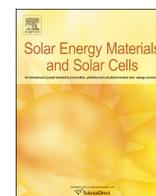




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## Structure property relationship for carbazole and benzothiadiazole based conjugated polymers

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## ABSTRACT

A series of conjugated polymers with carbazole monomer/dimer/trimer as the donor unit or benzothiadiazole monomer/trimer as the acceptor unit were synthesized and used as donor materials for polymer solar cells (PSCs). The influence of polymer structure on the optical properties and performance of PSCs was investigated in detail. P1 showed a power conversion efficiency (PCE) of 5.8%. The incorporation of longer donor or acceptor unit leads to a blue shift of absorption spectrum and the polymers became more amorphous due to the large torsion angles in the polymer backbone. After increasing the length of donor or acceptor, the PCE decreased dramatically to 0.43% for P2, 0.23% for P3, and 1.23% for P4. Our results have offered a useful insight to structure–property relationship for high performance polymer solar cells.

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## 1. Introduction

Bulk-heterojunction (BHJ) organic photovoltaic (OPV) cells have aroused a great interest for their potential applications and impressive device efficiency achieved in the past decade [1–3]. The progress of polymer solar cells (PSCs) is extremely encouraging and exciting. However, the achievement of PSCs still cannot meet the requirement of market for their exorbitant cost, low power conversion efficiency (PCE) and short device lifetime [4–6]. To obtain high PCE, the efficient absorption of solar energy for the active layer is very crucial [7]. The optical absorption profile of polymers should be matched well with the solar spectrum. Many experimental methods and new molecular design strategies have been applied to achieve strong light-absorbing ability [8–11]. Hopefully, broad absorptions can be obtained by using donor and acceptor alternating polymer backbone design strategy via the internal charge transfer (ICT) from the donor to the acceptor unit. Decreasing the band gap can make the polymers absorb more efficiently and lowering the HOMO level can maximize the open circuit voltage ( $V_{oc}$ ) of devices [12]. Narrow band gap polymers can be constructed by alternating an electron-rich donor (D) and an electron-deficient acceptor (A) segment in the polymer main chain [13–15]. The ICT effect can produce a pivotal light absorption in the region of visible light [16]. From the perspective of material structure–property, the

influence of length of donor or acceptor segment on the optical properties of polymers and the photovoltaic performance of devices has not been intensively explored. In this contribution, we synthesized a series of conjugated polymers with carbazole monomer/dimer/trimer as the donor unit and benzothiadiazole monomer/trimer as the acceptor unit (Scheme 1). The influence of polymer structure on the optical properties of polymers and the performance of PSCs was studied in detail.

