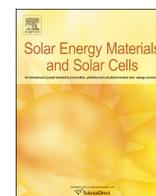




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Small molecules based on tetrazine unit for efficient performance solution-processed organic solar cells

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ABSTRACT

Two D2-A-D1-A-D2 type small molecules using Benzo[1,2-*b*:4,5-*b'*]dithiophene (BDT) as central building block, tetrazine (Tz) as an electron accepting moiety, bithiophene or terthiophene as end donor units were synthesized. The optical and electrochemical properties of synthesized molecules indicate that these molecules can absorb sunlight in a broad spectral range from 300 to 700 nm and show suitable energy level for efficient exciton dissociation. The introduction of tetrazine unit in these molecules effectively reduces the highest occupied molecular orbital (HOMO) energy levels of these molecules, thus increases air stability of these molecules as well as the open circuit voltage (V_{oc}) in photovoltaic devices. Bulk heterojunction organic solar cells were fabricated by blending of these molecules with [6,6]-phenyl-C₇₁-butyric acid methyl ester (PC₇₁BM) on indium tin oxide/glass substrates. This work affords promising power conversion efficiencies over 5.0%, with a large V_{oc} of 0.98 V, measured under air mass 1.5 global irradiation of 100 mW/cm².

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1. Introduction

Organic solar cells (OSCs) have attracted much attention because of the potential as a competitive technology of green energy with the advantages of solution processability, low cost, light weight and high mechanical flexibility [1–4]. Over the past decades, polymer based OSCs with bulk heterojunction (BHJ) architecture made great progress in achieving high power conversion efficiencies (PCEs) [5–8]. Recently, PCE has increased remarkably and approached greater than 10% based on polymer donors and fullerene derivative acceptors [9–11]. However, it cannot be denied that there are disadvantages for polymer based OSCs, such as undefined molecule weight, polydispersity, low purity, and batch-to-batch variations. In contrast, small molecule (SM) donors have been intensively researched as competitive alternative to their polymer counterparts due to their advantages of monodispersity, simple synthesis, high purity, greater solubility, good reproducibility and easier band structure control [12–15]. Up to now SMs have shown a great potential for solar cell application, with the highest PCEs over 9% [16–19]. However further

advancement towards commercialization still requires the design and synthesis of new SMs.

One feasible approach for obtaining organic conjugated molecule is to design donor-acceptor (D-A) architecture with alternating electron donor and electron acceptor moiety among the organic molecular backbone. The D-A type organic molecules can not only narrow band gap by utilizing intramolecular charge transfer transition between electron donor unit and acceptor unit inside molecules, but also adjust the HOMO and LUMO energy levels through selecting different donor or acceptor moiety into the molecular backbone [20–22]. The HOMO energy level of organic molecules is an important parameter for designing donor material of OSCs because the V_{oc} of BHJ OSCs is determined by the difference between of the LUMO level of PCBM and the HOMO level of organic molecule [23–25].

Tetrazine (Tz) has been a promising building block as a electron acceptor unit in D-A conjugated polymers, because relatively strong electron withdrawing ability of Tz would help to lower HOMO and LUMO energy levels of corresponding conjugated polymers, which is conducive to improving V_{oc} in BHJ OSCs [26–29]. For instance, it has been reported that a narrow band gap copolymer, PCPDTTBT, composed of cyclopenta[2,1-*b*:3,4-*b'*]dithiophene (CPDT) and benzothiadiazole (BT) as the D and A units, respectively, shows HOMO and LUMO energy levels of –5.12 and –3.39 eV, respectively [27]. When the BT unit in PCPDTTBT is replaced by Tz unit, the copolymer (PCPDTTz) exhibits lower

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HOMO and LUMO energy levels of -5.35 and -3.52 eV, respectively [28]. Another copolymer (PBDD-TTz) composed of Benzo[1,2-b:4,5-b']dithiophene (BDT) as D unit and Tz as A unit also exhibits relatively low HOMO and LUMO energy levels of -5.42 and -3.58 eV [29]. It suggests that the introduction of Tz moiety in D-A polymer backbone effectively reduce the HOMO energy levels of the copolymers and thus enhance the V_{oc} of photovoltaic device. In addition, the band gap of corresponding copolymer has not suffered from obvious increase after incorporating Tz unit [30]. This suggests us to design new Tz-based SMs to achieve high V_{oc} without significant losses in J_{sc} .

On the other hand, BDT is one of the most commonly employed electron donating building block of conjugated polymer materials for organic optoelectronic applications, especially for OSCs devices [31–33]. Because its relatively large and planar conjugated structure greatly enhance facial π - π stacking of the molecules, thus it benefit charge transportation and red shift of the absorption spectra of these conjugated polymers. The unique properties of BDT structure leads to the BDT-based polymer possess the advantage of not only high hole mobility in field effect transistor (FET) but also high PCE in OSCs. Therefore, the BDT is a promising electron donating unit in designing novel organic molecules for high performance photovoltaic cells.

In this paper, we designed and synthesized two new organic molecules with a D2-A-D1-A-D2 architecture, where D1 is BDT structure as a center and electron donating unit, thiophene or bithiophene as π -bridge, A is Tz as an electron withdrawing unit, and D2 is bithiophene or terthiophene as a electron donating unit and π -conjugation extender. We investigated the effects of π -bridge length and end groups on absorption, energy level and photovoltaic properties of these molecules. The photovoltaic devices fabricated from the two SMs with a structure of ITO/PEDOT/SM:PC₇₁BM/LiF/Al afforded PCEs of 5.01% and 5.29% under one sun of AM 1.5 solar simulator illumination (100 mW/cm^2). It is worthwhile to mention that the high V_{oc} s of 0.88 and 0.98 V derived from these devices due to the deep HOMO energy levels of these two molecules.

