Determining electro-optics of PBDB-T-2F /ITIC-4F organic solar cells film

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Solution-processed organic photovoltaic technologies (OPV) 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-fullerene acceptors (NFA) based molecules are of great interest.[3] However, understanding of the optical constants of the PBDB-T-2F and ITIC-4F is crucial for their applications in organic photovoltaics. In this work, we report the optical characterizations and modeling to investigate the intermolecular interactions and electronic transition of PBDB-T-2F donor and ITIC-4F NFA molecules, presumably playing a key role affecting both PCE and stability. 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). 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.

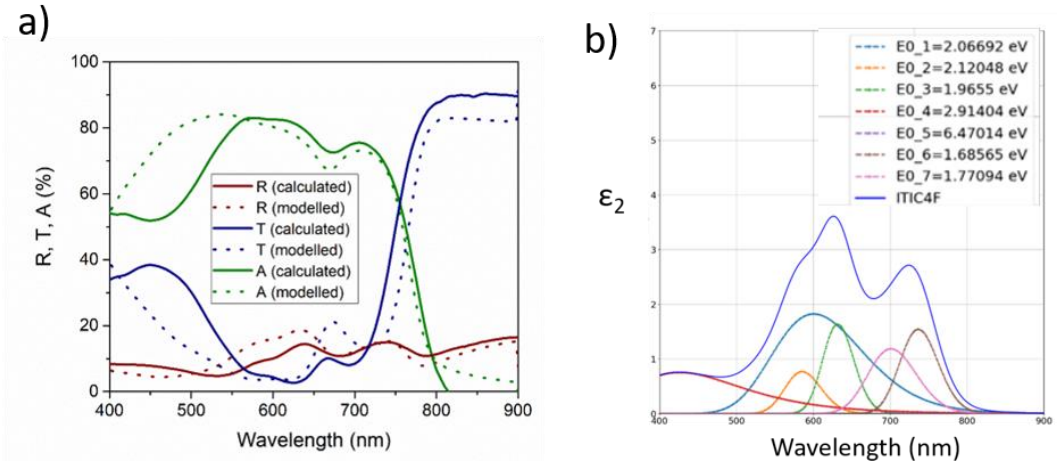

Figure 1. (a) Comparison between experimental measurements of R, T, A (solid lines) and optical simulations of R, T, A (dotted lines) for PBDB-T-2F/ITIC-4F thin films for different thicknesses. (b) Imaginary part of the dielectric function of the PBDB-T-2F/ITIC-4F thin films.

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References:

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(3) Li et al.. *Nat. Commun.* **2021**, *12* (1), 1–9.