

Chemical optimization of benzo-dithiophene and benzo-[2,1,3]thiadiazole copolymers for the high performance, green-solvent-processed polymer solar cells

YunXiang Chen^a, Guofeng You^a, Xinyu Lin^a, Xiyue Yuan^b, Ding Zou^a, Wen Wang^a, Renqing Yang^b, Hongyu Zhen^{a,*}, Qidan Ling^{a,*}

^a College of Chemistry and Materials Science, Fujian Key Laboratory of Polymer Materials, Fujian Normal University, Fuzhou 350007, PR China

^b CAS Key Laboratory of Bio-based Materials, Qingdao Institute of Bioenergy and Bioprocess Technology, Chinese Academy of Sciences, Qingdao 266101, PR China

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ABSTRACT

In this work, we demonstrate the chemical optimization of benzo[1,2-b:4,5-b']dithiophene (BDT)-5,6-difluorobenzo-[2,1,3]thiadiazole (FBT) D-A alternating copolymer for obtaining the efficient polymeric donors for the environment-friendly solution processed polymer solar cells (PSCs). Three polymers PBTF, PBTF-C₆ and PBTF-H, in which one or two alky thiophene units are inserted into the backbone of BDT-FBT alternating copolymer, present much different performances either in the PSCs processed from halogenated solvent and additive or in the PSCs processed from non-halogenated solvent and additive. With an alky thiophene and a bare thiophene as the spacer, PBTF-H performs best among the three. Especially when the devices processed from 1,2,4-trimethylbenzene and diphenyl ether, in which the highest PCE of 6.80% is achieved with a V_{oc} of 0.77 V, a J_{sc} of 13.67 mA cm⁻² and a FF of 64.2%. We think these results will cast light on developing new polymeric donors of the green-solvent-processed PSCs.

1. Introduction

Polymer solar cells (PSCs) have attracted a great deal of attention due to their distinctive advantages, including light weight, mechanical flexibility/stretchability, and solution-based device fabrication techniques, such as inkjet printing and roll-to-roll coating (Yu et al., 1995; Zhou et al., 2012; Lin et al., 2012; Chen et al., 2013; Kim et al., 2015). Recent years, there are rapid developments of materials and devices in the field of PSCs, power conversion efficiency (PCE) of bulk heterojunction (BHJ) PSCs has been promoted to be over 13% (Casey et al., 2015; Lin et al., 2015; Zhang et al., 2015; Li et al., 2016; Zhao et al., 2016a, 2016b; Kan et al., 2017; Li et al., 2017; Zhang et al., 2017; Zhao et al., 2017a, 2017b). But the efficient devices were always processed from the halogenated solvents, such as chloroform (CF), chlorobenzene (CB) and 1,2-dichlorobenzene (O-DCB). Together with the solvent, additives that contain halogenated elements like 1,8-diiodooctan (DIO), and 1-chloronaphthalene (1-CN) are also employed to improve morphology of active layers (You et al., 2013; Liu et al., 2014). Solvents and additives are the primary condition for the formation of optimal BHJ morphology, which is attributed to miscibility/solubility and interaction between donor, acceptor, solvent and additive (Chen et al., 2009;

Deng et al., 2015; Fan et al., 2017). PSC is considered as a green energy source, but halogenated solvents and additives are toxic and environment unfriendly (Ceballos et al., 2014; Chen et al., 2014). Therefore, developing efficient PSCs that can be processed from environment-friendly solvents and additives is necessary (Deng et al., 2015; Cai et al., 2015; Zhao et al., 2015b; Duan et al., 2016; Farahat et al., 2016; Park et al., 2017; Wu et al., 2017). There are many successful examples that employing non-halogenated solvents (Zhang et al., 2017; Chen et al., 2009; Deng et al., 2015; Cai et al., 2015), but it is still required intensive study on the chemical modification of the high efficiency donor for different kinds of solvents, especially for the non-halogenated ones.

