



Influence of substrate temperature on the film morphology and photovoltaic performance of non-fullerene organic solar cells



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ABSTRACT

A novel 1,8-naphthalimide-based small molecular acceptor (NI-T-C8) was designed and synthesized. The LUMO level of NI-T-C8 was high-lying, which would reduce the energy loss of WBG polymer PCDTBT-C12 based devices. When non-fullerene devices based on PCDTBT-C12: NI-T-C8 were spin-coated from substrates with a temperature of 30 °C, the aggregation of NI-T-C8 would lead to an unoptimized film morphology and result in a low power conversion efficiency (PCE) of 2.68%. After elevating the substrates from 30 to 45 °C, the domain size of blend films was decreased and a PCE of 3.61% with a high open circuit voltage (V_{oc}) of 1.28 V was acquired, but the aggregation of NI-T-C8 for blend films fabricated in 45 °C based substrates was still influence the exciton dissociation in the active layers, lower J_{sc} values for NI-T-C8 based devices in comparison to PC₇₁BM based ones were therefore acquired. This is the first single junction organic solar cell with a PCE higher than 3% could achieve a V_{oc} higher than 1.2 V. Our results also demonstrated that elevating the temperature of substrates could reduce the domain size of non-fullerene acceptors, which could provide a strategy to adjust the film morphology of active layer comprising easy-aggregating non-fullerene acceptor.

1. Introduction

Organic solar cells (OSCs), which generally adopt conjugated polymers or small molecules as the donor and fullerene derivatives such as (6,6)-phenyl-C71-butyric acid methyl ester (PC₇₁BM) as the acceptor have attracted tremendous attentions in the last two decades due to their merits of flexibility, light weight and low toxicity. [1–6] Driving by the synthesis of novel donor materials and the developing of device fabrication technology, power conversion efficiency (PCE) of 11.7% has been achieved for single junction devices. [7,8] Although fullerene derivatives have displayed a good performance as acceptor materials, the shortcoming of low absorption in visible region, difficulty in synthesis, separation and modification hamper the further improvement of PCE and future industrial application. [9,10] In comparison with fullerene derivatives, non-fullerene organic acceptors not only can absorb more sunlight in the visible region, but also possess an easy tuning energy level, making them potential acceptors to replace fullerene derivatives in OSCs. [11–14] Recently, a power conversion

efficiency (PCE) over 11.2% has been achieved [15], indicating that non-fullerene OSCs have enormous potential to approach performance similar and even superior to that of fullerene derivatives based devices. To achieve high J_{sc} and FF in devices, high electron mobility is generally demanded for non-fullerene acceptors. Planar molecules usually possess strong intra-molecular interaction, endowing them high electron mobilities when blended with donor materials. [16–19] However, planar acceptors constructed with a large and rigid electron withdrawing unit like perylene diimide (PDI) usually exhibit an inferior performance due to the formation of large aggregates in the active layer. [20,21] To solve this problem, a twisty bridge is usually introduced to increase the dihedral angle of adjacent PDI units, the planarity and crystallinity of acceptors could be therefore reduced. [20,22,23] However, this route might also decrease the electron mobility of acceptor materials. [21] Using high boiling point solvents such as DIO or 1-CN as the processing additive to reduce the domain size of the blend film in non-fullerene devices has also been reported. [10,20,21] Nevertheless, this strategy sometimes couldn't play a

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positive role in the tuning process [22,24], enriching the technique of tuning the aggregation of small molecular acceptors in blend films was therefore important and demanded.

Elevating the substrate temperatures could slow down the film-forming process of the blend film and achieve better mix properties for the active layers, making it a common method to fabricate devices based on donor materials with poor solubility. [25–28] However, adjusting the aggregation of non-fullerene acceptors via changing the temperature of substrates was yet to be investigated. The influence of temperature of substrates on the film morphology and photovoltaic performance of non-fullerene OSCs was still unclear.

In our previous work, a novel 1,8-naphthalimide (NI)-based small molecular acceptor with one thiophene bridged with two NI end groups was synthesized to reduce the LUMO level energy loss of wide band gap (WBG) polymer PCDTBT-C12 based devices. [29] In this contribution, by reducing the length of flexible chains on NI unit, new acceptor NI-T-C8 was designed and synthesized. The LUMO level of NI-T-C8 was high-lying, which was beneficial to reduce the energy loss of WBG polymer PCDTBT-C12 based devices. [11,26] In addition, NI-T-C8 was planar and crystalline, which would also be beneficial to achieve superior electron mobility in devices. [30,31] Although the planar and crystalline structure of NI-T-C8 was beneficial for the enhancement of electron transport when blended with donor materials, the resulting unoptimized film morphology would obviously influence the exciton separation in the donor/acceptor interface in the active layers, inferior J_{sc} in comparison to PCBM based acceptors was therefore acquired. When NI-T-C8 was used as acceptor to fabricate organic devices on a substrate with a normal temperature of 30 °C, big domain of PCDTBT-C12 and NI-T-C8 lead to a lower J_{sc} and resulting PCE. Elevating the temperature of substrates from 30 to 45 °C, the domain size of the blend films was obviously reduced, leading to a significantly enhanced PCE of 3.61% with a high open circuit voltage (V_{oc}) approached to 1.3 V. This is the first single junction organic solar cell device with a PCE higher than 3% could achieve a V_{oc} of approximate 1.3 V, revealing that NI-T-C8 is a potential acceptor to pair with WBG polymer donor. Our results also demonstrated that elevating the temperature of substrates could reduce the domain size of non-fullerene acceptors, which provide a strategy to tune the morphology of active layer comprising easy-aggregating non-fullerene acceptor.

