Nano Energy 40 (2017) 495–503

Contents lists available at ScienceDirect

Nano Energy

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

Full paper

Single-junction fullerene solar cells with 10% efficiency and high open-circuit voltage approaching 1 V

Dangqiang Zhu[a,1], Xichang Bao[a,1], Dan Ouyang[a,1], Junyi Wang[a], Xiyue Yuan[a], Qian Wang[b], Di Zhou[a], Shuguang Wen[a], Renqiang Yang[a,c,*]

[a] CAS Key Laboratory of Bio-based Materials, Qingdao Institute of Bioenergy and Bioprocess Technology, Chinese Academy of Sciences, Qingdao 266101, China
[b] College of Materials Science and Engineering, Harbin University of Science and Technology, Harbin 150080, China
[c] State Key Laboratory of Luminescent Materials and Devices, South China University of Technology, Guangzhou 510641, China

ARTICLE INFO

Keywords:
Polymer solar cell
Thieno[3, 4-*b*]thiophene
D-A(π)-Q-A(π) type
High open-circuit voltage

ABSTRACT

It has been proven that the introduction of F atom and the replacement of alkyl side-chain with alkylthio substituent could be the effective side-chain strategies, to obtain the deep highest occupied molecular orbital (HOMO) energy level with little influence on the optical absorption, and in turn, the small photo energy loss (E_{loss}). In this work, we combine the advantages of D–A(π)–Q–A(π) strategy and the above side chain engineering, to construct a series of high-performance polymers P1-P3 with high open-circuit voltage (V_{OC}) of exceeding 0.90 V in the conventional solar cells. Meanwhile, small E_{loss}s of 0.73–0.78 eV are achieved accompanying high V_{OC} and almost unchanged optical bandgaps of ~ 1.70 eV, which are the smaller values in comparison with that of the other high-performance polymer systems. More encouragingly, P2-based solar cells exhibit high PCE of 10.30% and V_{OC} of 0.97 V, which is one of the highest values for polymer/fullerene based solar cells. Our work not only demonstrates a series of high-efficiency new materials, but also strongly confirms that the combination of D–A(π)–Q–A(π) arrangement and rational side chain engineering is a very promising strategy to construct high-performance photovoltaic polymers with reduced energy loss.

1. Introduction

Polymer solar cells (PSCs) would be a promising renewable energy technology due to the advantages of large-area fabrication of flexible photovoltaic modules via ease of solution processing and low energy payback time [1–3]. In the past few years, the bulk heterojunction (BHJ) PSCs have undergone rapid developments in new light-harvesting polymers, interfacial engineering, and device processing technologies, and in turn, the power conversion efficiency (PCE) of over 11% has been reported in the single-junction fullerene-based solar cells [4]. Moreover, open-circuit voltage (V_{OC}) is one important parameter that determines the photovoltaic efficiency, and high V_{OC} could be more desirable in the multi-junction PSCs or under low light intensity for practical applications [5]. Generally, V_{OC} is closely related to the active materials in organic photovoltaic devices under traditional device processing. Among the representative high-performance PSCs (PCE > 9%) with various optical bandgaps as shown in Fig. 1 [4,6–29], photovoltaic devices with PCEs exceeding 10% based on low bandgap PBDTTT or PBT*n*T family only exhibit moderate V_{OC} of ~ 0.80 V [4,6–11]. In contrast, high V_{OC} of > 0.9 V usually can be found in wide bandgap polymers-based solar cell (E_g of ≥ 1.80 eV) [24–31], and only a few polymers exhibited the V_{OC} over 1.0 V but with relatively low PCEs of < 8% [32–34]. Moreover, photo energy loss ($E_{loss} = E_g - eV_{OC}$) according to the optical bandgap of the main light-harvesting materials (here means donor polymers for fullerene-based solar cells) is an important factor to evaluate the performance of active materials. As far as experience is concerned, the minimum E_{loss} of 0.6 eV could realize efficient charge generation and high external quantum efficiency (EQE) [35,36], and decreasing E_{loss} will be in favor of high V_{OC} at the same optical bandgap. However, the typical efficient polymers with high V_{OC} usually exhibit large E_{loss} of 0.8–0.9 eV as shown in Fig. 1. Therefore, in order to get further breakthroughs in the PCE and V_{OC} of PSCs, developing new light-harvesting polymers with low energy loss is an effective strategy and becomes particularly important.

In our previous work, a new D–A(π)–Q–A(π) construction strategy with incorporating weak acceptor unit as π bridge into the main

* Corresponding author at: CAS Key Laboratory of Bio-based Materials, Qingdao Institute of Bioenergy and Bioprocess Technology, Chinese Academy of Sciences, Qingdao 266101, China.
E-mail address: yangrq@qibebt.ac.cn (R. Yang).
[1] These authors contributed equally to the paper.

http://dx.doi.org/10.1016/j.nanoen.2017.08.062
Received 18 July 2017; Received in revised form 22 August 2017; Accepted 31 August 2017

