

Synthesis and photovoltaic properties of a small molecule acceptor with thienylenevinylene thiophene as π bridge



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ABSTRACT

A new *n*-type organic semiconductor (*n*-OS) acceptor with (*E*)-5-(2-(5-(2-ethylhexyl)thiophen-2-yl)vinyl)-thiophene-2-yl (TVT) functional group as π -bridge to link indacenodithiophene (IDT) core and 3-(dicyanomethylene)indan-1-one (IC) terminals, named ITVT, was synthesized and applied in polymer solar cells (PSCs). It is the first time employing TVT unit in *n*-OS small molecule acceptor. Benefited from the conjugated TVT side groups, the small molecule ITVT shows a strong absorption at the short wavelength range (300–500 nm). In addition, ITVT exhibits a low optical band gap (E_g^{opt}) of 1.48 eV and a medium electron mobility of $1.85 \times 10^{-4} \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$. A wide band gap polymer PBZ was chosen as donor to fabricate an inverted BHJ PSCs because of the complementary absorption and matched molecular energy levels. The as-cast PSCs yield a power conversion efficiency (PCE) of 5.84% with an open-circuit voltage (V_{oc}) of 0.96 V and a short-circuit current density (J_{sc}) of 14.22 mA cm^{-2} under the illumination of AM 1.5 G at 100 mW cm^{-2} .

1. Introduction

Bulk-heterojunction (BHJ) polymer solar cells (PSCs) have attracted considerable attention as a renewable and clean energy harvesting technology to form flexible, large-area and semi-transparent photovoltaic panels by low-cost solution processing techniques [1–8]. Indeed, the utilization of semiconducting materials as photoactive layer including both donors (D) and acceptors (A) has been extensively studied. Nowadays, the PSCs based on the *n*-type organic semiconductor (*n*-OS) small molecule acceptor have opened a new page for molecular design, especially for the linear small molecules with A-D-A structure, such as IEIC [9], ITIC [10], and the other derivatives on the basis of these linear small molecules. Modifying the D or A units of these linear small molecules, allows the energy levels to be fine-tuned, opening the possibility of a low-bandgap *n*-OS acceptor. This might be an effective approach to extend absorption range, which would be beneficial to achieving higher J_{sc} [11]. Since then, many strategies have been applied to modify the structure of IDT (indacenodithiophene) or IDTT (indacenodithiophene [3,2-*b*]thiophene)-based small molecules in order to adjust the absorption spectra and energy levels to further improve the power conversion efficiency (PCE), for example, by changing the side chains [12,13], extending the conjugation length [14–21], and

substituting the end groups [22–31]. To date, a great number of single-junction PSCs based on these *n*-OS acceptors have achieved a PCE of over 10% and even up to 14% [18–20,22,24–26,29,31–38].

Besides, the π -bridge in the linear small molecule acceptors with A- π -D- π -A structure can affect the absorption spectrum of active layer and then directly improve the J_{sc} of the PSCs. Hou and coworkers synthesized a low bandgap *n*-OS acceptor IEICO through utilizing a spacer (alkoxy thiophene) to enhance the intramolecular charge transfer (ICT) effect and electron delocalization. The IEICO-based PSC device showed a maximum PCE of 8.4%, and a higher PCE (10.7%) of tandem device based on IEICO was exhibited [39]. Although these modification on the electron-donating D unit, the electron-withdrawing A unit, and the π -bridge of these linear small molecules can broaden their absorption spectra in the long-wavelength region, the absorption strength in the short-wavelength region is weak, even though some interesting results have been achieved in a new family of conjugated polymers with conjugated side chains as donor materials [7,40–42]. This type of polymers features high hole mobility thanks to the overlapping of the side chain interactions with the conjugated main chains, and broad absorptions deriving from both the main chains and the conjugated side chains. After introducing thienylenevinylene thiophene (TVT) side groups onto the BDT units, the polymer PBDTTVT-DTTPD thin film was

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able to harvest a broad solar spectrum covering the range from 300 to 700 nm. Especially, the absorption intensity of PBDTTVT-DTTPD at 400 nm was significantly higher than that of the alkylthienyl-substituted polymer (PBDDT-DTTPD) [43]. Similarly, the polymer PBT-TVT exhibited stronger absorption spectrum and higher hole mobility compared to that of PTB7 because of its prolonged conjugation of the conjugated side groups (TVT) on BDT units [44].

In this work, a new *n*-OS acceptor with (*E*)-5-(2-(5-(2-ethylhexyl)thiophen-2-yl)vinyl)-thiophene-2-yl (TVT) functional group as π -bridge to link indacenodithiophene (IDT) core and 3-(dicyanomethylidene)indan-1-one (IC) terminals, named ITVT, was synthesized and applied in PSCs. Benefited from the conjugated TVT side groups, the small molecule ITVT shows a strong absorption at the short wavelength range (300–500 nm). ITVT exhibits a low optical band gap (E_g^{opt}) of 1.48 eV and a medium electron mobility of $1.85 \times 10^{-4} \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$. The inverted BHJ PSCs were fabricated with a wide band gap polymer PBZ as the donor. The PBZ:ITVT blend films show complementary absorption spectrum from 300 to 850 nm. The PSCs without additional treatment yield a PCE up to 5.84% with an open-circuit voltage (V_{oc}) of 0.96 V, a short-circuit current density (J_{sc}) of 14.22 mA cm^{-2} and a fill factor (FF) of 42.7% under AM 1.5 G (100 mW cm^{-2}) conditions.