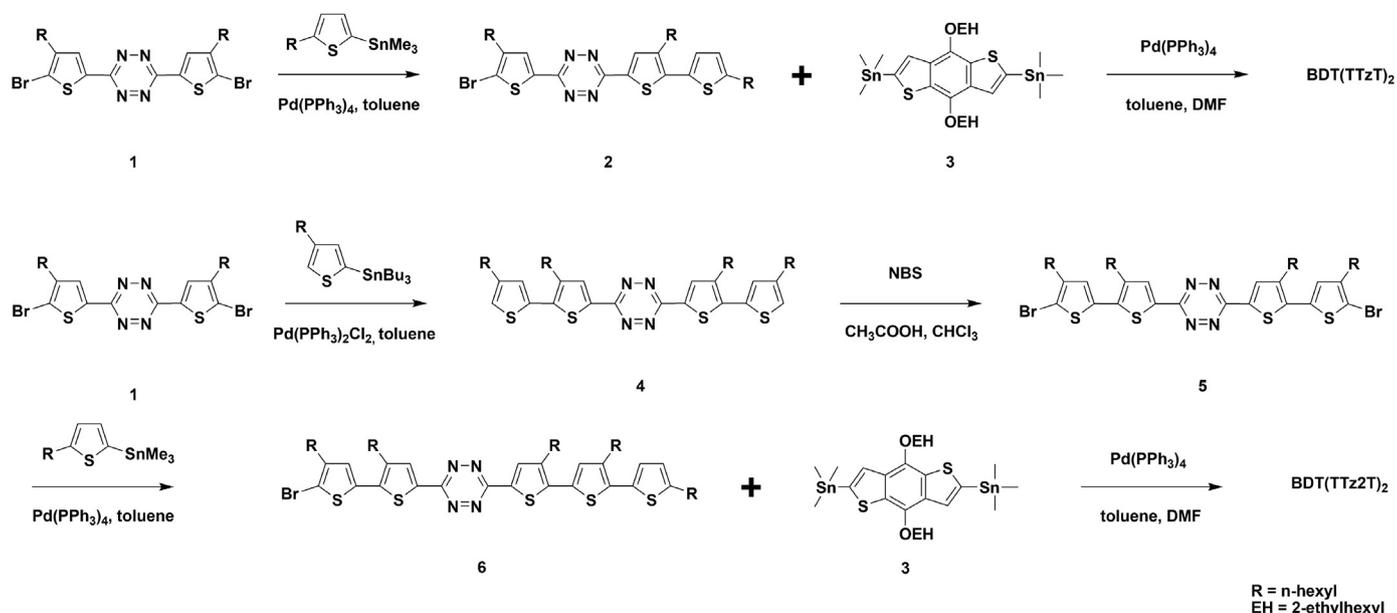
2. Results and discussion

2.1. Synthesis and characterization

The synthesis routes of these two D2-A-D1-A-D2 type SMs are presented in Scheme 1. Compounds 1 [27] and 3 [31] were synthesized according to the references. The new intermediate compound 2 and 6 were synthesized via stille coupling reaction between compound 1 or compound 5 and trimethyl(5-hexylthiophene-2-yl)stannane [34,35] using $\text{Pd}(\text{PPh}_3)_4$ as catalyst. Bromination of 4 with *N*-bromosuccinimide afforded compound 5 in a mixture of chloroform and acetic acid with a yield of 88%. At last, compound 3 was reacted with compounds 2 and 6 to obtain the two SMs BDT(TTzT)₂ and BDT(TTz2T)₂ though Stille coupling reaction. These synthesized molecules exhibited good solubility in common organic solvents such as dichloromethane, chloroform, and chlorobenzene at room temperature, which provides the solution-processed thin films for photovoltaic applications Fig. 1.

2.2. Optical properties

The UV–vis absorption spectra of the synthesized molecules in dilute chloroform solution and in solid films are shown in Fig. 2, and the main optical properties are summarized in Table 1. Both molecules exhibited a relatively broad absorption range covering the wavelength from 300 to 600 nm in solution. The maximum absorption (λ_{max}^{sol}) of BDT(TTz2T)₂ was 489 nm, which was red-shifted by 10 nm compared with that of BDT(TTzT)₂, because the extending π -bridge and end group in BDT(TTz2T)₂ backbone lead to extending molecular conjugated length. The molar absorption coefficients of BDT(TTz2T)₂ solution is $1.27 \times 10^5 \text{ M}^{-1} \text{ cm}^{-1}$ at the maximum absorption wavelength, quite larger than $7.29 \times 10^4 \text{ M}^{-1} \text{ cm}^{-1}$ of BDT(TTzT)₂ solution. Fig. 2(b) shows optical absorption spectra of thin film of these molecules. The absorption spectra of thin films exhibit broader response range than that in solution. The maximum absorption peaks of thin films are red-shifted 49 and 43 nm respectively compared with that in solution, and thus indicating a strong intermolecular π - π interaction in solid state [36]. The absorption coefficients of thin film of



Scheme 1. Synthetic routes of BDT(TTzT)₂ and BDT(TTz2T)₂.

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