



Synthesis and photovoltaic properties of conjugated copolymers with benzo[1,2-b:4,5-b']dithiophene and thiadiazolo[3,4-c]pyridine moieties

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ARTICLE INFO

Article history:

Received 4 March 2013

Received in revised form 28 May 2013

Accepted 10 June 2013

Available online 18 June 2013

Keywords:

Polymer solar cells

Conjugated polymers

Benzo[1,2-b:4,5-b']dithiophene

Thiadiazolo[3,4-c]pyridine

Horner–Wadsworth–Emmons reaction

Stille coupling polymerization

ABSTRACT

A series of main-chain and side-chain type D–A copolymers containing benzo[1,2-b:4,5-b']dithiophene (BDT) and thienylbenzo[1,2-b:4,5-b']dithiophene (BDTT) electron-donating units and an electron-withdrawing unit based on thiadiazolo[3,4-c]pyridine, PBDDT-DTPyT, PBDDT-T-DTPyT, and PBDTT-T-DTPyT were synthesized for polymer solar cells (PSCs). The copolymers exhibit good thermal stability, strong absorption in the visible region, and relatively lower HOMO energy levels from -5.22 to -5.38 eV. The results indicate thiadiazolo[3,4-c]pyridine led to enhanced π – π stacking of the polymer film owing to its stronger polarity. PBDTT-T-DTPyT exhibited a high hole mobility of $1.2 \times 10^{-2} \text{ cm}^2 \text{ V}^{-1} \text{ S}^{-1}$. The interaction of the thiadiazolo[3,4-c]pyridine in the polymers and the hole extraction layer led to a non-ohmic contact at the interface. The conventional and inverted bulk heterojunction polymer solar cells based on PBDDT-T-DTPyT as the electron donor and (6,6)-phenyl-C₆₁-butyric acid methyl ester (PC₆₁BM) as the electron acceptor exhibited power conversion efficiencies of 1.68% and 2.08%, respectively.

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1. Introduction

Bulk heterojunction (BHJ) polymer solar cells (PSCs) based on conjugated copolymers as electron donors and fullerene derivatives as the electron acceptor [1] have been intensively studied in recent years for their low cost, light weight, mechanical flexibility, fast/cheap roll-to-roll production and easy tunability of chemical properties of the photovoltaic materials [2–5]. In the past two years, a lot of new donor–acceptor (D–A) low band gap polymers have been reported for PSCs. However, only a few high perfor-

mance polymers have been reported with efficiencies surpassing 9% [6].

To simultaneously lower the HOMO energy level and the band gap as required by the ideal polymer, a “weak donor–strong acceptor” strategy was proposed [7]. A few low band gap conjugated polymers, incorporating weak donor moieties based on fused aromatic systems and a strong acceptor based on 4,7-dithien-2-yl-2,1,3-benzothiadiazole (DTBT), have been successfully demonstrated with high efficiency in BHJ devices [8,9]. What's more, we have already reported a new benzodithiophene-based copolymer PT-DTBT with dithienyl-benzothiadiazole-vinylene side chains, which exhibits excellent film-forming ability, a deep HOMO energy level, and good miscibility with PC₇₁-BM. Bulk heterojunction polymer solar cells fabricated from PT-DTBT and PC₇₁BM showed a promising power conversion efficiency (PCE) over 5% [10,11].

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Compared with benzene, pyridine is π -electron deficient. Therefore, thiadiazolo[3,4-c]pyridine (PyT) is a stronger acceptor than 2,1,3-benzothiadiazole (BT). A similar strategy has been demonstrated recently by You et al. [12], Jen et al. [13] and Leclerc et al. [14]. In addition, prominent PCEs up to 6.7% have been achieved for small molecule photovoltaic material based PyT [15]. However, some polymers based on carbazole or indacenodithiophene unit and dithiophene thiadiazolo[3,4-c]pyridine (DTPyT) exhibit only moderate efficiencies [13,14].

Here, we synthesized a series of side-chain type copolymers (PBDT-T-DTPyT and PBDTT-T-DTPyT, Scheme 1), which introduced DTPyT as the conjugated side chain and benzo[1,2-b:4,5-b']dithiophene (BDT) and thienylbenzo[1,2-b:4,5-b']dithiophene (BDTT) as the electron-donating units in these copolymers, which have been proved to be very good electron-donating units [16–18]. To enhance the coplanarity of the polymer backbone, the DTPyT moiety was attached to the polymer via vinylene bonds. In addition, we also synthesized a main-chain type copolymer (PBDT-DTPyT, Scheme 1) for comparison.

