Charge transfer induced by MoO3 at SubPc/6T heterojunction interface

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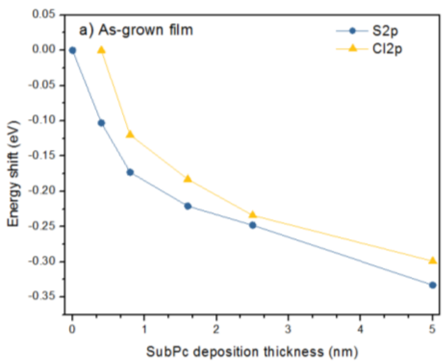
In the past years, many works have been dedicated to understanding the origin of the band bending in organic thin films and the energy-level alignment at organic-semiconductor and organic-organic interfaces. For organic materials, the electrical proprieties are intimately connected with the growth condition, thus not only the intrinsic electronic proprieties must be study, but also the intermolecular interactions and the physical proprieties must be considered [1]. Recently, one cascade heterojuntion solar cell has received much attention, it was reported that it was achieved an power conversion efficiency of 8.4%, using as acceptor boron subphthalocyanine chloride (SubPc) and boron subnaphthalocyanine chloride (SubNc), which are highly polar molecules, with α-sexithiophene (6T) donor [2]. The study of the energy-level alignment for these materials has already been reported in the literature, however the substrate used was p-doped silicon [3]. In this work, it was analyzed the energy-level alignment at SubPc/6T interface deposited on molybdenum trioxide (MoO3), which is commonly used as hole layer transportation in organic photovoltaic devices, using ultraviolet photoelectron spectroscopy (UPS) and X-ray photoelectron spectroscopy (XPS) and to check about the relation between the physical and electrical proprieties the same experiments were conducted, annealing the sample after each step of the SubPc deposition. In Fig.1 a), the energy shift from the sulfur 2p (related to 6T) and chorine 2p (related to SubPc) in function of the deposition thickness of SubPc for the as-grown film is displayed. We can see that with the increment of the SubPc film, the position of S2p and C2p has shifted to a higher binding energy, which characterizes a band bending. However, for the annealed film, fig. 1 b), the same pattern is not observed. Even though, some fluctuations are inserted, it is clearly that the shift was reduced and consequently the band bending and charge transfer was drastically reduced for the annealing film. After annealing the tail states were reduced creating a well-orientated SubPc film, which causes a reduction of the density of states, thus less states are available to the charge be transferred causing a reduction of the band bending.



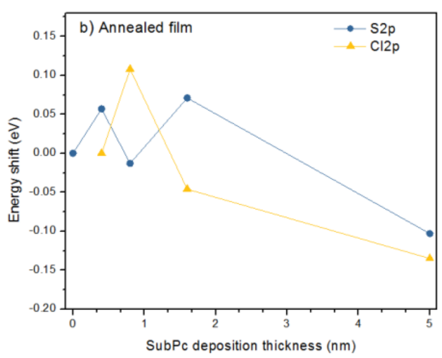


Fig. 1. Energy shift of the S2p and Cl2p peak in function of the SubPc thickness deposited on 6T (5 nm)/MoO3 (5 nm), a) for the as-grown film and b) for the annealed film.

[1] K. Yonezawa, et al., Adv. Mater. Interfaces. 1, 1400004 (2014).
[2] K. Cnops, B. P. Rand, D. Cheyns, B. Verreet, M. A Empl, P. Heremans, Nat. Commun. 5, 3406 (2014).
[3] J. Endres, I. Pelczer, B.P. Rand, A. Kahn, Chem. Mater. 28, 794, (2016)