# Advanced optical characterizations of Non-Fullerene-Acceptor based organic solar cells: correlation between material-interactions and stability

**A. K. Bharwal*, C.M. Ruiz, D. Duché, L. Escoubas, J.J. Simon**
Aix Marseille Université, CNRS, IM2NP UMR 7334, Marseille, France
**Y. A. Avalos-Quiroz, O. Margeat, C. Videlot-Ackermann, J. Ackermann**
Aix Marseille Université, CNRS, CINAM, Marseille, France
*Email contact : anil.bharwal@im2np.fr*

Solution-processed organic photovoltaic technologies (OPV), being the thin-film technology that shows one of the highest improvements of photoconversion efficiency (PCE) in recent years, have the capability to compete with the different PV technologies already at industrial scale.[1,2] In order to achieve a firm cost reduction for an existing market, non-fullerenes (NFA) based molecules are required. The NFA-15 project "Non-Fullerene-Acceptor based polymer solar cells with 15% efficiency and 10-year lifetime" addresses this challenge.[3]
However, increasing the PCE requires an improved understanding of the factors limiting the device efficiency and stability.[4] In this work, we report the ellipsometric technique and optical modeling to investigate the intermolecular interactions and electronic transition of non-fullerene PBDB-T-2F donor and ITIC-4F acceptor molecules, presumably playing a key role affecting both PCE and stability. In this study, the energies of the optical transitions and the bandgap of the PBDB-T-2F and ITIC-4F as well as of their blends are determined using a Gaussian model and compared to the experimental results obtained from UV-photospectrometry (figure 1a) and the photoluminescence. Small changes in optoelectronic transitions in the blends as compared to pure materials are attributed to the material-interactions (figure 1b) which resulted in improved stability of the solar cell. Additionally, we performed a comparison between fresh and aged samples based on both pure and blend materials by optical measurements. The optical results showed that the blend materials in both fresh and aged conditions were more stable than the pure ones, further confirming that the stability of blends based solar cells is improved by material-interactions.

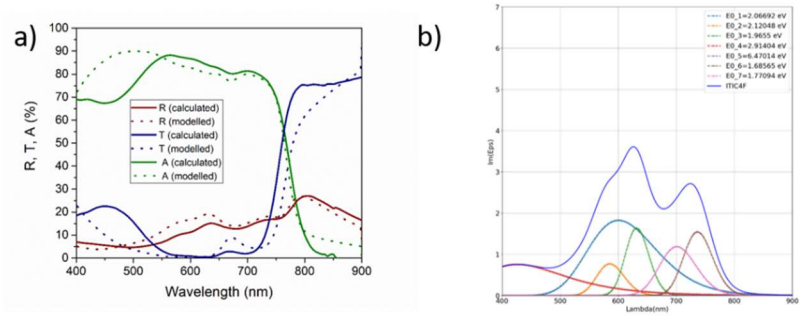


**Figure 1**. (a) Comparison between experimental measurements of T, A, R (solid lines) and optical simulations of T, A, R (dotted lines) for PBDB-T-2F/ ITIC-4F thin films for different thicknesses. (b) Imaginary part of the dielectric function of the PBDB-T-2F/ ITIC-4F thin films.

**References:**

(1) Colsmann, A.; Röhm, H.; Sprau, C. *Sol. RRL* **2020**, *4* (6), 2000015.
(2) ARMOR solar power films | Armor Corporate https://www.armor-group.com/en/aspf).
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(4) Köntges, W.; Perkhun, P.; Kammerer, J.; Alkarsifi, R.; Würfel, U.; Margeat, O.; Videlot-Ackermann, C.; Simon, J.-J.; Schröder, R. R.; Ackermann, J. *Energy Environ. Sci.* **2020**, *13* (4), 1259–1268.