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Fluorene-centered perylene monoimides as potential non-fullerene acceptor in organic solar cells

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ABSTRACT

A fluorene-centered perylene monoimide dimer, PMI-F-PMI with a partly non-coplanar configuration has been developed as a potential non-fullerene acceptor for organic solar cells (OSCs). The optimum power conversion efficiency (PCE) of the OSC based on PMI-F-PMI as acceptor and poly (3-hexyl thiophene) (P3HT) as donor is up to 2.30% after annealing at 150 °C. The PCE of 2.30% is the highest value for the OSCs based on P3HT donor and non-fullerene acceptor lies in that PMI-F-PMI's lowest unoccupied molecular orbital (LUMO) level around −3.50 eV matches well with the donor P3HT to produce higher open-circuit voltage (V_{oc}) of 0.98 V. Meanwhile, PMI-F-PMI makes remarkable contribution to devices' light absorption as the maximum EQE (30%) of the devices is at 512 nm, same to the maximum absorption wavelength of PMI-F-PMI. The other favorable characteristics of PMI-F-PMI in bulk heterojunction (BHJ) active layers is proved through the photo current density measures, the relatively balanced electron–hole transport, and the smooth morphology with root mean square (RMS) value of 1.86 nm. For these advantages, PMI-F-PMI overwhelms its sister PMI-F and parent PMI as an acceptor in BHJ solar cells.
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1. Introduction

The field of bulk heterojunction (BHJ) organic solar cells (OSCs) is undergoing rapid development and has become a hot research field in recent years [1,2]. The record of power convert efficiency (PCE) of the OSCs is being constantly refreshed [3–20], which should be mainly attributed to the evolution of electron donor materials, e.g., from conventional poly(3-hexyl thiophene) (P3HT) to the novel DERHD7T [21], PBDTT-DPP, PTB7 [22], PBDTTT-C-T [23] and PffBT4T-2DT [24] etc. However, the electron acceptors as another indispensable part of BHJ active layers are relatively underdeveloped. To date, fullerene derivatives, especially, [6,6]-phenyl C_{61} butyric acid methyl ester ($PC_{61}BM$) and [6,6]-phenyl C_{71} butyric acid methyl ester ($PC_{71}BM$) hold the dominant status, despite of the difficulty in their syntheses and/or purifications and their poor absorbance in solar spectrum [25].

Currently, seeking suitable non-fullerene acceptors has attracted considerable attention [26–44]. Although these materials' performances in BHJ cells are still inferior to fullerenes, from them, some fundamental laws can be summed up to guide the further molecular design. Taking the frequently applied perylene diimides (PDIs) as a representative example of non-fullerene acceptors, they have two unfavorable aspects (see Scheme 1). Firstly, their relatively low lowest unoccupied molecular orbital (LUMO) level around −4.0 eV is unsuitable with the high HOMO of donor materials, e.g., P3HT, which is decisive for the smaller open-circuit voltage (V_{oc}) [45–47]. Secondly, PDIs' large, rigid and planar conjugation skeletons make them tend to excessively aggregate [48], which may reduce the quality of the BHJ films. So, modifications on bay sites to lift PDIs' LUMO level, and constructions of non-coplanar PDI polymers/oligomers to improve the film morphology have proved efficient strategies [29]. Very recently, BHJ solar cells using an alkoxy-substituted PDI dimer of twisted configuration as the acceptor and PffBT4T-2DT as the donor have achieved a PCE of 6.3% which is the highest for all the reported non-fullerene acceptors [24].

Herein, we designed PMI-F-PMI, a fluorene-centered dimer of perylene monoimide as shown in Scheme 1. Although PDI is very popular building block to develop acceptors for BHJ solar cells, we believe that PMI (perylene monoimide [49]) is better, because the remove of one imide segment means remarkable raise of LUMO and therefore higher V_{oc}. Fluorene's 2,7-positions are coupled to the peri-position of two PMI moieties, because we want to utilize the steric hindrance effect to construct a large conjugated molecule with a partially non-coplanar configuration (distorted angles ~57° between fluorene and PMI moiety, as estimated by

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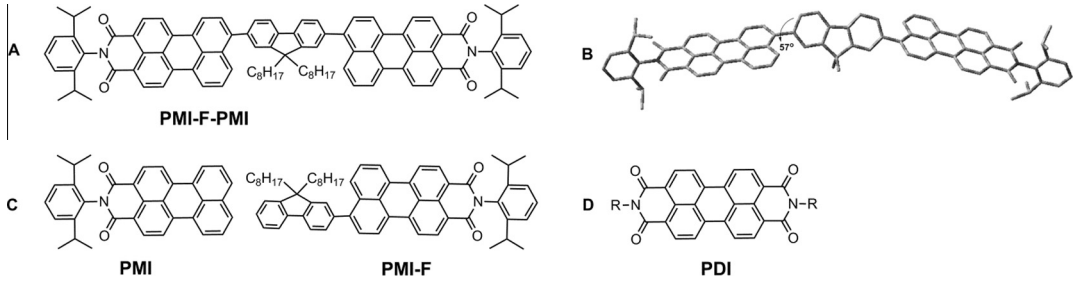


Scheme 1. (A) The chemical structure of PMI-F-PMI; (B) the optimized geometry structure of PMI-F-PMI showing a distorted configuration; (C) the chemical structures of PMI and PMI-F; (D) the general structure of PDI molecules.

density functional theory (DFT) calculation, see Scheme 1) favorable for modulating the morphology of BHJ active layers.