2. Experimental section

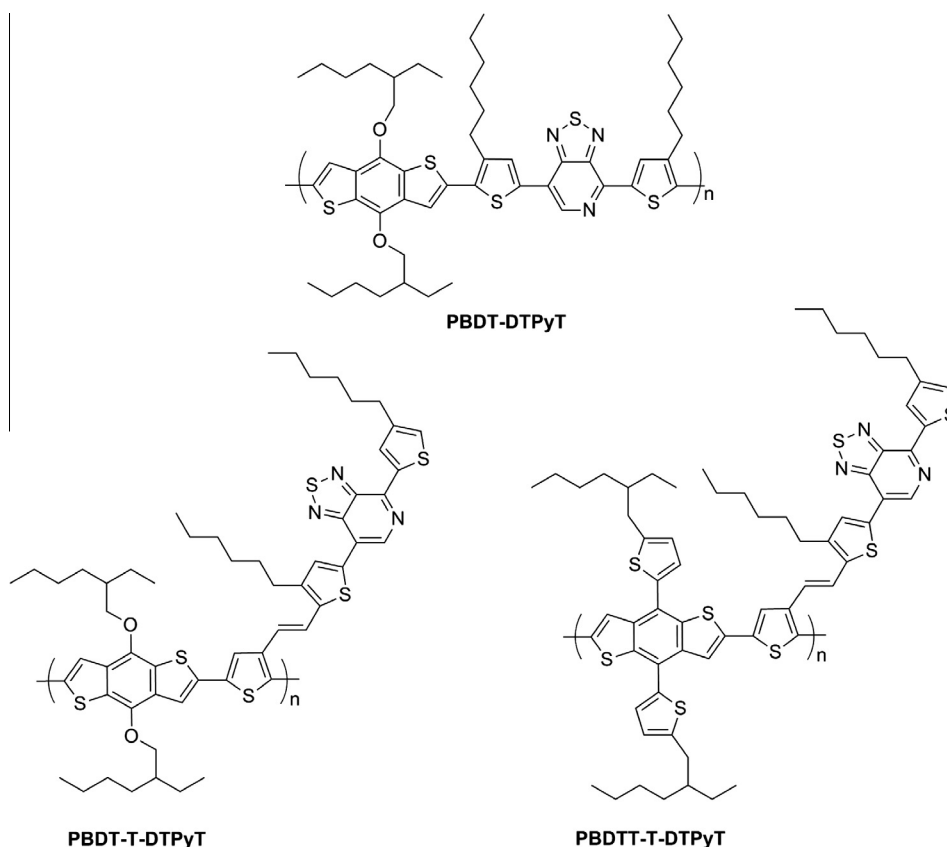
2.1. Materials

4,7-bis(4-hexylthiophen-2-yl)-[1,2,5]thiadiazolo[3,4-c]pyridine (DTPyT) [12–14], 3-hexyl-5-(4-(4-hexylthiophen-2-yl)-

[1,2,5]thiadiazolo[3,4-c]pyridin-7-yl)thiophene-2-carbaldehyde (DTPyT-CHO) [10,11], (2,5-dibromothiophen-3-ylmethyl)phosphonic acid diethylester (1) [19], (4,8-bis((2-ethylhexyl)oxy)benzo[1,2-b:4,5-b']dithiophene-2,6-diyl)bis(trimethylstannane) (**M3** BDT) [20], (4,8-bis(5-(2-ethylhexyl)thiophen-2-yl) benzo[1,2-b:4,5-b']dithiophene-2,6-diyl)bis(trimethylstannane) (**M4** BDTT) [17,18] were synthesized according to literature procedures. All the chemicals were purchased from Alfa Aesar and Energy Chemical. Tetrahydrofuran (THF) and toluene were refluxed over sodium and benzophenone and distilled. Dimethyl formamide (DMF) was dried and distilled under reduced pressure. All other commercially available materials were used as received unless noted otherwise. Column chromatography was performed on silica gel (Qingdao Haiyang Chemical Co., LTD, 200–300 mesh).

2.2. Characterization

^1H NMR and ^{13}C NMR spectra were recorded with Bruker AVANCE 400 spectrometer. UV–vis spectra and photoluminescence (PL) spectra of the copolymers were obtained on Perkin–Elmer Lamada 25 spectrometer and Perkin–Elmer LS-50 luminescence spectrometer, respectively. FT-IR spectra were measured on Perkin–Elmer Spectra One. Molecular mass was determined by matrix assisted laser desorption–ionization time-of-flight mass spectrometry (MALDI-TOF MS) using a Bruker Aupoflex-



Scheme 1. Molecular structures of the polymers.

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