Designing donor (electron-rich) and acceptor (electron-deficient) alternating copolymers to form an internal charge transfer system is a promising strategy for the achievement of efficient PSCs (Chu et al., 2011; Casey et al., 2015; Blouin et al., 2008; Zhou et al., 2010; McCulloch et al., 2012; Mo et al., 2017; Sung et al., 2017; Li et al., 2018). Employing alkyl side chain to the backbone of the polymer is necessary to increase solubility in organic solvent and miscibility with acceptor (Hu et al., 2015). Length, size and the substitution position of alkyl chain can significantly affect the solubility, steric hindrance, charge mobility and intermolecular stacking of polymeric donors

* Corresponding authors.

E-mail addresses: rainy_ch@126.com (H. Zhen), qdling@fjnu.edu.cn (Q. Ling).

(Stevens et al., 2011; Zhao et al., 2015a; Huang et al., 2016; Qin et al., 2018). Furthermore, the insertion of one thiophene unit as a spacer between donor and acceptor unit can promote the planarity of the polymer backbone effectively (Wang et al., 2013; Gao et al., 2016). On the whole, the chemical optimization on alkyl chains and spacers of donor polymers is an eternal issue of PSCs.

In this work, three polymers named by PBTF, PBTF-C₆ and PBTF-H were synthesized and studied, in which different number of thiophene with and without alkyl side chains were incorporated into the backbone of benzo[1,2-b:4,5-b']dithiophene (BDT)-5,6-difluorobenzo[2,1,3]thiadiazole (FBT) D-A alternating copolymer. PBTF possesses the simplest chemical structure, in which 2-octyldodecyl (2-OD) substituted thiophene were inserted between BDT and FBT unit. One thiophene unit with and without a hexyl chain was added into backbone of PBTF, the resulting polymers are called by PBTF-C₆ and PBTF-H respectively. Two solvent-additive systems, the halogenated O-DCB doped with DIO and the non-halogenated 1,2,4-trimethylbenzene (TMB) doped with diphenyl ether (DPE), were used for the formation of BHJ. Due to the modification in the spacer, three polymers presented distinctly different photovoltaic effect in their PSCs processed from any agent system. PBTF:PC₇₁BM based PSCs presented close PCEs in the range of 4–5% when processed from both agent systems. For the other two polymers, PCE of the PSCs increased from 1.28% of PBTF-C₆ to 5.85% of PBTF-H by using O-DCB and DIO,

which is attributed to the steric hindrance of the hexyl side chain. More interesting, the PSCs based on PBTF-H:PC₇₁BM exhibited more promising device performances when processed from TMB and DPE, in which the highest PCE of 6.80% was achieved with a V_{OC} of 0.77 V, a J_{SC} of 13.67 mA cm⁻² and a FF of 64.2%. To find out the structure-property-device performance relationships, the study on molecular conformations, photophysical and electrochemical properties, charge transport and morphology of BHJ were carried out.

2. Experimental section

2.1. Materials and synthesis

All the starting materials were purchased from SunaTech Inc. Acceptor PC₇₁BM was purchased from American Dye Source Inc. Toluene was fresh distilled from CaH₂. Other solvents and reagents were commercially available and used as received, unless otherwise specified.

The synthesis routes of polymers are shown in Fig. 1. PBTF was synthesized via Stille coupling reaction between 4,7-bis(5-bromo-4-(2-octyldodecyl)thiophen-2-yl)-5,6-difluorobenzo[1,2,5]thiadiazole (1) and (4,8-bis(5-(2-ethylhexyl)thiophen-2-yl)benzo[1,2-b:4,5-b']dithiophene-2,6-diyl)bis(trimethylstannane) (2) with Pd₂(dba)₃ as the catalyst and P(o-tol)₃ as the ligand in toluene. 5,6-difluoro-4,7-bis(4'-hexyl-3-

