The impact of the oxide transport layer on the energy band alignment of the frontier orbitals in non-fullerene acceptor organic solar cells

Noemi Vannucchi[1,2], Fredrik O.L. Johansson[2], Mariam Ahmad[3,4], Tanya Kumari[3], Chun Yuen Ho[3], Kun Wang[3], Cathy Vang[1], Hervé Cruguel[1], Morten Madsen[3,4], Andreas Lindblad[2] and Nadine Witkowski[1]

[1] *Institut des Nanosciences de Paris, Sorbonne Université, UMR CNRS 7588, Paris, France*
[2] *Division of X-ray Photon Science, Uppsala University, Uppsala, Sweden*
[3] *SDU Centre for Advanced Photovoltaics and Thin-Film Energy Devices, Mads Clausen Institute, University of Southern Denmark, Sønderborg, Denmark*
[4] *SDU Climate Cluster, University of Southern Denmark, Odense 5230, Denmark*

The transition from fullerene to non-fullerene acceptors (NFAs) has drastically increased the power conversion efficiency (PCE) of organic photovoltaics, reaching PCEs above 20% [1]. The PM6:Y7 polymer donor:NFA binary blend is one of the most promising systems [2] thanks to its broad absorption range, which favors high photocurrents in such based devices [3]. Frontier orbital band alignment between the active layer and the oxide charge transport layers is a key factor affecting the device's efficiency. This aspect remains unexplored in the PM6:Y7 blend system, especially with varying donor-acceptor ratios. This work investigates the impact of the charge transport layers ZnO and MoO_3 on the electronic structure and the band alignment of spin-coated PM6:Y7 thin films as a function of the donor-to-acceptor mass ratio. To map this energetic landscape, we employed synchrotron techniques such as X-ray and UV photoemission spectroscopy to access the core level electronic structure, the work function, and the HOMO onset, and X-ray absorption spectroscopy for determining the LUMO onset. We observed that the optimal charge transport preventing recombination at both oxide interfaces is obtained for a 1:2 donor-to-acceptor mass ratio blend film, corresponding to the lowest bandgap (Fig. 1). Moreover, when films are prepared on ZnO substrate, a reversed p-n junction for charge extraction is observed, driven by interface dipoles at the oxide/organic interface. In conclusion, our work has shed light on the impact of oxide transport layers in shaping band alignment within an organic solar cell stack— a crucial factor in achieving optimal device efficiency.

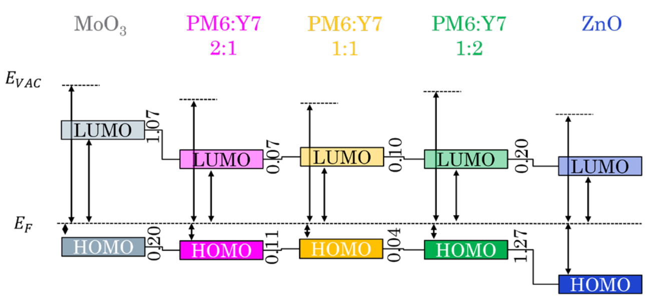

Figure 1. Frontier orbital band alignment at the interface between the organic blend PM6:Y7 with different mass ratios and the oxide transport layers

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