

Molecular Design and Synthesis of Semiconducting Conjugated Polymers Based on Diketopyrrolopyrrole for High Performance Polymer Solar Cells

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Polymer solar cells (PSCs) provide special opportunities for low-cost, printable, light-weight, flexible, and portable energy sources. For the past few years, a great advance to improve the efficiency of polymer solar cells has been achieved owing to development of new semiconducting polymers, understanding of organic semiconductor physics and advancement in the device optimization including interface engineering. As a result, the power conversion efficiency (PCE) has continuously increased to its current value over 8%. Nevertheless, further development of PSCs is still needed for commercialization, which requires the PCE higher than 10%. To enhance the PCE, many approaches has been proposed: (i) synthesis of low bandgap conjugated copolymers to harvest the solar spectrum more effectively, (ii) synthesis of semi-conducting polymers with deep HOMO levels to enhance V_{OC} , (iii) synthesis of planar conjugated polymers to afford high hole mobility, (iv) synthesis of new fullerene derivatives as acceptor material, and others.

Diketopyrrolo[3,4-c]pyrrole (DPP) has emerged as a promising building block of low band-gap conjugated polymers for the optoelectronic applications including both organic field effect transistors (OFETs) and PSCs. Its highly conjugated structure leads to strong π - π interaction, and the electron deficiency provides the DPP with the potential use of electron-accepting unit for synthesis of low band-gap conjugated polymers. We report synthesis of novel low band-gap conjugated polymers, PDTTDPP, composed of dithieno[3,2-b:2',3'-d]thiophene (DTT) and DPP, and PBDTDPP composed of unsubstituted benzo[1,2-*b*:4,5-*b'*]dithiophene (BDT) and DPP.

We demonstrates that a novel low bandgap polymer (PDTTDPP), composed of electron-rich extended heteroarene unit (DTT) and electron-deficient unit (DPP), can be used as a *p*-type conjugated polymer for both OFETs and OPVs. The strong intermolecular π - π stacking of PDTTDPP contributes to achieve the high hole mobility of $0.68 \text{ cm}^2/\text{V}\cdot\text{s}$ in OFETs without post treatment. The PDTTDPP also shows a low bandgap of 1.22 eV due to strong intra-molecular charge transfer between DTT and DPP. Consequently, the high hole mobility and broad light absorption of PDTTDPP achieves a promising power conversion efficiency (PCE) of 6.05% with $J_{sc} = 13.9 \text{ mA}/\text{cm}^2$, $V_{oc} = 0.66 \text{ V}$, and $FF = 65.7\%$. This work clearly demonstrates that extended heteroarene unit (DTT) is a promising building block in the molecular design of new polymers for high performance organic electronics.

PBDTDPP is another interesting polymer and expected to exhibit a low-lying HOMO level to afford high V_{oc} , because alkoxy group is removed from alkoxy-substituted BDT. Alkoxy group has strong electron-donating power, and therefore it raises the HOMO level of D-A conjugated polymer. Since the V_{oc} of PSCs is proportional to the difference between the HOMO level of donor and the LUMO level of acceptor, PBDTDPP with low-lying HOMO level due to removal of alkoxy group exhibits higher V_{oc} while the conjugated polymer (PBDTDPP-OR) with alkoxy group exhibits lower V_{oc} due to its high-lying HOMO level. Consequently, the removal of the alkoxy side group from alkoxy-substituted BDT leads to achieve a promising PCE of 5.16% with a high V_{oc} of 0.82V. These values are much higher than those of alkoxy-substituted BDT-based polymer (2.24% and 0.61 eV).