Organic Electronics 35 (2016) 112–117

Contents lists available at ScienceDirect

Organic Electronics

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

A systematical investigation of non-fullerene solar cells based on diketopyrrolopyrrole polymers as electron donor

Cheng Li, Andong Zhang, Guitao Feng, Fan Yang, Xudong Jiang, Yaping Yu, Dongdong Xia, Weiwei Li*

Beijing National Laboratory for Molecular Sciences, CAS Key Laboratory of Organic Solids, Institute of Chemistry, Chinese Academy of Sciences, Beijing, 10090, China

ARTICLE INFO

Article history:
Received 16 April 2016
Received in revised form
8 May 2016
Accepted 8 May 2016
Available online 20 May 2016

Keywords:
Diketopyrrolopyrrole
Non-fullerene solar cells
Perylene diimide

ABSTRACT

Diketopyrrolopyrrole (DPP)-based conjugated polymers have been successfully applied in high performance field-effect transistors and fullerene-based solar cells, but show limited application in non-fullerene solar cells. In this work, we use four DPP polymers as electron donor and a perylene bisimide dye as electron acceptor to construct non-fullerene solar cells. The donors and acceptor have complementary absorption spectra in visible and near-infrared region, resulting in broad photo-response from 300 nm to 1000 nm. The solar cells were found to provide relatively low power conversion efficiencies of 1.6–2.6%, which was mainly due to low photocurrent and fill factor. Further investigation reveals that the low performance is originated from the high charge recombination in photo-active layers. Our systematical studies will help better understand the non-fullerene solar cells based on DPP polymers and inspire new researches toward efficient non-fullerene solar cells with broad photo-response.

1. Introduction

Perylene bisimide (PBI) derivatives with comparable electron affinities to fullerenes have been widely used as electron acceptor in non-fullerene solar cells during the last few years [1–24]. In contrast to the limited fullerene-based materials, the chemical structures of PBI compounds can be intensively engineered in terms of absorption spectra, energy levels, crystal properties and electron mobilities so as to provide the possibility to improve the photovoltaic performance. PBIs tend to form large π-stacked aggregation with size >1 μm in thin films, but in bulk-heterojunction solar cells the domain size of 10–20 nm for the acceptor is required to provide efficient charge separation and transport [25]. In order to reduce the intermolecular interactions and avoid the strong tendency toward large crystalline aggregation of the conjugated backbone, a dimeric PBI compound, SdiPBI (Fig. 1a), was developed [19–21]. The bulk-heterojunction thin films containing SdiPBI showed favorable micro-phase separation, and hence SdiPBI and its derivatives could provide high power conversion efficiencies (PCEs) above 8% [23].

The PCEs of solar cells depend on the physical properties of photo-active layers, such as the absorption spectra, the alignment of energy levels between donor and acceptor and the micro-phase separation. Since SdiPBI shows the narrow absorption band in the visible spectrum, the conjugated materials with absorption spectra in the near-infrared (NIR) region are required in order to sufficiently harvest sunlight. When SdiPBI as acceptor was blended with a wide band gap polymer PDBT-T1 [23] as donor, a PCE of 8.42% could be achieved but with narrow photo-response in the range of 300–700 nm, which also presented the highest performance for PBI-based solar cells. The photo-response could be further extended to 800 nm when using a well-known electron donor PBDTT-F-TT, but the cells provided a low PCE of 5.9% after applying a modified interface [19]. The low efficiency could be due to the unbalanced hole and electron mobilites (4.36×10^{-2} and 3.32×10^{-5} $cm^2 V^{-1} s^{-1}$) of donor and acceptor, resulting in enhanced charge recombination in solar cells [19].