2. Results and discussion

2.1. Material synthesis and characterization

As shown in Fig. 1a, NI-T-C8 was synthesized by facilely direct C-H activation via excessive N-dodecyl-4-bromo-1,8-naphthalimide and

thiophene using Pd(OAc)₂ and PCy₃HBF₄ as catalyst precursors, which is similar to our previous small molecular acceptor NI-T-NI (only with shorter end chains); PCDTBT-C12 was also synthesized according to the literature procedures (with different molecular weight). [29] The weight average molecular weight (M_w) and dispersity (D) of PCDTBT-C12 were determined by gel permeation chromatography (GPC) at 90 °C using CB as an eluent to be 78.2 kg mol⁻¹ and 1.21, respectively (see Supplementary Fig. 1). NI-T-C8 exhibited good solubility and could be fully dissolved in dichloromethane (DCM), chlorobenzene (CB) and 1,2-dichlorobenzene (DCB) at room temperature, whereas PCDTBT-C12 is only soluble in DCB at elevated temperature. As shown in Supplementary Fig. 2, thermo gravimetric analysis (TGA) experiments revealed that PCDTBT-C12 and NI-A-C8 are of good thermo stability with a 5% weight loss temperature of 325 and 434 °C, respectively. Differential scanning calorimetry (DSC) traces displayed a melting peak at 196 °C and a crystallization peak at 167 °C for NI-T-C8, revealing that NI-T-C8 is crystalline, whereas no obvious glass transition was observed for PCDTBT-C12, demonstrating that PCDTBT-C12 could be amorphous (see Supplementary Fig. 3 [29]). Computer calculation was carried out to shed light on the planarity of NI-T-C8. Density functional theory (DFT) approaches (B3LYP/6–31 G(d)) was used and alkyl group was simplified as methyl to decrease the computational load. [10] As shown in Fig. 1b, NI-A-C8 tends to form an approximately planar conformation with a dihedral angle of 11° between two NI groups. For NI based small molecular acceptors, increasing their planarity has been demonstrated to be beneficial for enhancing the electron mobility and giving rise to larger short circuit current density (J_{sc}) for devices [30,32,33], suggesting that NI-A-C8 could be a promising acceptor in non-fullerene OSCs. To further investigate the crystallinity of PCDTBT-C12 and NI-T-C8, wide angle XRD images of PCDTBT-C12 film and PCDTBT-C12: NI-T-C8 blend films were measured. As shown in Fig. 2, PCDTBT-C12 film only displays a weak 100 peak at 5.02°, revealing that PCDTBT-C12 is amorphous. When the blend of PCDTBT-C12 and NI-T-C8 was cast onto a 30 °C substrate, the film XRD image displayed a sharp 100 peak at 5.52° and a 010 peak at 24.2°, corresponding to a lamellar distance of 17.58 Å and a π - π stacking distance of 3.71 Å for NI-T-C8, demonstrating that NI-T-C8 is crystalline. When the blend films were spin-coated onto a substrate with an elevated temperature of 45 °C, the intensity of 100 and 010 peaks of NI-T-C8 significantly decreased, revealing the aggregation of NI-T-C8 in the blend films could be reduced by elevating the temperature of the substrate.

2.2. Optical properties

As shown in Fig. 3a, the optical properties of PCDTBT-C12 and NI-

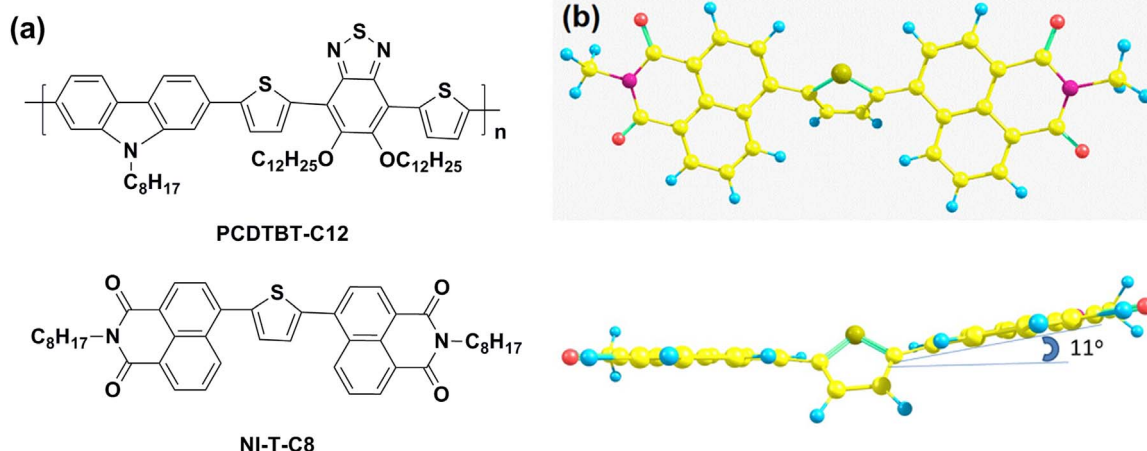


Fig. 1. (a) Chemical structure of PCDTBT-C12 and NI-T-C8; (b) Top view and side view of NI-T-C8.

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