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Synthesis and photovoltaic properties of conjugated polymers with an asymmetric 4-(2-ethylhexyloxy)-8-(2-ethylhexylthio)benzo[1,2-*b*:4,5-*b*′]dithiophene unit

Yuanshuai Huang, Fen Wu, Min Zhang, Suli Mei, Ping Shen, Songting Tan*

College of Chemistry, and Key Laboratory of Environmentally Friendly Chemistry and Applications of Ministry of Education, Xiangtan University, Xiangtan 411105, PR China

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ABSTRACT

Two novel copolymers containing an asymmetric 4-(2-ethylhexyloxy)-8-(2-ethylhexylthio)benzo[1,2-*b*:4,5-*b*′]dithiophene and different conjugated side groups were designed and synthesized for polymer solar cell applications. The thermal, optical, and electrochemical properties were investigated by thermal gravimetric analysis, UV–Vis absorption, and cyclic voltammetry, respectively. The two copolymers showed a good thermal stability and solubility in common organic solvents, and relatively deep highest occupied molecular orbital (HOMO) energy levels with the values of −5.56 eV for 5,6-difluoro-benzodiathiazole-based copolymer and −5.48 eV for isoindigo-based copolymer. The polymer photovoltaic devices based on 5,6-difluoro-benzodiathiazole-based polymer/phenyl-C_{71}-butyric acid methyl ester exhibited a high open circuit voltage (V_{oc}) of 0.92 V and the power conversion efficiency of 5.0%.

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1. Introduction

Polymer solar cells (PSCs) based on blends of conjugated polymers and fullerene derivatives have received great attention as renewable energy sources for their compatibility with fabricating large-area, flexible, and cost-effective devices via roll-to-roll processing techniques [1–9]. The power conversion efficiencies of polymer bulk heterojunction (BHJ) solar cells have recently exceeded 10% because of significant developments in conjugated polymers and device technologies [10–14]. However, the low PCE is still the largest challenge in commercial application of PSCs. Consequently, the improvement of the PCE by the synthesis of novel materials is the key aim in PSCs [15–20].

The most powerful strategy to design a low band gap conjugated polymer is to incorporate electron-rich donor (D) and electron-deficient acceptor (A) segments to form internal donor-acceptor (D-A) structures, because the absorption range of the polymers can be extended to longer wavelengths and their electronic properties can be easily tuned by varying the donor and acceptor segments [21,22]. Based on this strategy, a new family of polymers with conjugated side groups has been developed by several research groups [23–28]. This type of polymers featured deep HOMO energy levels and high absorption coefficients owing to the overlapping of the conjugated side chains interactions with the conjugated main chains, which demonstrated prominent device performances in PSCs [23].

Among the various conjugated polymers, alternating copolymers based on dialkoxy-substituted benzo[1,2-*b*:4,5-*b*′]dithiophene (**BDT**) units have attracted considerable interest as electron-donating building blocks in PSCs application, due to their excellent features including structural symmetry, planarity as well as rigid and π-extended conjugation, which enhance electron delocalization and intermolecular interactions to improve charge mobility [29–34]. Based on these copolymers, the power conversion efficiency (PCE) over 8% were obtained [35]. It was reported that a dialkylthio-substituted **BDT** homopolymer was developed with deep HOMO energy level resulting in a high V_{oc} up to 0.99 V [36]. In addition, BHJ polymer solar cells based on dialkylthio-substituted **BDT** showed the hitherto reported a high PCE of 9.3% [37]. After an extensive investigation on the **BDT**, asymmetric 4-(2-ethylhexyloxy)-8-(2-ethylhexylthio)benzo[1,2-*b*:4,5-*b*′]dithiophene (**SBDT**), as a structural hybrid of 4,8-bis(2-ethylhexyloxy)benzo[1,2-

* Corresponding author.
E-mail address: tanst2008@163.com (S. Tan).

