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Synthesis of Pyrimidine-Based Polymers Consist of 2-{4-[4,6-Bis-(4-Hexyl-Thiophen-2-yl)-Pyrimidin-2-yl]-Phenyl}-Thiazolo[5,4-B]Pyridine with Deep HOMO Level for Photovoltaics

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Abstract : Photovoltaics, which have many advantages in cost, easy processing, and light-weight, have attracted attention. We synthesized pyrimidine-based conjugated polymers with 2-{4-[4,6-bis-(4-hexyl-thiophen-2-yl)-pyrimidin-2-yl]-phenyl}-thiazolo[5,4-b]pyridine (pPTP) which have an ability of powerful electron withdrawing and introduced into the PSCs. By Stille polymerization, we designed the conjugated polymers, pPTPBDT-12, pPTPBDT-EH, pPTPBDTT-EH and pPTPTTI. The HOMO energy levels of four polymers (pPTPBDT-12, pPTPBDT-EH, pPTPBDTT-EH and pPTPTTI) were at -5.61 ~ -5.89 eV, their LUMO (Lowest Unoccupied Molecular Orbital) energy levels were at -3.95 ~ -4.09 eV. The device including pPTPBDT-12 and PC71BM (1:2) indicated a V_oc of 0.67 V, a J_sc of 1.33 mA/cm², and a fill factor (FF) of 0.25, giving a power conversion efficiency (PCE) of 0.23%. The device including pPTPBDT-EH and PC71BM (1:2) indicated a V_oc of 0.72 V, a J_sc of 2.56 mA/cm², and a fill factor (FF) of 0.30, giving a power conversion efficiency of 0.56%. The device including pPTPBDTT-EH and PC71BM (1:2) indicated a V_oc of 0.72 V, a J_sc of 3.61 mA/cm², and a fill factor (FF) of 0.29, giving a power conversion efficiency of 0.74%. The device including pPTPTTI and PC71BM (1:2) indicated a V_oc of 0.83 V, a J_sc of 4.41 mA/cm², and a fill factor (FF) of 0.31, giving a power conversion efficiency of 1.13%. Therefore, pPTPBDT-12, pPTPBDT-EH, pPTPBDTT-EH, and pPTPTTI were synthesized by Stille polymerization. And We find one of the best efficiency for these polymers, called pPTPTTI. Their optical properties were measured and the results show that pyrimidine-based polymers especially like pPTPTTI have a great promise to act as the donor of the active layer.

Keywords : polymer solar cells, pyrimidine-based polymers, photovoltaics, conjugated polymer
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