

Electronic Structure, Core-Valence Spectroscopy and Femtosecond Charge Transfer Dynamics of Organic Solar Cells Active Layer Components PTB7-Th and ITIC

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Synergic effects concerning electronic structure and morphology in the PTB7-Th polymer and the non-fullerene acceptor ITIC molecule has resulted in state-of-art systems for organic solar cells (OSCs), achieving over 12% PCE values [1]. Furthermore, the substitution of harmful halogenated solvents to environmentally friendly solvents that do not compromise PCE values has become a subject of great interest in the literature [2].

In this work, we employed sulfur K-edge Angle-Resolved Near-Edge X-ray Absorption Fine Structure (NEXAFS), Resonant Auger (RAS), and the Core-Hole Clock spectroscopies in an attempt to gain information on the effect of different processing methods on the electronic and morphological properties of these systems. These spectroscopic measurements (NEXAFS, RAES and XPS) were carried out at the SXS beamline of the Brazilian Synchrotron Light Laboratory (LNLS).

In order to compare the use of an conventional acceptor molecule, we have performed Steady State and Time-Resolved Photoluminescence (TRPL) experiments for neat PTB7-Th and blends with ITIC and PCBM. TRPL measurements were carried at the Swansea's Material Research Centre.

To a better comprehension of the sulfur excited states involved in the electronic transitions probed by the synchrotron-based-spectroscopic methods, theoretical calculations were performed utilizing Restricted-Excitation-Window Time-Dependent Density Functional Theory (REW-TD-DFT). In order to probe the extent of relativistic effects present in these transitions, we employed different Hamiltonians (ZORA, DKH, X2C) in our calculations.

We also explored different chemical descriptors (the Donor-Acceptor and Aromatic-Quinoid approaches) to obtain information at valence level in both ground and low-lying excited states. All calculations were performed in NWChem 7.0, Gaussian16 and Amsterdam Density Functional (ADF).

References

- [1] Jianhui Hou et al. “Organic solar cells based on non-fullerene acceptors”. In: *Nature materials* 17.2 (2018), pp. 119–128.
- [2] Jingbo Zhao et al. “Efficient organic solar cells processed from hydrocarbon solvents”. In: *Nature Energy* 1.2 (2016), pp. 1–7.