

Impact of acceptor unit copolymerization on the degradation of thiophene-based conjugated polymer donors for organic photovoltaic applications

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Donor-acceptor (D-A) copolymers have been gradually replacing thiophene-based homopolymers like poly(3-hexylthiophene-2,5-diyl) (P3HT) as electron donors in organic solar cells (OSCs). As D-A copolymers have a broader absorption compared to P3HT, they generally produce higher power conversion efficiencies compared to P3HT-based OSCs. Despite being the most popular monomer, thiophene-based OSCs are usually not durable. For example, the relatively quick deterioration of P3HT-based OSCs is associated with the fast oxidation dynamics of the thiophene homopolymer. Here, we compare the degradation dynamics of P3HT and of several D-A copolymers employing terthiophenes (3T) as the D unit. For this comparative study, we employed benzodithiophene (BDT) core and an isoindigo (IID) A units.

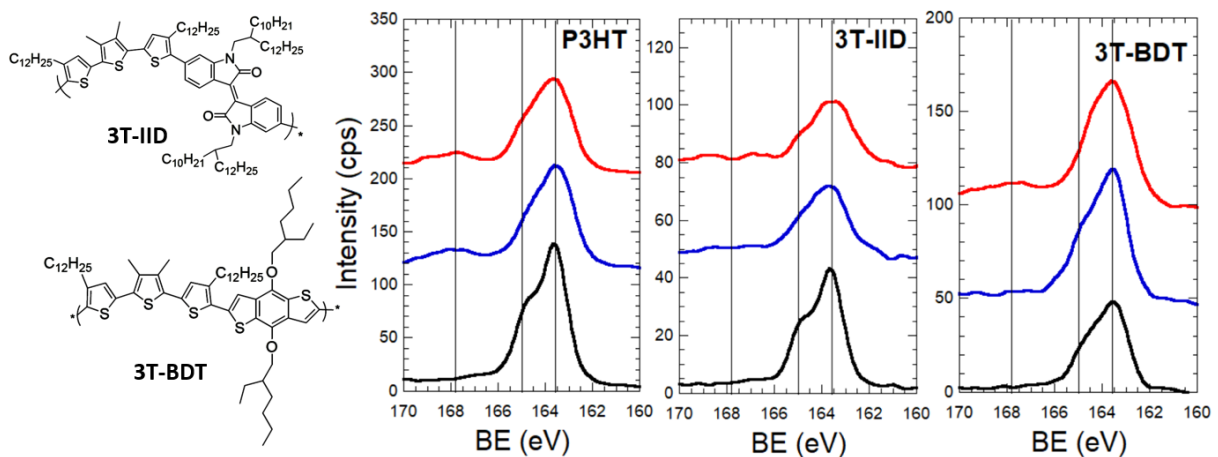


Fig. 1: Molecular structure and XPS analysis of the S_{2p} peak for the three studied polymer donors.

The molecular structures of the studied D-A copolymers, referred to as 3T-BDT and 3T-IID, can be found in Fig. 1. X-ray photoelectron spectroscopy (XPS) analysis confirm that annealing P3HT at 85°C leads to the rapid formation of oxidized sulfur moieties. XPS results also reveal that the inclusion of the A units notably delays the oxidation of thiophene-based conjugated polymers. Despite the similar oxidation dynamics of 3T-BDT and 3T-IID, the photovoltaic performances of 3T-IID OSCs degrade much faster than those of 3T-BDT ones. For each of the studied polymers, our systematic morphological and spectroscopic analysis enables us to identify whether the decrease in performance results from a drop in intrinsic properties of the semiconductor (broken conjugation) or from undesired phase separation in the OSC active layer. The study presented here should thus help establishing ground rules for the design of conjugated polymer donors that can be used to produce efficient and durable OSCs.