Å and 50Å. The appearance of a new peak can be regarded as a generation of interface state.

In addition to the case of BCP on Ca, interface states were observed for BCP on Mg, Al, and Ag. BCP is well known as a strong chelating ligand forming coordinated compounds, therefore, it may be easy to form chemical bonding between BCP and metal atoms such as Ca, Mg, Al, and Ag. Such chemical bond may correspond to the interface state observed by UPS. It may be possible to consider that electrons can through from LUMO of BCP to metal via interface state. We think such effect of the interface state results in the improvement of the device performance.

Summary

The electronic properties of BCP on metals were investigated by UPS. New interface states were observed in the case of BCP on Ag, Al, Mg, and Ca. The interface state may play an important role in improving electrical properties at the interface between BCP and electrode.

References

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