



Comparison of conventional and inverted structures in fullerene-free organic solar cells[☆]

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ABSTRACT

A *n*-type small molecule DC-IDT2F, with 4,4,9,9-tetrakis(4-hexylphenyl)-indaceno[1,2-*b*:5,6-*b'*]dithiophene as a central building block, furan as π -bridges, and 1,1-dicyanomethylene-3-indanone as end acceptor groups, was synthesized and used as an electron acceptor in solution-processed organic solar cells (OSCs). DC-IDT2F exhibited good thermal stability, broad and strong absorption in 500–850 nm, a narrow bandgap of 1.54 eV, LUMO of –3.88 eV, HOMO of –5.44 eV and an electron mobility of $6.5 \times 10^{-4} \text{ cm}^2/(\text{V}\cdot\text{s})$. DC-IDT2F-based OSCs with conventional and inverted structures exhibited power conversion efficiencies of 2.26 and 3.08%, respectively. The effect of vertical phase separation and morphology of the active layer on the device performance in the two structures was studied.

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1. Introduction

Organic solar cells (OSCs) have been studied extensively over the past decade because of its advantages over traditional silicon solar cells, which include low cost, light weight and flexibility [1–7]. Most OSCs are processed based on a bulk heterojunction of a polymer donor and a fullerene acceptor, and the power conversion efficiencies (PCE) have reached the milestone of 10% [8–11]. In spite of the quick development of the donor materials, the development of acceptor materials have far lagged behind [12–14]. Compared with fullerene and its derivatives, which have been the dominant acceptors, non-fullerene *n*-type organic semiconductors have drawn increasing attention because of their broad absorption, relatively low cost and tunability of energy levels [15,16]. In the last few years, considerable efforts have been devoted to developing potential non-fullerene acceptors [17–22], and fullerene-free OSCs have achieved PCEs of up to 4–8% [23–32], which gives us an encouraging prospect of developing new non-fullerene acceptors aiming at being comparable or even better than their fullerene counterparts.

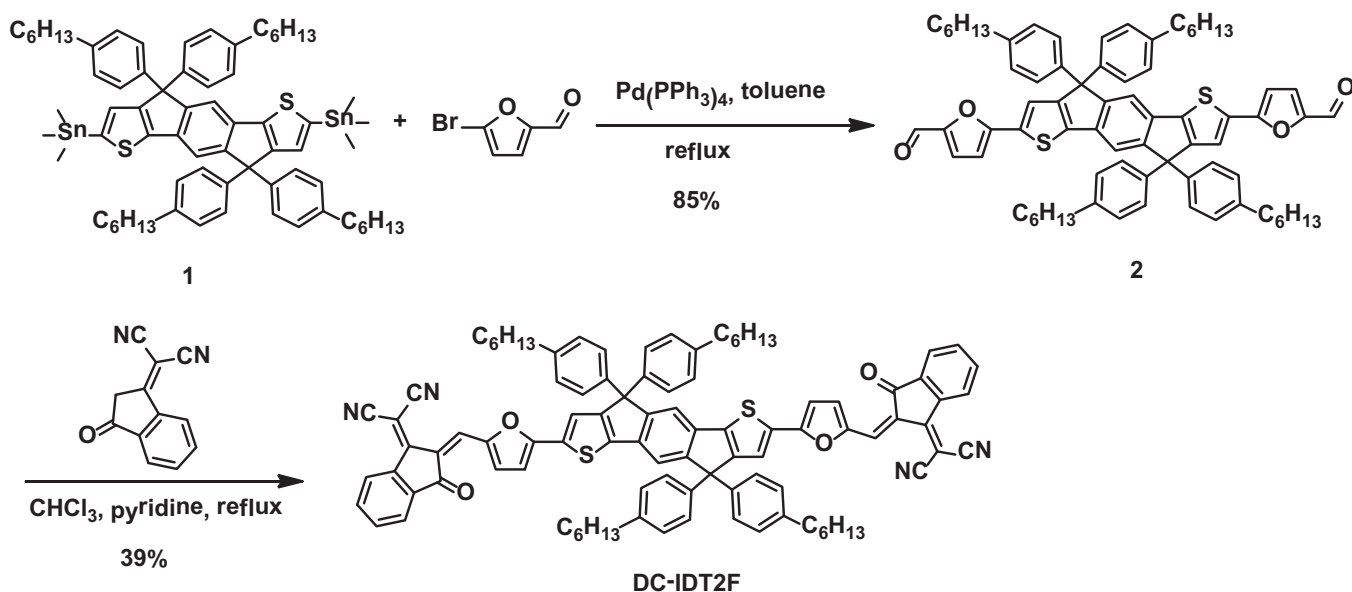
Vertical phase separation plays an important role in device performance, since it affects the dissociation of excitons as well as transportation, recombination and extraction of the charge carriers [33–37]. Extensive research investigated the effect of vertical phase separation in traditional fullerene-based OSCs and found that donor enriched at the anode and acceptor enriched at the cathode can facilitate the performance of the devices [38–40]. However, the role of vertical phase separation in fullerene-free OSCs has rarely been studied.