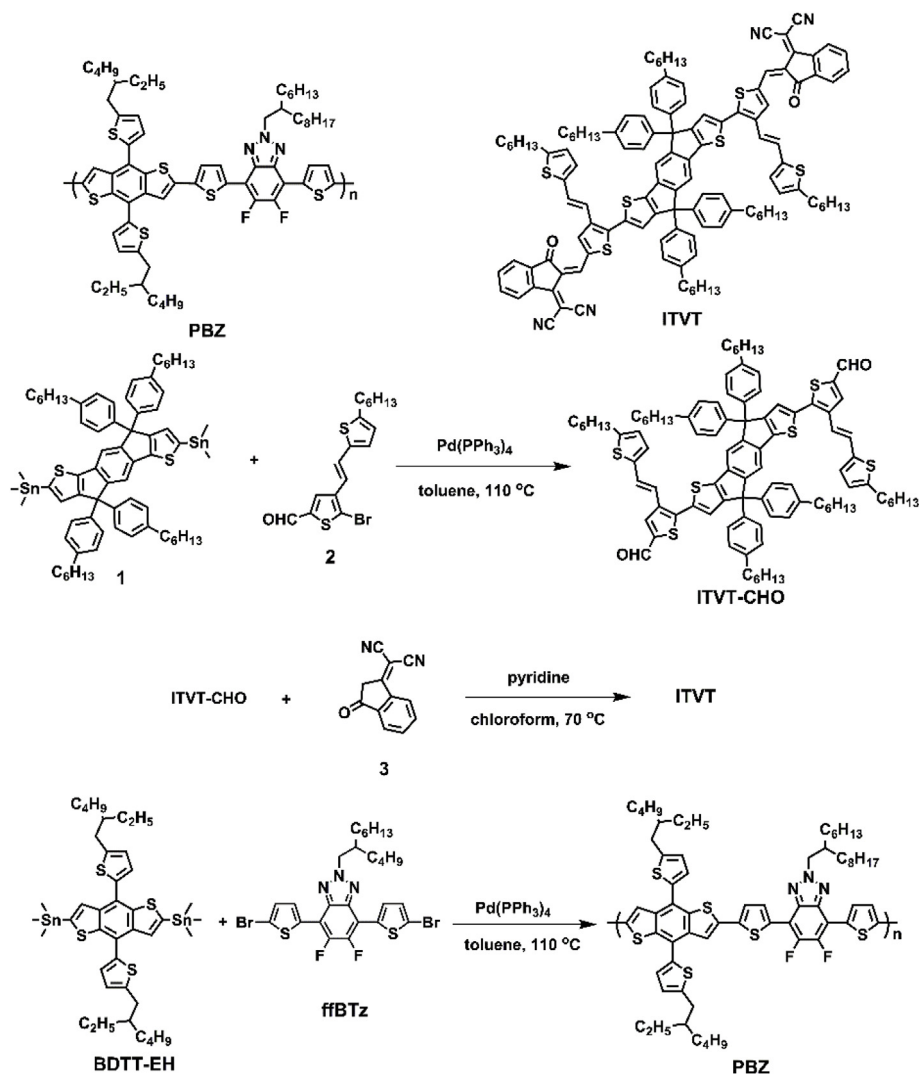
2. Results and discussion

2.1. Synthesis and characterization

ITVT was synthesized *via* facile reactions (Scheme 1). The intermediate compound ITVT-CHO was synthesized through the Stille coupling reaction between compounds 1 and 2 with $\text{Pd}(\text{PPh}_3)_4$ as catalyst. Then a typical Knoevenagel condensation reaction of ITVT-CHO with compound 3 afforded the small molecule ITVT. The chemical structure of ITVT was fully characterized using ^1H NMR, ^{13}C NMR, MALDI-TOF and elemental analysis techniques in Supporting Information (SI). ITVT exhibits good solubility in common organic solvents, such as chloroform (CF), chlorobenzene (CB) and *o*-dichlorobenzene (*o*-DCB) at room temperature. The thermal stability of ITVT was evaluated by thermogravimetric analysis (TGA) (Fig. S1, SI) under nitrogen atmosphere. The molecule did not decompose until 340 °C, which is adequate for the application in PSCs.

2.2. Absorption spectra and electronic energy levels

The UV–vis absorption spectra of the small molecule acceptor ITVT and the polymer donor PBZ in thin film are shown in Fig. 1a. The absorption spectrum of ITVT in dilute chloroform solution is shown in Fig. S2 in SI. A chloroform solution of ITVT displays absorption in the region of 500–800 nm with a maximum extinction coefficient of $1.42 \times 10^5 \text{ M}^{-1} \text{ cm}^{-1}$.



Scheme 1. Chemical structures of PBZ and ITVT, and synthetic route of ITVT.

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