Area 4: Organic and Dye-Sensitized Solar Cells

Π-CONJUGATION EFFECTS OF OLIGO(THIENYLENEVINYLENE) SIDE CHAINS IN SEMICONDUCTING POLYMERS ON PHOTOVOLTAIC PERFORMANCE

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The 2D-conjugated polymers composed of the donor-acceptor (D-A) main chains and the conjugated side chains have been studied on polymer solar cells (PSCs). Zhou *et al.* reported that the introduction of the tris(thienylenevinylene) (tris-TTV) side chain to D-A polymers in a ratio of 20% greatly improved PCE by 25–43% compared with the original polymers owing to the increase of short circuit current (J_{SC}) and fill factor (FF) regardless of the main chain structures.[1] However, the origin of the enhancement effect is still unclear because of the lack of systematic studies.

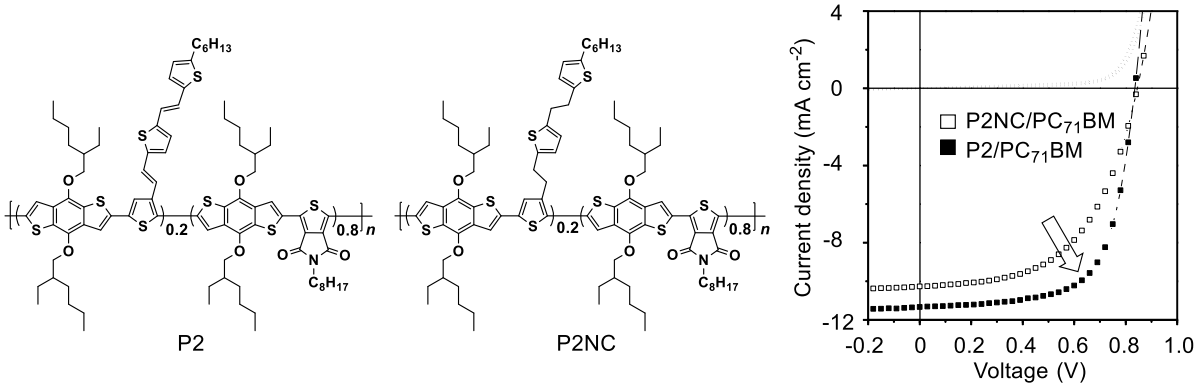

Figure 1. Chemical structures of polymers and *J-V* curves of the polymers:$PC_{71}BM$ PSC devices.

In this work, semiconducting polymers based on benzo[1,2-*b*:4,5-*b*']dithiophene (BDT) and thieno[3,4-*c*]pyrole-4,6-dione (TPD) as a main chain containing an oligo(thienylenevinylene) side chain and an analogous non-conjugated side chain, respectively (Figure 1), were synthesized to examine the effects of the conjugated side chain on the PSC performance. P2-based device showed a higher J_{SC} and FF compared with the reference polymer P2NC with "broken conjugation" at the side chain, resulting in an increase of power conversion efficiency (PCE) of 10–22%. Measurements of hole mobility by space-charge-limited current (SCLC) and internal quantum efficiency (IQE) indicated that introducing the π-conjugated side-chain units can facilitate both charge transport and charge separation in the polymer:$PC_{71}BM$ blend films. Furthermore, we also discussed the effects of the length of the conjugated side chain on the PSC performance and calculated the frontier molecular orbitals of their model pentamers by density functional theory (DFT) at the CAM-B3LYP/6-31G(d, p) level. In this presentation, these results will be reported in detail.

(1) Zhou, E.; Cong, J.; Hashimoto, K.; Tajima, K. *Energy Environ. Sci*. **2012**, *5*, 9756-9759.