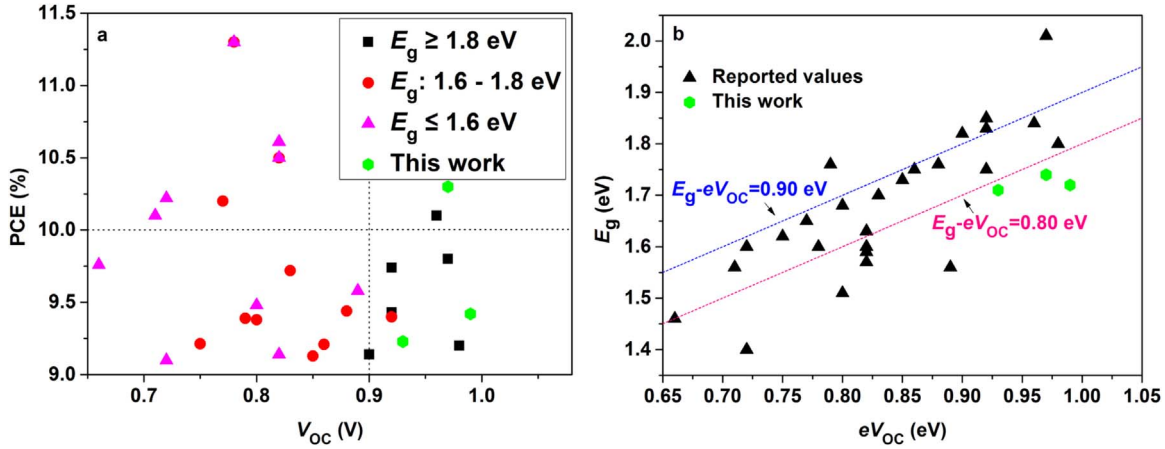
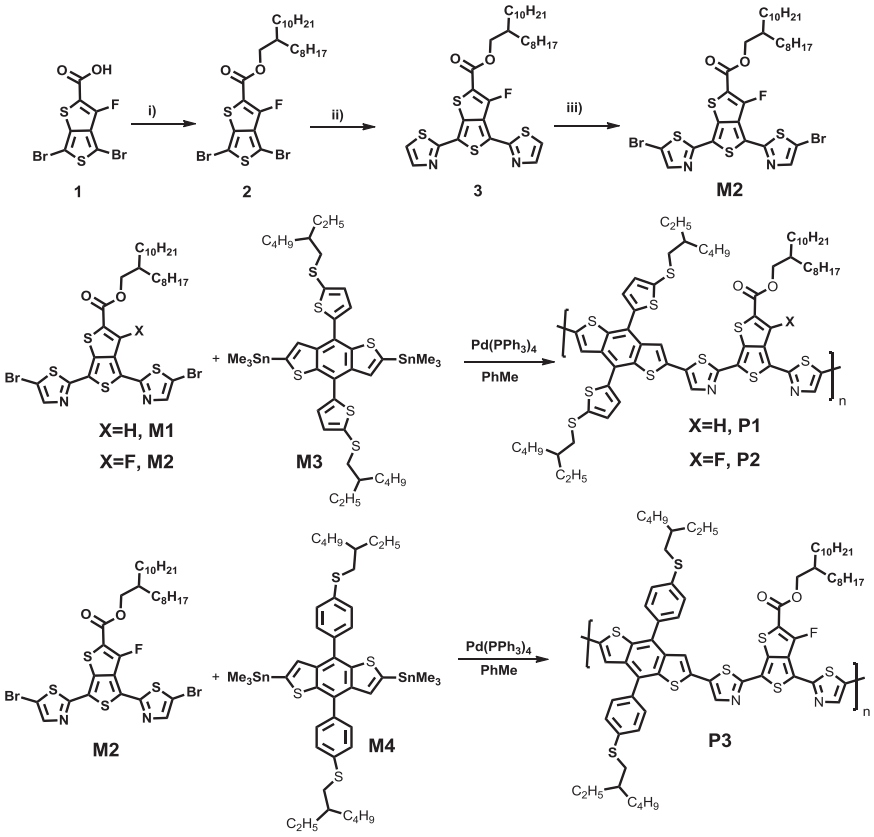


Fig. 1. Maximum PCE vs V_{OC} (a) and E_g vs eV_{OC} (b) for reported highly efficient polymer solar cells (the details are shown in Table S1).



Scheme 1. Synthetic routes of the monomers and polymers.

backbone of the quinoid polymer was proposed, which combines the advantages of employing the A unit to decrease the highest occupied molecular orbital (HOMO) energy level and the Q unit to maintain the broad optical absorption. The new polymer PTBTz-2 exhibits high efficiency of 9.72%, significantly higher than that of the reference polymer PBDTTT-E-T just without π-spacer (6.21%), but with high energy loss of 0.87 eV calculated from the optical bandgap of 1.70 eV and optimal V_{OC} of 0.83 V [37]. In many D-A systems, it has been proven that the strategy of replacement of alkyl side chain with alkylthio substituent could increase V_{OC} with little influence on the optical absorption. Li reported the alkylthio substituted polymer PBDTT-S-TT, which exhibits the nearly same optical bandgap of ~1.57 eV to that of analog PBDTT-TT with alkyl side chain. However, PBDTT-S-TT-based devices exhibit the V_{OC} of 0.84 V, higher than that of PBDTT-TT (0.77 V), resulting in a decreased E_{loss} of 0.07 eV [38]. In addition, fluorine (F) atom also plays an important role in decreasing E_{loss}. Compared with PTB5 just without F substituent, the polymer PTB4 with F atoms shows a higher V_{OC} and a decreased E_{loss} of 0.08 eV [11]. Employing the above strategies and side chain engineering, three new polymers P1, P2, and P3 (see Scheme 1) were designed and synthesized upon the introduction of fluorine (F) atom on TT, and the replacement of alkyl side-chain thiophene with alkylthio thiophene or benzene. The devices based on the three polymers with conventional structures show high V_{OC} of > 0.93 V, especially, it can reach 0.99 V for P3-based solar cells, and their E_{loss}s (0.73–0.78 eV) were markedly decreased, which were rarely reported in the present high-performance systems with E_gs > 1.70 eV. More encouragingly, P2-based photovoltaic device showed a PCE of 10.30% and V_{OC} of 0.97 V, both are among the highest values for polymer/fullerene solar cells. Our work not only demonstrates a series of high-performance donor polymers with high V_{OC} and