Incorporation of ester groups into low band-gap diketopyrrolopyrrole containing polymers for solar cell applications

To increase the open circuit voltage (VOC) of polymer solar cells based on diketopyrrolopyrrole (DPP) containing polymers, the weakly electron-withdrawing thiophene-3,4-dicarboxylate unit was introduced into the polymer backbone. Two ester group functionalized DPP containing polymers, PCTDPP with a random structure and PDCTDPP with a regular structure, were designed and synthesized by the Stille coupling reaction. The resulting copolymers exhibit broad and strong absorption bands from 350 to 1000 nm with low optical band gaps below 1.40 eV. Through cyclic voltammetry measurements, it is found that regular PDCTDPP’s HOMO energy level is 0.18 V lower than that of the corresponding random PCTDPP (~5.14 eV for PCTDPP and ~5.32 eV for PDCTDPP). Preliminary photovoltaic properties of the copolymers blended with [6,6]-phenyl-C61-butyric acid methyl ester (PCBM) as an electron acceptor were investigated. The PSC based on a PCTDPP:PCBM blend shows a power conversion efficiency (PCE) up to 3.52%, with a VOC of 0.66 V, a short circuit current (ISC) of 8.53 mA cm−2, and a fill factor (FF) of 0.63. For the PDCTDPP:PCBM blend, the highest VOC reaches a value of 0.84 V, and a final PCE (0.92%) is limited by the poor hole mobility of the active layer.

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