In this article, the focus is on the BHJ solar cells using PMI-F-PMI as acceptor and P3HT as donor. P3HT is a very common and commercially available donor for BHJ solar cells, so devices using P3HT, rather than the novel efficient donors, can better clarify the potential of newly developed non-fullerene acceptors. And to gain deep insight into the relationship between molecular structures and the device performances, a thorough comparison study on PMI-F-PMI, the parent PMI and the sister PMI-F has been carried out. The optimum PCE of PMI-F-PMI:P3HT solar cells is up to 2.30%, which is among the highest values for non-fullerene small molecule acceptors using P3HT as the donor. Furthermore, it should be noted that the area of the OSC devices with a conventional architecture is 0.20 cm^2, which is larger than those of the reported ones [12,29].

2. Experimental

2.1. Materials and measurements

Compound PMI [50], 1 [51], 2 [52], 9,9′-dioctyl-2-bromofluorene [53] and 9,9′-dioctyl-2,7-dibromofluorene [54] are synthesized according to reference procedure. The synthetic routes of PMI, PMI-F and PMI-F-PMI are shown in Scheme 2. All other reactants are purchased from commercial sources. NMR spectra are measured with a 400 MHz Bruker spectrometer using TMS as reference for ^1H and ^{13}C NMR. Accurate mass correction is measured with MALDI TOF Mass Spectrometer (MALDI micro MX). Cyclic voltammetry (CV) is performed in 0.05 M solution in CH_2Cl_2 with a standard commercial electrochemical analyzer in a three electrode single-component cell under argon with a scan rate of 100 mV/s. Working electrode: glassy carbon; reference electrode: Ag/AgCl; auxiliary electrode: Pt disk; internal standard: ferrocene (Fc). The energy of Fc/Fc^+ is 5.08 eV relative to vacuum [55]. UV–vis absorption spectrum is measured with UV–vis Spectrophotometer (HP8453). Thermal gravimetric analyse (TGA) are carried out using a Mettler Toledo TGA/SDTA 851e at a heating rate of 10 °C min^{-1} under nitrogen flow of 20 mL min^{-1}.

2.2. Fabrication of SCLC model device

The SCLC in this case of mobility depending on the field can be approximated by [33]:

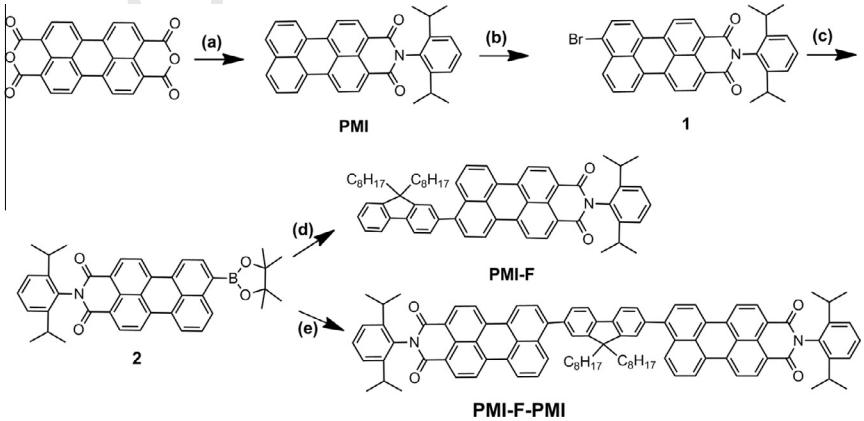
$$J = \frac{9}{8}\varepsilon\varepsilon_0\frac{E^2}{L}\mu_0 \exp(0.89\gamma\sqrt{E}) \quad (129)$$

where E is the electric field across the sample, ε and ε_0 are the relative dielectric constant and the permittivity of the free space, respectively, and L is the thickness of the organic layer, with μ_0 the zero-field mobility and γ describing the field activation of the mobility.

The device structure for the measurement of the hole mobilities is ITO/PEDOT:PSS/PMI-F or PMI-F-PMI:P3HT/Au and the device structure for the measurement of the electron mobilities is Al/PMI-F or PMI-F-PMI:P3HT(1:1, w/w)/LiF/Al with annealed at 150 °C.

2.3. Photocurrent density (J_{photo}) measurements

The photocurrent density is defined as $J_{photo} = J_{light} - J_{dark}$, where J_{light} and J_{dark} are current densities of the device measured under illumination and in the dark [34]. The effective applied



Scheme 2. Synthesis of PMI-F and PMI-F-PMI: 2,6-diisopropylaniline, zinc acetate, H_2O, imidazone, 190 °C, 23 h; (b) Br_2, chlorobenzene, 50 °C, 5 h; (c) Bis(pinacolato) diboron, potassium acetate, toluene, 80 °C, 14 h, argon; (d) 9,9′-dioctyl-2-bromofluorene, 2 M K_2CO_3 solution, Pd $(PPh_3)_4$, THF, 70 °C, 16 h, argon; (e) 9,9′-dioctyl-2,7-dibromofluorene, 2 M K_2CO_3 solution, Pd $(PPh_3)_4$, THF, 70 °C, 14 h, argon.

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