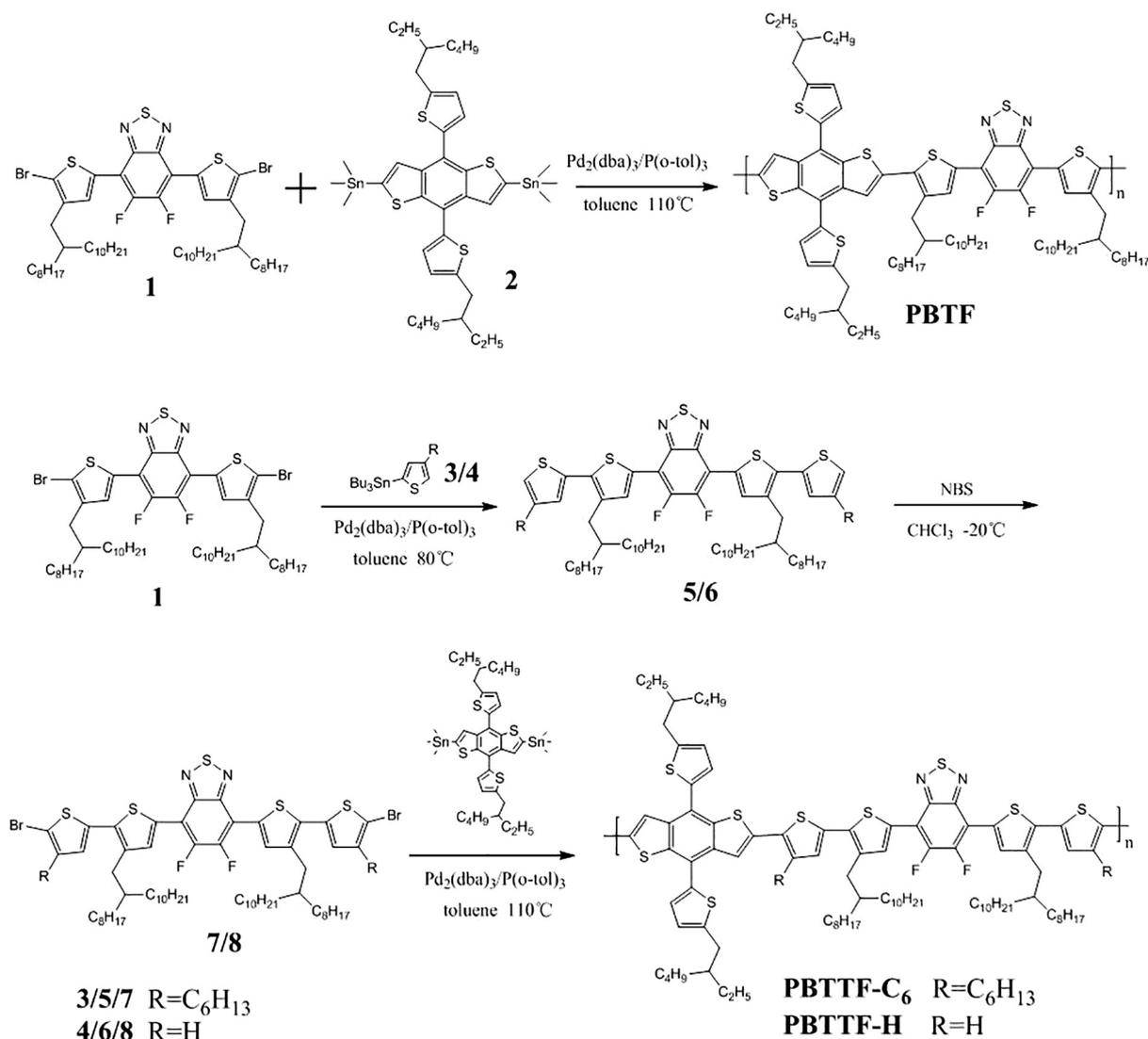


Fig. 1. Synthetic route and chemical structures of PBTF, PBTF-C₆ and PBTF-H.

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