

Narrow band gap isoindigo-based small molecules for solution-processed organic solar cells with high open-circuit voltage



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ABSTRACT

Isoindigo, one of the latest reported amide-based electron-accepting units, was introduced into two new D- π -A- π -D typed organic small molecules with triphenylamine as electron-donating unit for organic solar cells. Both (TPAEB)₂il and (TPACB)₂il possess narrow band gaps of 1.57 and 1.71 eV, respectively. Notably, (TPACB)₂il with 2-phenylacrylonitrile as π -bridge exhibited a high open-circuit voltage of 1.06 V and an improved power conversion efficiency of 3.57%, which is the best performance for isoindigo-triphenylamine based solution-processed organic photovoltaic devices so far. The high open-circuit voltage is primarily attributed to its higher electrochemical oxidation potential by molecular design. The relatively higher photovoltaic performance of (TPACB)₂il-based device relative to (TPAEB)₂il is shown to originate from the reasonably higher hole-transporting capacity, more optimized active layer morphology and higher degree of crystallinity. These results indicate that isoindigo-based small molecules are a kind of promising photovoltaic materials.

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1. Introduction

Bulk heterojunction organic solar cells (BHJ OSCs) have been a hot topic in the field of solar cells owing to their distinctive characteristics of lightweight, low cost and flexibility [1]. In the past several years, intensive efforts have been devoted to polymer BHJ OSCs and the dramatic power conversion efficiencies (PCEs) over 10% have been reported [2]. As an alternative to polymer BHJ OSCs, solution-processed organic small molecules (OSMs) solar cells have received much attention due to their advantages of well-defined chemical structures with less batch-to-batch variation, easier chemical modification and facility of purification [3]. To date, OSMs-based BHJ devices exhibit outstanding photovoltaic (PV) performance with PCEs over 10% [4]. To realize high performance, it is believed that two straightforward strategies should be considered to design small molecular donors: (1) reducing the band-gap (E_g) to broaden the absorption range [1,5], and (2) lowering the highest occupied molecular orbital (HOMO) to increase open-circuit voltage (Voc) [6]. In this regard, developing new electron donor-acceptor (D-A) conjugated structure has become an efficient strategy, because this design can not only

reduce the E_g through intramolecular charge transfer (ICT) process, but also efficiently control the energy levels through employing appropriate electron-donating and electron-accepting units [7]. Among multitudinous electron-donating and electron-accepting moieties, great attention has been paid to triphenylamine (TPA) [8], diketopyrrolopyrrole (DPP) [9] and benzothiadiazole (BT) [10] by reason of their good performance for BHJ OSCs.

Isoindigo (il), one of the latest reported amide-based A units for OSCs, is the isomer of the famous dye indigo [11]. il possesses superior characters similar to DPP, such as great planarity, easy synthesis in bulk quantities, deep-lying HOMO levels and strong electron-withdrawing ability [12]. It is worth mentioning that il displays some unique advantages, such as easily obtained from natural products and easily functionalized with multi-positions on il building-block [11]. The application of il compound in OSCs was first reported by Reynolds et al. in 2010 [13]. As far as we know, the research activities of il-based OSCs have been mostly focused on polymers with PCEs up to 9.1% [14]. However, the PV performance of il-based BHJ devices is still behind those of their polymer counterparts [11,15]. In general, the PCEs obtained from il-based molecules are around in the 3–4% range. For example, Loo et al. reported a competitive PCE of 3.4% for il-based solution-processed OSM solar cells [16]. To date, PCEs of il-TPA based solution-processed OSM solar cells are under 1% [7,17]. These reported il-based molecules were prone to crystallization into large domains,

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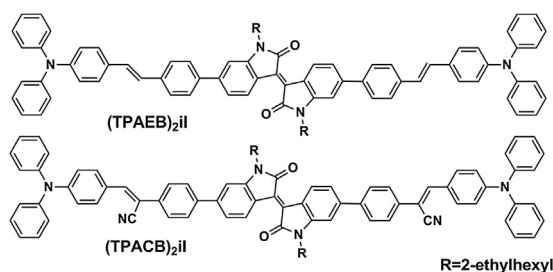
which hindered the charge separation, and thus prevented to give better PCE over 4%. In addition, low V_{OC} is also an important element imposed restriction on improving PV performance of i -based solar cells. In a word, the basic reason determining PV performance of BHJ device is the characteristics of OSMs [11,15]. According to our previous investigation, the introduction of π -bridges into D- π -A- π -D-typed OSMs, such as acrylonitrile or ethylene-linkage, can result in the improvement of PV performance [18].

