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Solar Energy Materials & Solar Cells

journal homepage: www.elsevier.com/locate/solmat

Toward high open-circuit voltage by smart chain engineering in 2D-conjugated polymer for polymer solar cells

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ARTICLE INFO

Article history:

Received 25 November 2015

Received in revised form

14 January 2016

Accepted 17 January 2016

Keywords:

Polymer solar cells

2D-conjugated polymer

Molecular energy levels

Electron-donating side-chains

ABSTRACT

Two electron-donating side chain (octylthio and methoxy) were strategically attached on BDTT unit to develop two new polymers (**PBDTT-OS-TT-EF** and **PBDTT-OS-TT-CF**) as donor materials for polymer solar cells. **PBDTT-OS-TT-EF** and **PBDTT-OS-TT-CF** show broad absorption spectra with narrow optical band-gap of 1.52 and 1.56 eV, and low-lying HOMO energy level of -5.34 and -5.46 eV, respectively. A high V_{oc} of 0.92 V was obtained from the PSC devices based on **PBDTT-OS-TT-EF**. Particularly, the V_{oc} of PSC device based on **PBDTT-OS-TT-CF** is as high as 1.00 V, which is the highest value for the devices based on TT-base polymers. The results indicate that the engineering two electron-donating side chains in BDTT unit is an effective strategy to narrow the band-gap and manipulate the energy levels of polymers, which can be potentially applied to design polymer donor materials with high V_{oc} values.

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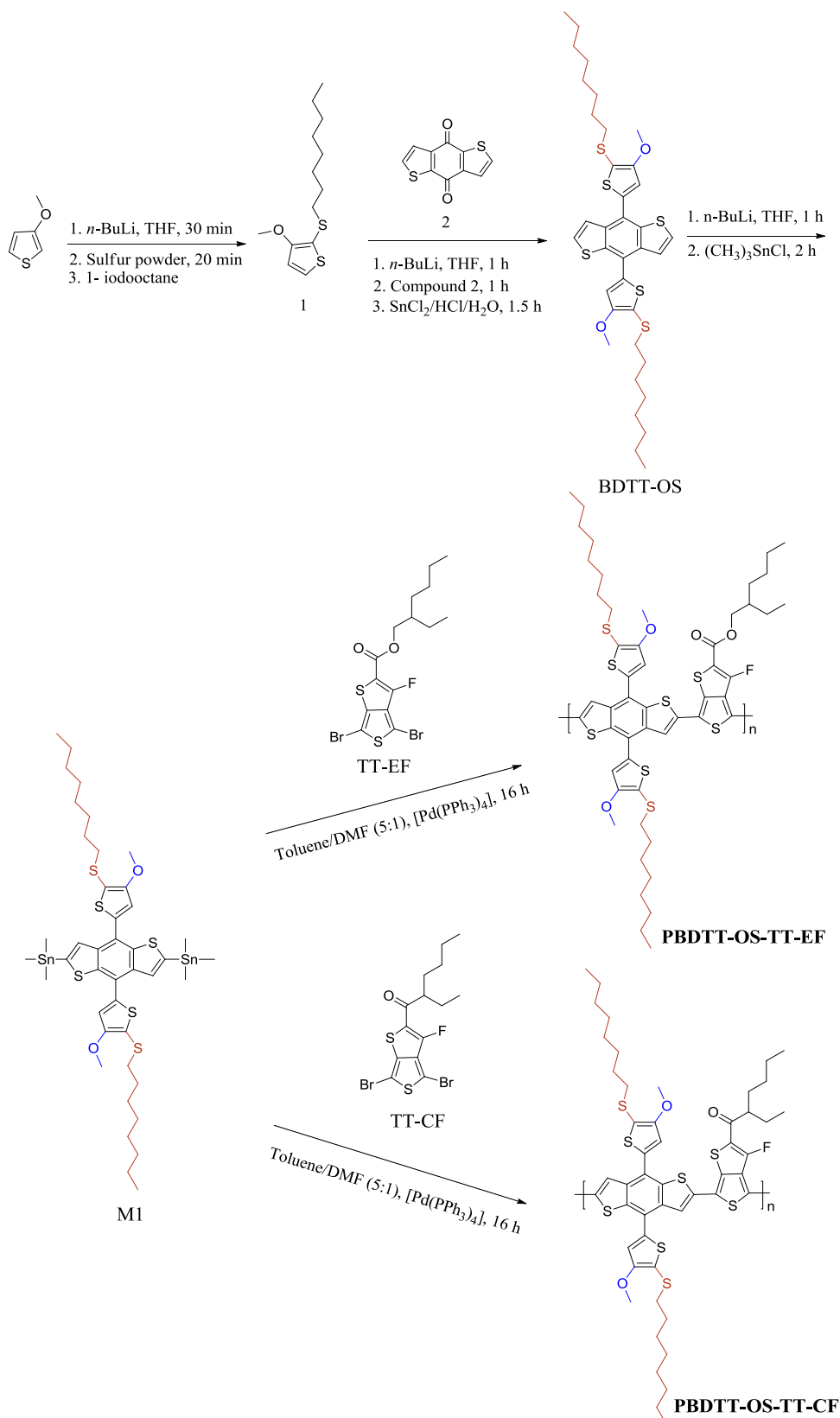
1. Introduction

