The effect of molecular geometry on the photovoltaic property of diketopyrrolopyrrole based non-fullerene acceptors - DTU Orbit (13/12/2018)

The effect of molecular geometry on the photovoltaic property of diketopyrrolopyrrole based non-fullerene acceptors

The non-fullerene acceptors with different geometric structures have great impact on light absorption, exciton dissociation, and charge transportation in the active layer of organic solar cells (OSCs). In this paper, we designed and synthesized two diketopyrrolopyrrole based non-fullerene acceptors, Ph(DPP)2 and PhMe(DPP)2 with similar chemical components but different molecular geometries. Due to its more twisted molecular conformation, PhMe(DPP)2 shows more blue-shifted absorption bands, higher electron mobility, and better miscibility with the polymer donor poly(3-hexylthiophene) (P3HT) while compared to Ph(DPP)2. Therefore, the resulting P3HT:PhMe(DPP)2 based OSCs shows a better power conversion efficiency (PCE) of 0.65%, higher than that from P3HT:Ph(DPP)2 based OSCs (0.48%), which can be ascribed to more efficient exciton dissociation and electron transportation in the active layer of P3HT:PhMe(DPP)2.

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