

**TRANSIENT INSIGHTS INTO ORGANIC SOLAR CELLS: FROM
FULLERENE TO Y-FAMILY ACCEPTORS**

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Organic photovoltaics (OPV) are a pivotal technology for transition towards renewable energy. The remarkable progress in power conversion efficiency (PCE) in the last decades is mainly attributed to the evolution from fullerene-based molecular acceptors (PCE ~ 3-4%) to non-fullerene systems (PCE over 20%) [1,2]. In a typical bulk heterojunction (BHJ) architecture, the active layer is composed of an electron donor and acceptor (macro)molecular blend. The efficiency of the BHJ organic solar cell (OSC) is governed by a delicate balance between exciton dissociation into free charges at donor/acceptor interfaces and charge carrier extraction at electrodes, while charge recombination within the active layer diminishes the power output. In this research, we have acquired Transient Photocurrent (TPC)/ Transient Photovoltage (TPV) simultaneously to Transient Absorption (TA) measurements. TPC offers insights on charge extraction dynamics, while TPV is supposed to probe the charge recombination dynamics. This approach provides a direct correlation between optical measurements of carrier population within the active layer and electronic signals due to charge transport and recombination. We have investigated a wide range of active layers: initial fullerene-based blends as P3HT:PC61BM and PTB7-Th:PC71BM, small molecule acceptors (PBDB-T:IDIC), and the high

efficiency state-of-art non fullerene blend PM6:Y6. In the comparative analysis in the short-circuit regime, charge extraction lifetime shortens as materials evolve to higher mobilities. While TA and TPC dynamics align in some systems, a contrast is apparent in high-efficiency materials, when the primary extraction occurs on timescales faster than 1 μ s. The difference indicates that the RC time constant of the optical apparatus is limiting the analysis. Furthermore, fullerene materials exhibit TA decay constants shorter than the TPV counterparts, a signature of high recombination rates that limit the fill factor and device performance. The outline of this work demonstrates that simultaneous TA and TPC/TPV is a robust methodology to probe charge dynamics in OSCs, and shows that suppressing recombination remains one of the primary frontiers for the next generation of OPV materials engineering.

References:

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Palavras-chave: organic solar cells; transient absorption spectroscopy; non-fullerene acceptors.