In this work, we report design and synthesis of a new A–D–A-type non-fullerene acceptor (DC-IDT2F) based on 4,4,9,9-tetrakis(4-hexylphenyl)-indaceno[1,2-*b*:5,6-*b'*]dithiophene as a central building block, 1,1-dicyanomethylene-3-indanone as electron-withdrawing end groups and furan as π -bridges (Scheme 1). The strong electron-withdrawing capability of 1,1-dicyanomethylene-3-indanone enabled this molecule to have deep LUMO level of –3.88 eV. Moreover, DC-IDT2F exhibited a broad, strong absorption with a narrow bandgap of 1.54 eV. OSCs with conventional and inverted structures were fabricated using DC-IDT2F as an acceptor and a low-bandgap polymer PBDTTT-C-T (Figure S1, Supporting Information) as an electron donor. The conventional and inverted OSCs exhibited PCEs of 2.26 and 3.08%, respectively. Vertical phase separation and morphology of the active layer play important roles in determining the performance of the fullerene-free OSCs.

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Scheme 1. Synthetic route for DC-IDT2F.

2. Experimental

2.1. Synthesis

Unless stated otherwise, all the solvents and chemical reagents used were obtained commercially and were used without further purification. Toluene was distilled from sodium benzophenone under nitrogen before use. Compound **1** was synthesized according to a literature procedure [41].

Compound 2. To a three-necked round bottom flask were added compound **1** (986 mg, 0.8 mmol), 5-bromofuran-2-carbaldehyde (350 mg, 2.0 mmol), and toluene (30 mL). The mixture was deoxygenated with argon gas for 15 min, and then Pd(PPh₃)₄ (70 mg, 0.06 mmol) was added. The mixture was refluxed for 24 h and then allowed to cool to room temperature. A volume of 40 mL KF solution (0.1 g/mL) was added, and the mixture was stirred at room temperature overnight to remove any tin impurities. Water (150 mL) was added and the mixture was extracted with CHCl₃ (2 × 150 mL). The organic phase was dried over anhydrous MgSO₄. After removing the solvent, the residue was purified using column chromatography on silica gel employing petroleum ether/CH₂Cl₂ (1:2) as an eluent, yielding a red-colored solid (745 mg, 85%). ¹H-NMR (400 MHz, CD₂Cl₂): δ 9.54 (s, 2H), 7.53 (s, 2H), 7.44 (s, 2H), 7.28 (d, *J* = 4 Hz, 2H), 7.19 (d, *J* = 8 Hz, 8H), 7.11 (d, *J* = 8 Hz, 8H), 6.69 (d, *J* = 4 Hz, 2H), 2.59 (m, 8H), 1.61 (m, 8H), 1.30 (m, 24H), 0.89 (m, 12H). ¹³C-NMR (100 MHz, CDCl₃): δ 176.48, 157.24, 155.12, 154.12, 151.41, 143.41, 141.92, 141.18, 135.35, 133.84, 128.58, 127.87, 124.07, 122.26, 117.88, 107.41, 63.08, 35.62, 31.77, 31.38, 29.15, 22.65, 14.16. MS (MALDI-TOF): *m/z* 1095 (M⁺). Anal. Calc. for C₇₄H₇₈O₄S₂: C, 81.13; H, 7.18. Found: C, 80.84; H, 7.20%.