Polymer solar cells (PSCs) have emerged as a promising outlook for low-cost renewable energy technology due to their unique advantages of light weight, easy fabrication and the capability to be produced on large area flexible substrates [1–4]. Conjugated polymer donor and fullerene derivative acceptor are the key photovoltaic materials in the photoactive layer of the PSCs. Photovoltaic materials innovation, especially the innovation of polymer donor materials plays very important role in driving the power conversion efficiency (PCE) of PSCs rapidly increasing from below 1% to over 10% in the past decades [5–11]. The PCE of PSCs is proportional to the values of open-circuit voltage (V_{oc}), short-circuit current density (J_{sc}), and fill factor (FF) of the devices. The key issues of molecular design for photovoltaic materials include engineering the band-gap and energy levels to achieve high J_{sc} and V_{oc} , enhancing planarity to attain high charge carrier mobility [1,6,12–15]. Especially, energy levels of photovoltaic materials play an important role in device performance. The gap between the LUMO (lowest unoccupied molecular orbital) level of the acceptor and the HOMO (highest occupied molecular orbital) level of the

donor determines the V_{oc} value, and the offset of LUMO or HOMO between the donor and acceptor materials provide driving force for the exciton dissociation which closely relate to the values of J_{sc} and FF [16–19]. Therefore, engineering suitable energy levels of polymer donor materials is crucial in material design, and several molecular design strategies have been developed to address this issue. For example, it is fairly easy to manipulate the energy levels of polymers by constructing the conjugated backbone via the donor–acceptor (D–A) approach, since the HOMO level is mainly located at the donor unit and the LUMO is mainly located at the acceptor unit in such D–A copolymer systems [19–22]. Introducing varied electronegativity groups such as carbonyl [23,24], ester [25] and fluorine [26–29] also effectively reduce the HOMO of the resulting polymers. Besides, flexible side-chains also play an important role in influencing the electronic energy levels of conjugated polymers [30–34]. Recently, we employed alkylthio side-chain into thienyl-substituted benzodithiophene (namely BDTT-S) to develop a new two-dimension (2D)-conjugated copolymer (namely PBDTT-S-TT), and the HOMO energy level of PBDTT-S-TT was effectively down-shifted by 0.11 eV in comparison with PBDTT-TT [35]. As a result, PBDTT-S-TT-based device yielded a high V_{oc} of 0.84 V, leading to a higher PCE of 8.42%. The results demonstrated a simply strategy to enhance the V_{oc} value of the polymers. On the other hand, the engineering of alkoxy side chain benefits to red-shift the absorption of the resulting polymer [35].

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

Considering the fact that the promising side-chain effect on down-shifting HOMO energy level and broadening absorption of polymer donor materials so that enhancing V_{oc} and J_{sc} of the PSCs, we attach two side chains of octylthio and methoxy on thiophene

conjugated side chain of BDTT unit (designated as BDTT-OS, as shown in [Scheme 1](#)) in the polymer donor. Linear octylthio and methoxy groups were chosen for reducing the molecular steric hindrance. 1-(4,6-Dibromo-3-fluorothieno[3,4-*b*]thiophen-2-yl)-2-

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