In this work, an interesting molecular design is aimed at obtaining PV materials with narrow E_g and high V_{oc} for BHJ OSCs. i l as A building block was introduced into two new D- π -A- π -D-typed OSMs with TPA as D unit, which were linked with 2-phenylacrylonitrile or styrene π -bridge, respectively. Scheme 1 shows the molecular structures of the synthesized compounds (TPAEB) $_2$ iI and (TPACB) $_2$ iI. Both of them possess narrow E_g^{CV} of 1.57 and 1.71 eV, respectively. It is worth mentioning that (TPACB) $_2$ iI with 2-phenylacrylonitrile group as π -bridge exhibited a deeper-lying HOMO level of -5.42 eV compared with (TPAEB) $_2$ iI, resulting in a high V_{oc} of 1.06 V and a PCE of 3.57%, which is the best performance for i -TPA based solution-processed BHJ OSCs so far. These results indicate that i -based small molecules are a kind of promising PV materials with narrow E_g and high V_{oc} .

2. Experimental section

2.1. Materials, measurement and characterization

All reagents were purchased and used without further purification unless specified. All reactions were performed under a nitrogen atmosphere with the standard Schlenk technique unless otherwise noted. Toluene was distilled over Na/benzophenone before use. $^1\text{H-NMR}$ and $^{13}\text{C-NMR}$ spectra were recorded on a Bruker AVANCE II 400-MHz spectrometer with CDCl_3 as solvent and TMS as the internal standard. High-resolution mass spectra (HRMS) were recorded with MALDI Micro MX spectrometer. The UV-vis absorption spectra in solution and in thin film were taken on Agilent Cary 5000 spectrophotometer. Cyclic voltammetry (CV) measurements were carried out on a CHI610D electrochemical workstation from CH Instruments, Inc., and it was performed in 0.1 M anhydrous $\text{Bu}_4\text{NBF}_4/\text{CH}_2\text{Cl}_2$ solution at a scan rate of 100 mV s^{-1} under nitrogen atmosphere, using the glass-carbon electrode, Ag/Ag^+ electrode (Ag in 0.1 M AgNO_3 solution of MeCN) and platinum wire electrode as the working electrode, reference electrode and counter electrode, respectively. In addition, Ferrocene-ferrocenium (Fc/Fc^+) couple was selected as internal standard. An aluminium layer of PV devices was deposited with high vacuum resistance evaporation coating machine (Beijing Technol Science Co., Ltd). The current density-voltage (J - V) characteristics of PV devices were recorded with a Keithley 2400 Source Measure Unit under simulated AM 1.5 G illumination with an intensity of 100 mW cm^{-2} . The incident-photons-to-current efficiency (IPCE) spectra were recorded with a SM-25 photoelectric conversion



Scheme 1. Molecular structures of (TPAEB) $_2$ iI and (TPACB) $_2$ iI.

analyzer. The hole mobility experiments of synthesized materials were achieved with the computer-controlled Keithley 2400 Source Measure Unit system in the dark. Atomic force microscopy (AFM) images were taken using a Nanoscope IIIa Dimension 3100. X-ray diffraction patterns (XRD) data were collected on X'Pert Powder.