These studies intrigue us to search conjugated polymers with NIR absorption spectra as electron donor for SdiPBI-based non-fullerene solar cells. Our group focus on developing diketopyrrolopyrrole (DPP)-based conjugated polymers for high performance

* Corresponding author.
E-mail address: liweiwei@iccas.ac.cn (W. Li).

http://dx.doi.org/10.1016/j.orgel.2016.05.011
1566-1199/

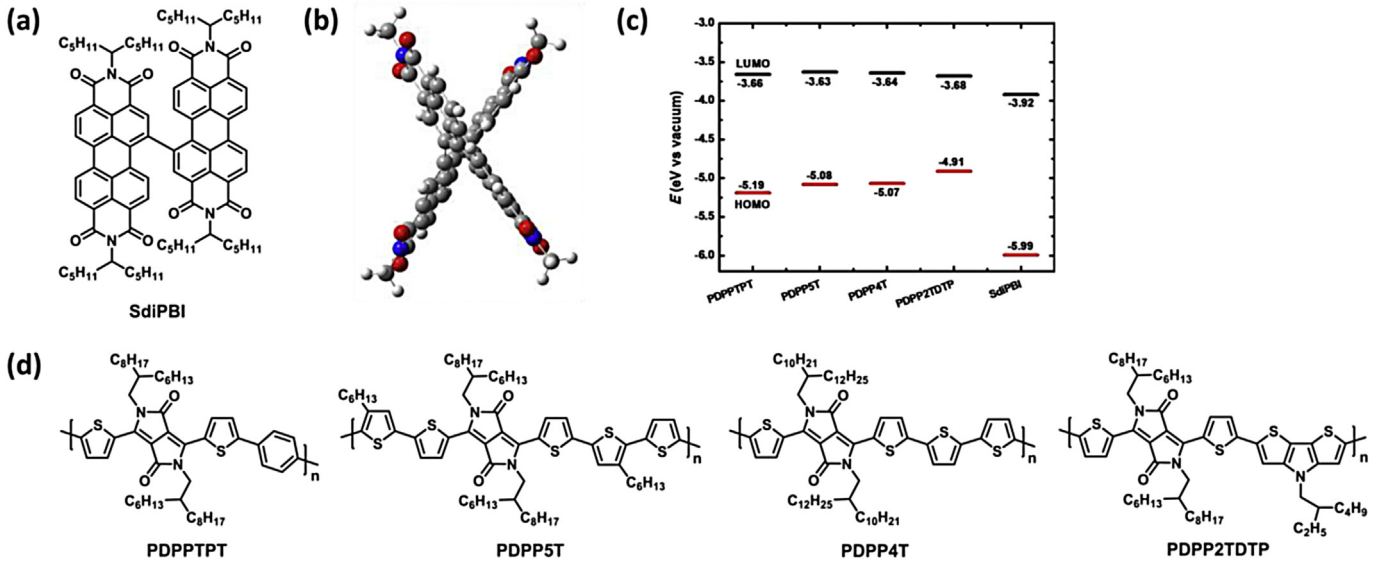

Fig. 1. (a) Chemical structures of electron acceptor SdiPBI; (b) The optimized geometry of SdiPBI obtained using DFT calculations at the B3LYP/6-31G*; (c) Energy levels of the donor and acceptor in this work; (d) Chemical structures of DPP polymers.

field-effect transistors (FETs) [26,27] and organic solar cells [28]. DPP unit has strong electron-withdrawing ability to construct small band gap conjugated polymers. By selecting electron-donating units, such as benzene [29], thiophene [30] and dithienopyrrole [31] units, the absorption onset can be easily tuned from 800 nm to 1000 nm. DPP polymers also exhibit good crystallinity and high hole mobilities above 10 $cm^2\ V^{-1}\ s^{-1}$ [27,32,33]. As a result, DPP polymers as electron donor have achieved high PCEs >9% in fullerene-based solar cells [34]. Therefore, it will be interesting to study the photovoltaic properties of DPP polymer:SdiPBI systems.