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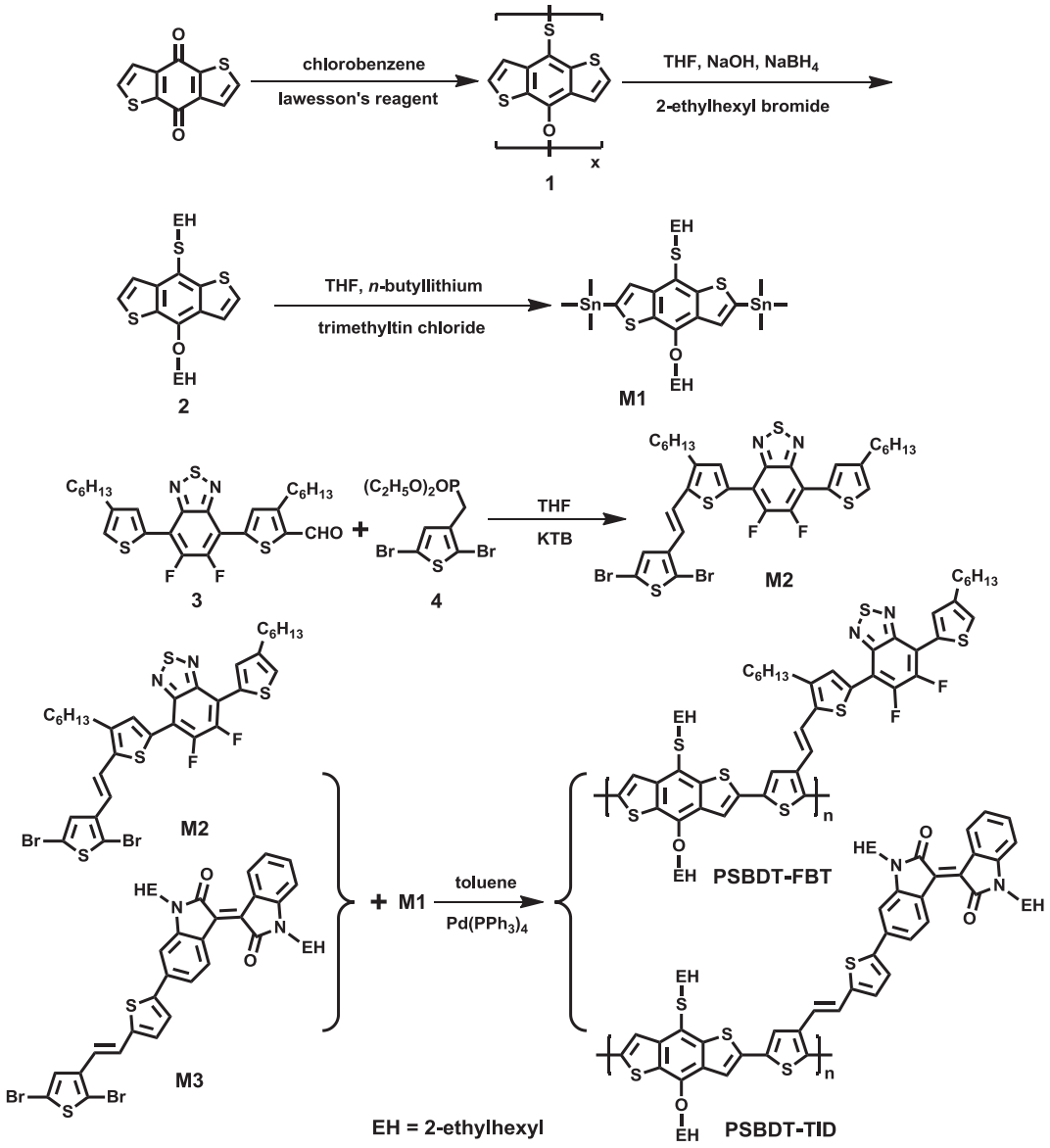
b:4,5-*b*′]dithiophene (**DOBDT**) and 4,8-bis(2-ethylhexylthio)benzo[1,2-*b*:4,5-*b*′]dithiophene (**DSBDT**), has not yet been explored. Our keen interest in **SBDT**-based chromophores stems from the assumption that they show remarkably different optoelectronic properties from **DOBDT** and **DSBDT** derivatives by replacement of an oxygen atom with a sulfur atom in the **DOBDT**. The sulfur atom plays an important role in **SBDT** molecules. The electron-donating ability of sulfur is weaker than oxygen resulting from the poorer overlap of its orbitals with the π-system on the polymer backbone. Furthermore, it is also amenable to further transformation to highly electron-withdrawing sulfoxide or sulfone functionality. Most importantly, it can be anticipated the excellent properties of the **SBDT** for PSCs applications, because sulfur and oxygen possess similar electronic properties. Finally, a synergetic effect of 2-ethylhexylthio and 2-ethylhexyloxy in the **SBDT** molecules is of great importance.

Herein, two new conjugated copolymers (**PSBDT**–**FBT** and **PSBDT**–**TID**) based on asymmetric **SBDT** were synthesized via a Stille coupling reaction (Scheme 1). In the molecular structures, **SBDT** and thiophene units were alternated to form the conjugated main chain and 5,6-difluoro-4,7-bis(4-(2-ethylhexyl)thiophen-2-yl)benzo[c][1,2,5]thiadiazole (**DTffBT**) groups or 6-(thiophen-2-yl)-di(2-ethylhexy)isoindigo (**TID**) groups were pended onto the thiophene units to build a side group by the linkage of a vinyl unit. The 2-ethylhexylthiol and 2-ethylhexyloxy on the **SBDT** could enhance solubility and affect optoelectronic properties. Therefore, the photophysical, electrochemical, and photovoltaic properties of the copolymers were investigated fully.

2. Experimental details

2.1. Materials and synthesis

All the chemicals were purchased from Alfa Aesar and Chem Greatwall Chemical Company (Wuhan, China) and used without further purification. THF and toluene were refluxed over sodium and benzophenone and distilled. All other commercially available materials were used as received unless noted otherwise.



Scheme 1. Synthetic routes and chemical structures of the copolymers.

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