

Influence of the Work Function of the Substrate in the Energy-Level Alignment at Organic-Organic Heterojunction Interface

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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. In this 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 MoO₃ and Cs₂CO₃. Their work function 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. First, we deposited 6T (5.0 nm) on these substrates and we observed that the high WF substrate induced a charge transfer from 6T in order to reach the thermodynamic equilibrium. On the other hand, Cs₂CO₃ induced a charge transfer on the opposite direction. Figure 1 shows the peak shift of the S 2p. After the first deposition of SubPc (0.4nm), a shift of the S 2p peak was observed in the films deposited on both substrates, which can be explained as a charge transfer due to the formation of the donor-acceptor heterojunction interface. After the following depositions, we observed that for the films deposited on MoO₃, the S 2p peak shifted for a high binding energy (BE) and for a low BE on the case of the Cs₂CO₃ substrate. The band bending in SubPc can be extracted by the Cl 2p – S 2p peak shift, displayed in Fig. 2, and we observed a shift for a low BE in the films deposited on both substrates, which can be explained as a charge transfer from 6T to the unoccupied tail states in SubPc. After annealing we observed a drastic reduction of the core-level shift at the organic films, 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 annealing, which reduces the available states to charge transfer to achieve the equilibrium.

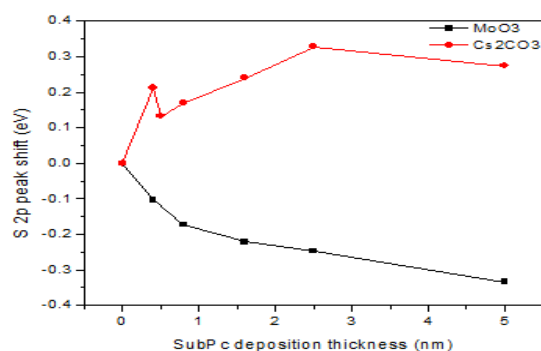


Fig. 1. S 2p peak shift in function of SubPc deposition thickness deposited on 6T/MoO₃ and 6T/ Cs₂CO₃.

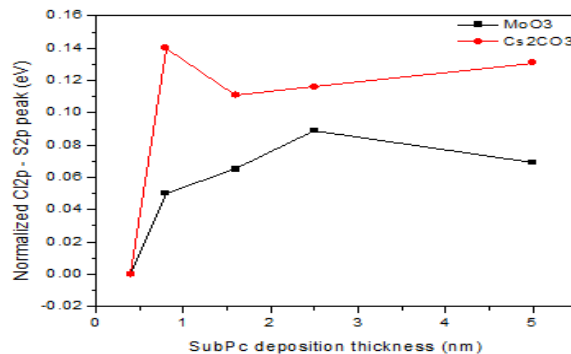


Fig. 2. Cl 2p - S 2p peak shift in function of SubPc deposition thickness deposited on 6T/MoO₃ and 6T/ Cs₂CO₃.