DC-IDT2F. Compound **2** (438 mg, 0.4 mmol) and 1,1-dicyanomethylene-3-indanone (103 mg, 0.53 mmol) were dissolved in CHCl₃ (30 mL). The mixture was deoxygenated with argon gas for 15 min. Three drops of pyridine were then added and the mixture was stirred and refluxed for 12 h under argon gas. After being allowed to cool to room temperature, water (100 mL) was added and the mixture was extracted with CHCl₃ (2 × 100 mL). The organic phase was dried over anhydrous MgSO₄. After removing the solvent, the residue was purified using column chromatography on silica gel employing petroleum ether/CHCl₃ (1:4) as an eluent, yielding a red-black-colored solid (226 mg, 39%). ¹H-NMR (400 MHz, CDCl₃)

(Figure S2, Supporting Information): δ 8.84 (s, 2H), 8.67 (d, *J* = 8 Hz, 2H), 8.48 (s, 2H), 7.89 (d, *J* = 8 Hz, 2H), 7.75 (m, 4H), 7.50 (s, 4H), 7.19 (d, *J* = 8 Hz, 8H), 7.12 (d, *J* = 8 Hz, 8H), 6.89 (s, 2H), 2.59 (m, 8H), 1.61 (m, 8H), 1.29 (m, 24H), 0.87 (m, 12H). ¹³C-NMR (100 MHz, CDCl₃) (Figure S3, Supporting Information): δ 187.37, 160.60, 158.04, 157.78, 154.60, 150.55, 145.62, 142.06, 140.81, 139.78, 137.10, 135.54, 134.83, 134.28, 133.90, 131.50, 128.62, 127.93, 127.77, 125.02, 123.57, 123.29, 122.54, 118.14, 114.78, 114.48, 111.98, 69.03, 63.07, 35.56, 31.69, 31.32, 29.11, 22.57, 14.08. MS (MALDI-TOF) (Figure S4, Supporting Information): *m/z* 1448 (M⁺). Anal. Calc. for C₉₈H₈₆N₄O₄S₂: C, 81.29; H, 5.99; N, 3.87. Found: C, 81.22; H, 6.06; N, 3.87%. λ_{s, max} = 702 nm (1.4 × 10⁵ M⁻¹ cm⁻¹).

2.2. Characterization

The ¹H and ¹³C NMR spectra were measured using a Bruker AVANCE 400 MHz spectrometer employing tetramethylsilane (TMS; δ = 0 ppm) as an internal standard. Elemental analysis was carried out using a Flash EA 1112 elemental analyzer. Mass spectra were measured using a Bruker Daltonics Biflex III MALDI-TOF Analyzer in the MALDI mode. Solution (chloroform) and thin film (on a quartz substrate) UV-vis absorption spectra were recorded using a Jasco V-570 spectrophotometer. Electrochemical measurements were carried out under nitrogen in a deoxygenated solution of tetra-*n*-butylammonium hexafluorophosphate (0.1 M) in acetonitrile using a potential scan rate of 100 mV/s employing a computer-controlled Zahner IM6e electrochemical workstation, a glassy-carbon working electrode coated with the DC-IDT2F film, a platinum-wire auxiliary electrode, and an Ag/AgCl electrode as a reference electrode. The potentials were referenced to a ferrocenium/ferrocene (FeCp₂⁺⁰) couple using ferrocene as an external standard. Thermogravimetric analysis (TGA) measurement was performed using a Shimadzu thermogravimetric analyzer (Model DTG-60) under flowing nitrogen gas at a heating rate of 10 °C/min. Differential scanning calorimetry (DSC) measurement was performed using a Mettler differential scanning calorimeter (DSC822e) under nitrogen gas at a heating rate of 10 °C/min.

X-ray diffraction (XRD) of the thin films was performed in the reflection mode at 40 kV and 200 mA using Cu-*K*α radiation in a 2 kW Rigaku D/max-2500 X-ray diffractometer. The nanoscale morphology of the blended films was observed using a Veeco Nanoscope V atomic

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