A planar indandione based small organic molecule for effective donor materials in organic solar cells

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A new and effective donor material of indandione based D- $\pi$ -A planar molecule, 2-(5"-hexyl-[2,2':5'2" terthiophen]-5-yl) methylene)-1H- indene-1,3(2H) dione, H3T-ID) was synthesized to fabricate the bulk-heterojunction organic solar cells (BIH-OSCs). A promising absorption behavior with the optical band gap of ~1.98 eV was recorded for H3T-ID molecule. The H3T-ID molecule with  $\pi$ -spacer and hexyl side chain showed in improving the thin film morphology, molecular packing and charge transport. H3T-ID organic molecule presented the deep H0MO of ~ -5.37 eV and higher LUMO of ~ -3.38 eV, these were well-matched with energy levels of PC<sub>61</sub>BM acceptor. Fabricated BHI-OSC using H3T-ID as donor and PC<sub>61</sub>BM as acceptor attained the maximum PCE of ~4.05 % with good  $J_{SC}$  = ~10.43 mAcm<sup>-2</sup>,  $V_{OC}$  = ~0.77 V and FF= 0.51. Importantly, the fabricated BHI-OSCs expressed showed good reproducibility and stability by retaining over ~80% of its initial PCE for 15 days without encapsulation.