Organic Electronics 15 (2014) 2270–2276

Contents lists available at ScienceDirect

Organic Electronics

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

Towards high-efficiency non-fullerene organic solar cells: Matching small molecule/polymer donor/acceptor

Pei Cheng [a,c], Xingang Zhao [a], Weiyi Zhou [a], Jianhui Hou [a], Yongfang Li [a], Xiaowei Zhan [b,*]

[a] Beijing National Laboratory for Molecular Sciences and CAS Key Laboratory of Organic Solids, Institute of Chemistry, Chinese Academy of Sciences, Beijing 100190, China
[b] Department of Materials Science and Engineering, College of Engineering, Peking University, Beijing 100871, China
[c] University of Chinese Academy of Sciences, Beijing 100049, China

ARTICLE INFO

Article history:
Received 22 May 2014
Received in revised form 19 June 2014
Accepted 20 June 2014
Available online 7 July 2014

Keywords:
Organic solar cells
Non-fullerene
Morphology
Charge transfer
Charge transport

ABSTRACT

Two low band-gap donors, small molecule p-DTS(FBTTh$_2$)$_2$ (S_D) and polymer PBDTTT-C-T (P_D), and two perylene diimide acceptors, small molecule PDI-2DTT (S_A) and polymer PPDIDTT (P_A), were used to fabricate non-fullerene organic solar cells. The effects of four donor/acceptor combinations, P_D/P_A, P_D/S_A, S_D/S_A and S_D/P_A, on the morphology, charge transfer, charge transport and photovoltaic performance were investigated. Power conversion efficiencies (PCEs) of P_D/P_A, P_D/S_A, S_D/S_A and S_D/P_A were 3.04%, 0.28%, 2.52% and 0.29%, respectively. The P_D/P_A blend and S_D/S_A blend exhibited relatively uniform and continuous morphology, efficient photoinduced charge transfer, high mobility and balanced charge transport relative to P_D/S_A and S_D/P_A blends, leading to much higher PCEs.

1. Introduction

Solar cells are one of the best candidates to overcome traditional energy depletion and environmental pollution. Especially, organic solar cells (OSCs) have been the focus of research in the past decade due to some advantages, such as simple and large area preparation, low cost, light weight, and flexibility [1–10]. Nowadays, bulk heterojunction (BHJ) OSCs based on interpenetrating networks of polymer donors and fullerene acceptors have shown the best performance with power conversion efficiencies (PCEs) that exceed 9% for single-junction devices [11–14] and 10% for tandem devices [15–17].

Fullerene derivatives are widely used as electron acceptors in OSCs duo to their high electron mobility [18], ultrafast photoinduced charge transfer at donor/acceptor (D/A) interfaces [3], and good ability to form favorable nanoscale network with donor polymers [19]. However, fullerene derivatives have some disadvantages. For instance, as a widely used fullerene acceptor, [6,6]-phenyl-C61-butyric-acid-methyl-ester ($PC_{61}BM$) exhibits weak absorption in the visible region; relatively low lowest unoccupied molecular orbital (LUMO) energy level (*ca.* −3.91 eV [20]) which decreases the open circuit voltage (V_{OC}); and easy aggregation which reduces long-term stability of devices [21].

In recent years, people have developed a number of small molecule and polymer non-fullerene electron acceptors [19,22–25] consisting of perylene diimide (PDI) [26–39], naphthalene diimide (NDI) [40–46], benzothiadiazole (BT) [47–53] and other electron-deficient groups [54–66]. The non-fullerene OSCs, which consist of a p-type semiconducting polymer or small molecule as an electron donor and an n-type semiconducting polymer or non-fullerene small molecule as an electron acceptor, have some advantages over fullerene based solar cells. Firstly, these non-fullerene acceptors can achieve broad and strong absorption via molecule design. Secondly, their LUMO energy levels can be adjusted to achieve a suitable charge

* Corresponding author.
E-mail address: xwzhan@pku.edu.cn (X. Zhan).

