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Novel donor-acceptor low band gap copolymers for bulk heterojunction (BHJ) solar cells

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Tremendous advances have been achieved over the past decade in the area of design and synthesis of novel conjugated polymers for bulk heterojunction (BHJ) solar cells and light emitting diodes (LEDs). With ingenious use of variety of synthetic techniques, researchers have synthesised copolymers with optimized physical properties. For instance, an organic photovoltaic (OPV) material showing record-breaking power conversion efficiency (PCE) of ca. 10% has been reported recently. In the design of semiconducting copolymers, the donor-acceptor (DA) approach has been found to afford low band gap (LBG) copolymers with broad absorption to efficiently harvest solar energy. Here we report the synthesis of two novel LBG copolymers (PFDEBT and PFDES) and studies of their photo-physical and electrochemical properties, for prospective use in organic electronics. PFDEBT with benzothiadiazole acceptor moiety demonstrated bathochromic shift of absorption from 578 nm in solution to 591 nm in the solid state with an optical band gap of 1.69 eV, while PFDES containing dibenzothiophene-S,S-dioxide unit showed absorption at 489 and 494 nm in both the liquid and solid states respectively with an optical band gap of 2.25 eV. Both polymers are highly emissive materials; with the former emitting in the red region of the emission spectrum attaining emission λ_{max} of 709 nm and 28% photoluminescence quantum yield (PL Φ) in solution, while the later emits in the green region with an emission λ_{max} of 517 nm and 55% PL Φ . The HOMO energy levels of the polymers estimated from cyclic voltammetry analysis are -4.9 and -5.1 respectively. Preliminary studies of BHJ solar devices of the blend of these copolymers with PC60BM showed PCE of 1.45% and 1.1% for PFDEBT and PFDES respectively for non-optimized devices.

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