In this work, we select a series of DPP polymers as donor for use in non-fullerene solar cells with SdiPBI as electron acceptor (Fig. 1). Although DPP polymers show high PCEs in fullerene-based solar cells, some studies revealed that DPP polymers performed low PCEs in non-fullerene solar cells [20,35–37]. In our previous work, we investigated the solar cells of DPP polymers as donor and a naphthalenediimide-based polymer as acceptor with PCEs below 2%, which was mainly due to the good miscibility of donor and acceptor polymers [38]. In this work, DPP polymer:SdiPBI solar cells provided better PCEs up to 2.6% with broad photo-response from 300 nm to 1000 nm. Further studies reveal that unbalanced hole and electron mobilities will enhance the charge recombination, which is mainly responsible for the low PCEs. Our results indicate that by designing new electron acceptors with high electron mobilities, DPP polymers can be used in efficient non-fullerene solar cells toward thermally stable and large-area flexible devices [39].

2. Experimental section

All chemicals were purchased from commercial suppliers and used without further purification unless otherwise specified. The four DPP polymers PDPPTPT [29], PDPP5T [40], PDPP4T [41], PDPP2TDTP [31] and the acceptor SdiPBI [9] were synthesized according to literature procedures. Poly(3-hexylthiophene) (P3HT) and [6,6]-phenyl-C_{71}-butyric acid methyl ester ([70]PCBM) were purchased from Solarmer Materials Inc.

The photovoltaic devices were fabricated with a structure of glass/ITO/ZnO/donor:acceptor/MoO_3/Ag. Zinc Acetate dehydrate (0.5 M) and ethanolamine (0.5 M) in 2-methoxylethanol was stirred at room temperature for 2 h. The solution was spin coated at 4000 rpm for 60 s onto precleaned, patterned ITO substrates and the thin film was thermal annealed at 150 °C for 10 min to form ZnO layer [42]. The photoactive layer was deposited by spin coating the DPP polymer:SdiPBI in chloroform solution with appropriate amount of processing additive such as 1,8-diiodooctane (DIO) or *ortho*-dichlorobenzene (*o*-DCB) in air. The photoactive layers based on P3HT:[70]PCBM (1:1) were fabricated from *o*-DCB solution (30 mg mL^{-1}) at 1000 rpm in air and thermal annealed at 150 °C for 10 min in N_2 filled glove box. MoO_3 (10 nm) and Ag (100 nm) were deposited by vacuum evaporation at ca. 4×10^{-5} Pa as the back electrode. The active area of the cells was 0.04 cm^2. The *J-V* characteristics were measured by a keithley 2400 source meter unit under AM1.5G spectrum from a solar simulator (enlitech model SS-F5-3A). Solar simulator illumination intensity was determined at 100 mW/cm^2 using a monocrystal silicon reference cell with KG5 filter.

Short circuit currents under AM1.5G conditions were estimated from the spectral response and convolution with the solar spectrum. The external quantum efficiency was measured by a Solar Cell Spectral Response Measurement System QE-R3011 (Enli Technology Co., Ltd.). The thickness of the active layers in the photovoltaic devices was measured on a Veeco Dektak XT profilometer.

Density functional theory (DFT) calculations were performed at the B3LYP/6-31G* level of theory by using the Gaussian 09 program package. AFM images were recorded using a digital instruments nanoscope IIIA multimode atomic force microscope in tapping mode.

The carrier mobilities were measured by space charge limit current (SCLC), where the device configuration of ITO/PEDOT:PSS/active layer/Au was used for hole-only devices and ITO/ZnO/active layer/LiF/Al was used for electron-only devices. The mobilities were calculated from the slope of the $J^{1/2}$-*V* curves, by fitting the dark current according to the model of a single carrier SCLC equation: $J = 9\varepsilon_0\varepsilon_r\mu_h(\mu_e)V^2/8d^3$, where *J* is the measured current density, ε_0 is the permittivity of free space, ε_r is the relative dielectric constant of the transport material, μ is the mobility, *d* is the thickness of the active layer. *V* is the difference between the applied voltage and the offset voltage.