http://dx.doi.org/10.1016/j.orgel.2014.06.025
1566-1199/

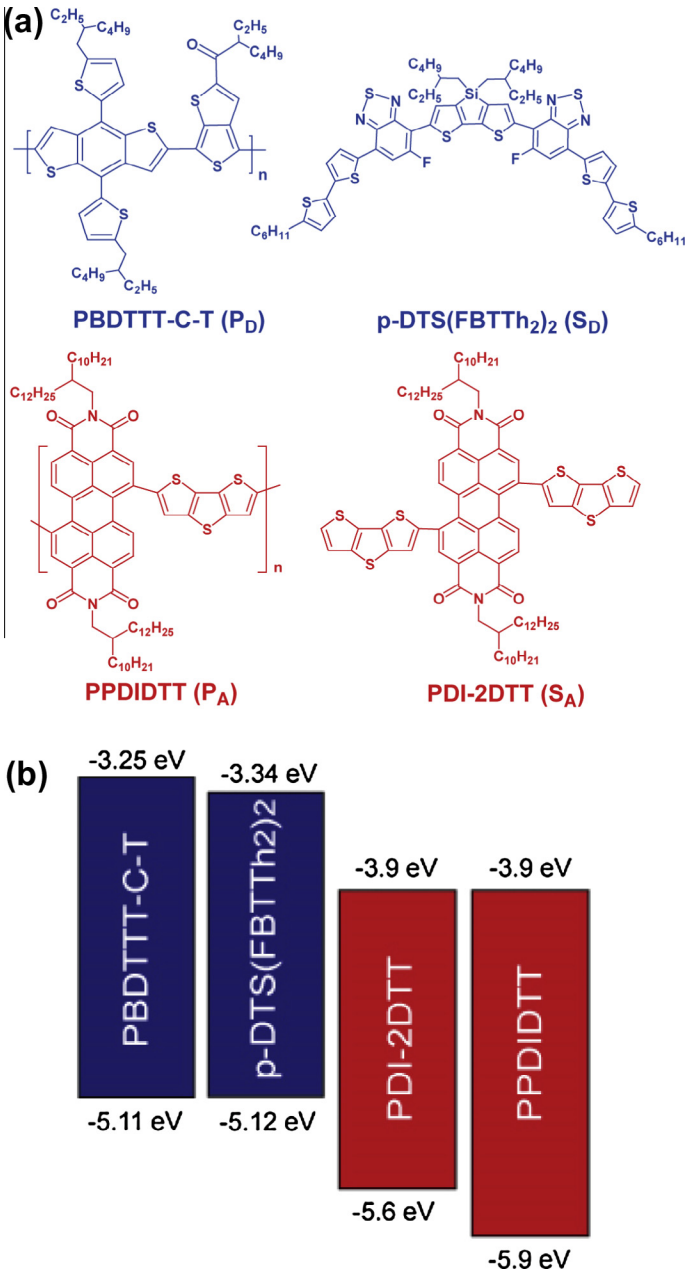

Fig. 1. (a) Molecule structure and (b) energy levels of PBDTTT-C-T (P_D), p-DTS(FBTTh$_2$)$_2$ (S_D), PPDIDTT (P_A) and PDI-2DTT (S_A).

separation driving force and high V_{OC}. Thirdly, non-fullerene OSCs exhibit good long-term stability [28] and good stability upon continuous bending [67].

Most reported non-fullerene OSCs used poly(3-hexylthiophene) (P3HT) as electron donors [38,43,45,46,48–53,56,58–66]. However, the highest occupied molecular orbital (HOMO) energy level of P3HT is very high (*ca.* −4.76 eV [68]), leading to low V_{OC}. Moreover, the absorption spectrum of P3HT is narrow (less than 650 nm), leading to low short circuit current density (J_{SC}). Accordingly, low band-gap small molecule and polymer donors with suitable HOMO level, high mobility and wide absorption are used in non-fullerene OSCs instead of P3HT [69]. Relative to polymer:PCBM blends and P3HT:non-fullerene acceptor blends, low band-gap donor:non-fullerene acceptor blends have more D/A combination choices. Non-fullerene OSCs with low band-gap donors have achieved PCEs exceeding 3% for polymer donor:polymer acceptor blend [28,31,40,41,44], polymer donor:small molecule acceptor blend [33–35,37,39] and small molecule donor:small molecule acceptor blend [36]. However, there have been no reports on small molecule donor:polymer acceptor blend. Thus, how to select D/A combination to achieve high efficiency of non-fullerene OSCs is an important and