2.2. Device fabrication

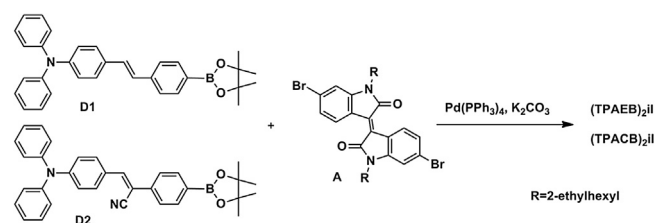
BHJ PV devices were fabricated with a conventional sandwiched architecture of ITO/PEDOT:PSS/OSMs:PC $_{61}$ BM/Al. The ITO glass substrate was cleaned successively in water, methanol, acetone, toluene and isopropyl alcohol for 10 min, respectively. Then a 40 nm thick layer of poly (3,4-ethylenedioxythiophene):poly (styrene sulfonate) (PEDOT:PSS) was spin-coated (4000 rpm s^{-1} , 60 s) on the ITO glass substrate. After being baked at 140°C for 15 min, the prepared substrate was transferred into a nitrogen-filled glove box. Subsequently, the active layer (80 nm) was spin-coated at 1500 rpm s^{-1} for 60 s with the mixed solution of OSMs and PC $_{61}$ BM (total concentration of 12 mg mL^{-1} in chloroform and with varied D/A weight ratios) on the top of prepared ITO/PEDOT:PSS substrate. Finally, an aluminium layer (100 nm) was deposited by vacuum thermal evaporation (ca. 10^{-4} Pa) through a shadow mask, yielding six individual devices with 5 mm^2 nominal area. The hole-only devices were fabricated for their hole mobility measurements with a structure of ITO/PEDOT:PSS/OSMs:PC $_{61}$ BM (1:2, w/w)/Au, and the gold (70 nm) was used as the negative electrode.

2.3. Synthesis

The synthetic routes of the compounds (TPAEB) $_2$ iI and (TPACB) $_2$ iI are shown in Scheme 2.

2.4. Synthesis of (TPAEB) $_2$ iI:

Toluene (12 mL), ethanol (6 mL) and deionized water (3 mL) were transferred to a mixture of compound A (194 mg, 0.3 mmol), D1 (355 mg, 0.75 mmol), $\text{Pd}(\text{PPh}_3)_4$ (35 mg, 0.03 mmol) and K_2CO_3 (1.66 g, 12 mmol). The resulting mixture was stirred at 110°C for 24 h. After being cooled to the room temperature, the mixture was poured into water (100 mL) and extracted with CH_2Cl_2 (40 mL \times 3). The combined extracts were dried over anhydrous sodium sulphate and evaporated under reduced pressure. The crude product was purified by silica chromatography, eluting with (CH_2Cl_2 : hexane = 1: 3) to give (TPAEB) $_2$ iI as a black solid (194 mg, 55%). M.p.: $107\text{--}109^\circ\text{C}$. $^1\text{H NMR}$ (400 MHz, CDCl_3 , ppm): δ 9.20 (d, $J = 8.2\text{ Hz}$, 2H), 7.61 (d, $J = 7.9\text{ Hz}$, 4H), 7.56 (d, $J = 8.0\text{ Hz}$, 4H), 7.39 (d, $J = 8.2\text{ Hz}$, 4H), 7.30–7.23 (m, 10H), 7.14–6.99 (m, 20H), 6.96 (s, 2H), 3.82–3.64 (m, 4H), 1.92–1.88 (m, 2H), 1.46–1.29 (m, 16H), 0.99–0.87 (m, 12H). $^{13}\text{C NMR}$ (100 MHz, CDCl_3): δ 168.73, 147.62, 147.54, 145.79, 144.32, 139.18, 137.74, 132.38, 131.32, 130.18, 129.32, 128.86, 127.50, 127.19, 126.84, 126.29, 124.61, 123.50, 123.16, 121.04, 120.47, 106.21, 44.24, 37.79, 30.86, 28.87, 24.26, 23.11, 14.10, 10.82. HRMS (MALDI-TOF): 1177.6372, $[\text{M}+\text{H}^+]$ (calcd for $\text{C}_{84}\text{H}_{80}\text{N}_4\text{O}_2$: 1177.6360).



Scheme 2. Synthetic routes of (TPAEB) $_2$ iI and (TPACB) $_2$ iI.

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