

In thin film, organic solar cells (OSCs) the stacked layers must respect an appropriate energy alignment to allow efficient charge separation and transport to the electrodes. Numerous studies report on the advantage of using an interfacial layer (IFL) to drain and/or collect charges at the electrode interfaces. In this field we demonstrated the efficiency of a highly crystalline thin layer of a dipyranylidene (**Figure 1**) derivative (DIPS-Ph₄) as a hole transport layer at the ITO anodic contact.[1] The efficiency of IFL and its electronic properties is strongly linked to the orientation of these conjugated flat molecules with respect to each other and with the substrate.[2]

After a thermal deposition under vacuum on Si₃N₄ substrates the layers were characterized by AFM and STXM on PolLux beamline.[3] From these measurements we firstly had access to the topography of the organic layer. Secondly, we got the organic structure at a molecular level changing the incidence angle (0° and 30° with the normal to the substrate). We performed the measurements for 2 nominal thicknesses (3 and 30·10¹⁵ cm⁻²) corresponding respectively to recovery ratios of 30% and 100%. This was done for DIPO-Ph₄ and DIPS-Ph₄. For the oxygenated compound, we also prepared 2 samples in the same conditions but followed by a thermal annealing at 170°C during 1h and 2 others with thermal deposition on a substrate at 100°C.

The organic layers grow forming islands on the top of the substrate. As a first result STXM highlights that there is no organic material between the islands which confirm a Volmer-Weber (3D mode) growth for dipyranylidene. Secondly, we observed a difference between the top and the edge of the island. Indeed, the ration between the π* and the σ* transitions change when looking at different zones on the islands (**Figure 2**). Such observations could be explained by a change of molecular orientation during the deposition. Molecules seem to lay parallel on the surface at the beginning of the

DIP interfacial layer in PV heterostructures using ITO as an electrode: impact of coating ratio and evaporation conditions on molecular orientation studied by STXM.

deposition. Then, molecule/molecule interactions becoming more important, the orientation seems to be more perpendicular to the surface. These results have been developed with the angle study. Finally, we highlighted the fact that in some samples presenting a twinned crystal, there is a difference of orientation between the two twins structure.

References

- [1] S. Beryny et al. ACS Appl. Mater. Interfaces **2** (2010) 3059–3068
- [2] D. Qi et al. J. Am. Chem. Soc. **129** (2007) 8084–8085
- [3] C. R. McNeill et al. Nanotechnology **19** (2008) 424015

Figures

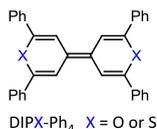


Figure 1: Dipyranylidene structure.

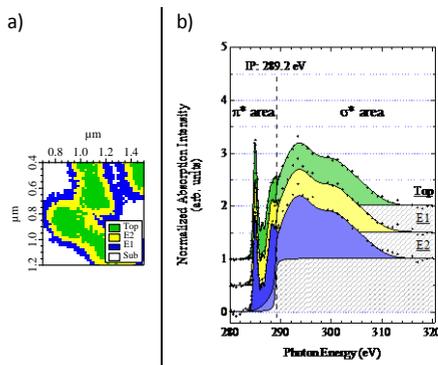


Figure 2: a) DIPO-Ph₄ layer (3·10¹⁵ cm⁻²) morphology and main area of interest; b) Absorption spectra for each area / Γ_{π*/σ*}: 0.23, 0.21 and 0.19 from Top to E2 area.