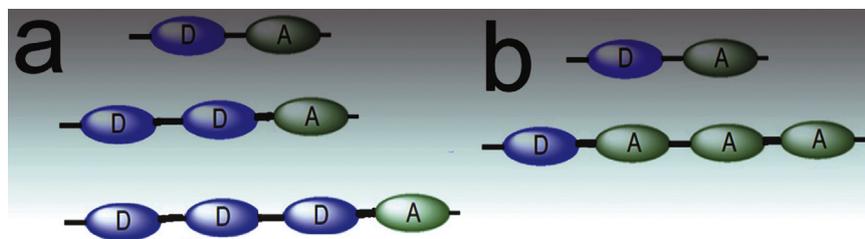
## 2. Results and discussion

## 2.1. Synthesis

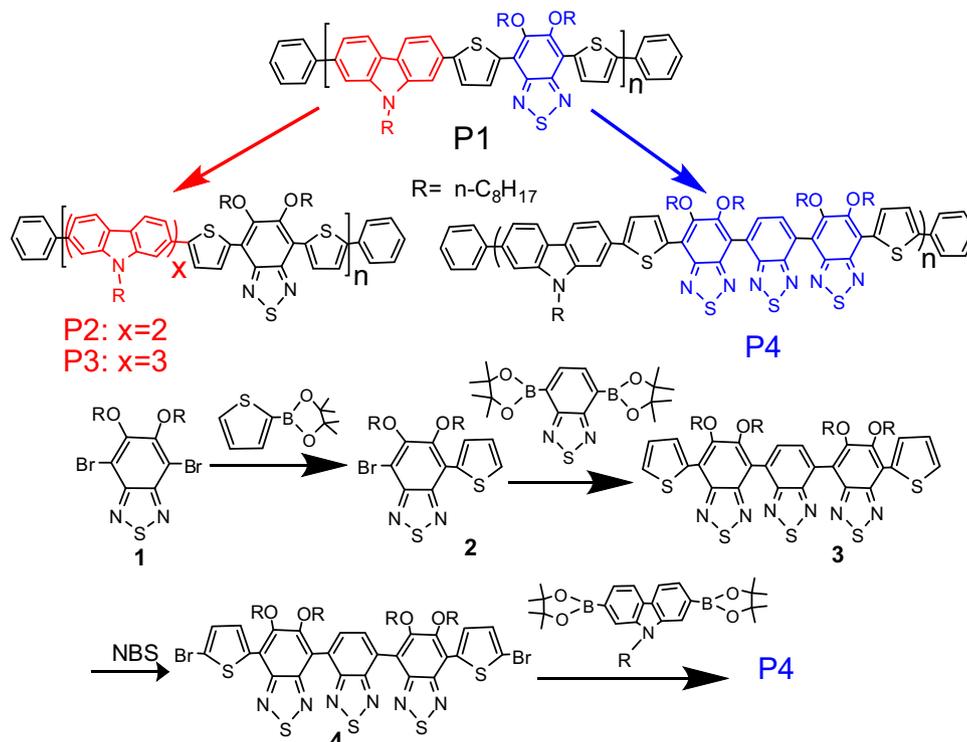
The syntheses of P1–4 are illustrated in Scheme 2. The structures of P1–4 were characterized by  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectroscopy (Figs. S1–7, Supporting information). Molecular weights of and molecular weight distributions of P1–4 were measured by GPC at room temperature using chloroform as an eluent and calibrated with polystyrene standards. The data are summarized in Table S1 (Supporting information). The relatively low molecular weight for polymer P3 and P4 was probably due to their poor solubility in the organic solvent used for polycondensation. P3 and P4 precipitated from the reaction media during the polycondensation. The precipitated polymers could be readily dissolved in chloroform (CF) and 1,2-dichlorobenzene (DCB). Degradation temperatures as determined by thermogravimetric analysis (TGA) indicated that all polymers have a good thermal stability. Glass transition temperatures ( $T_g$ ) of polymers are also listed (Table S1 in the

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**Scheme 1.** The structure of polymers with elongated donor carbazole D (a) and acceptor unit benzothiadiazole A (b).



**Scheme 2.** The chemical structure and synthetic routes.

**Supporting Information**). P2 and P4 showed relatively low  $T_g$ , namely 58.9 °C for P2 and 68.0 °C for P4. The low molecular weight and the poor crystalline caused by the larger torsion angle along the main chain may be responsible for this (Figs. 4 and S8).

## 2.2. Optical properties and powdery X-ray diffraction results

UV–visible absorption spectra of P1–4 in dilute THF solutions (a) and as films (b) are shown in Fig. 1. P1 showed a broad absorption in the visible region with two peaks located at 404 and 564 nm. The short wavelength absorption peak is due to the  $\pi$ – $\pi^*$  transition and the long wavelength peak is caused by the internal charge transfer (ICT) from the donor to the acceptor. Increasing the length of donor unit or acceptor unit, the resulted polymers exhibited blue-shifted absorption spectra. P2 showed an intense absorption peak at 396 nm and a weak absorption peak at 527 nm. P3 also showed an intense absorption peak at short wavelength region and a weak absorption in the long wavelength region with the two peaks located at 363 and 535 nm. P4 displayed narrow absorption ranged from 300 to 550 nm. The above result demonstrated that either increasing the length of donor unit or the acceptor unit will lead to a decreasing the effective conjugation length or the charge transfer effect from donor unit to the acceptor unit. In going from solutions to films, all these polymers showed

similar behavior as shown in Fig. 2b. All the absorption peaks became broader due to the aggregation of polymer chains in the solid state. Usually, the ICT absorption plays an important role to the performance of polymer solar cells (PSCs). Polymers such as PTB7 [17], PCDTBT [18], PffBT4T-2OD [2], DR3TSBDT [1], and PBDTT–SeDPP [19] with an intense ICT absorption usually gave high efficiency. The band gaps of these polymers were determined by the absorption onsets of polymer films. The highest occupied molecular orbital (HOMO) levels of these polymers were determined by cyclic voltammetry as described in the **Supporting information**. The lowest unoccupied molecular orbital (LUMO) levels were calculated by the equation

$$E_{\text{LUMO}} = E_{\text{HOMO}} + E_g$$

The energy levels of these polymers are shown in Fig. 2 (left). Increasing the length of donor unit, the band gap of P2 and P3 became slightly broader and the HOMO levels of P2 and P3 slightly decreased. The energy levels of polymers are believed depending on the donor and acceptor units, in which the HOMO level is mainly determined by the donor and the LUMO level mainly by the acceptor. Here, increasing the length of donor unit only slight influences the energy levels. Increasing the length of acceptor unit has a significant influence on the energy level. The HOMO level of P4 decreased to  $-5.42$  eV and the LUMO level increased to  $-3.11$  eV.

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