BL-3B, BL-13B/2016G584

Energy level alignment at hetero-interfaces in sub-phthalocyanine based solar cells

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1 Introduction

In the past years, many works have been dedicated to understand the origin of the band bending in organic thin films and the energy-level alignment (ELA) at organic-inorganic and organic-organic heterojunction (OOH) interfaces. [1] In our work, we are interested in understanding the influence of the substrate work function (WF) at donor/acceptor interface and the role of the tail states in the ELA. To do so, we used X-ray and ultraviolet photoelectron spectroscopy (XPS and UPS) to study the ELA of boron subphthalocyanine chloride (SubPc)/ α-sexithiophene (6T) deposited on MoO_3, [2] SiO_2, [3] and Cs_2CO_3. Their work function (WF) values are 5.9, 4.0, 3.0 eV, respectively. The ionization potential (IP) of SubPc and 6T were measured as 5.7 and 4.7 eV, respectively.

2 Experiment

The UPS/XPS measurements were mainly performed at BL-13B at Photon Factory (PF). The Si/SiO_2 substrate was grown on the surface of Si by using an UV-ozone treatment. The other substrate layers were obtained by the deposition of 5 nm of MoO_3 and Cs_2CO_3 deposited on cleaned Si substrate. Subsequently, 6T and SubPc were deposited step-by-step in a deposition chamber (<$5.0x10^{-9}$ Torr), until a thickness of 5 nm. To investigate the morphology dependence, the heterostructures were annealed for 60 s at 150 °C in the analysis chamber.

3 Results and Discussion

After the contact, for MoO_3, the binding energy (BE) of HOMO onsets were measured as 0.55 eV and 0.86 eV for 6T (5nm) and SubPc (5nm), respectively. For Cs_2CO_3, due to its low WF of, the HOMO onsets of the organic materials move away from the Fermi level to 1.16 eV and 1.14 eV for 6T and SubPc, respectively. And for the SiO_2, the HOMO onsets were measured as 0.73 eV and 1.24 eV for 6T and SubPc, respectively. We estimated qualitatively the charge accumulated at the OOH, analysing the evolution of S 2p and Cl 2p peaks position, which are associate with 6T and SubPc, respectively. Figure 1 shows the peak shift of S 2p and Cl 2p (straight lines), which exhibits the same tendency as described above by the UPS measurement. The band bending in SubPc can be extracted by the Cl 2p – S 2p peak shift (fig. 2). We observerd that SubPc layer deposited on $6T/Cs_2CO_3$, due to the substrate influence, the following deposition showed that the band bending occurred in upward direction. For the SubPc/6T deposited on SiO_2, almost no shift was observed. The upward band bending suggests that an electron is accumulate at the SubPc interface due to the acceptor property. After annealing the stack layers, we observed a drastic reduction of the core-level shift at the organic films, as displayed at Fig. 1 (dashed lines), which could be explained as reduction of the density of the SubPc tail states that controls the band bending at the OOH interface by better molecular stacking due to the annealing, which reduces the available states to charge transfer to achieve the equilibrium.

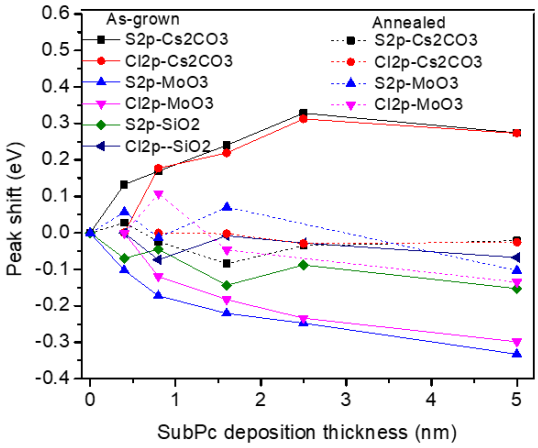

Fig. 1 Energy shift in function of the SubPc thickness deposited on 6T (5 nm)/ Substrate.

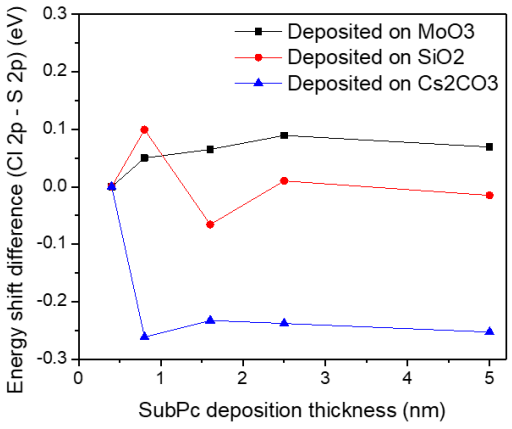

Fig. 2 Energy shift difference (Cl2p-S2p) for the organic stack layer deposited on the substrates in function of the SubPc thickness.

References

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