



Interface engineering on phenanthrocarbazole/thienopyrroledione-based conjugated polymer for efficient organic photovoltaic devices with ideal nano-morphology and improved charge carrier dynamics



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ABSTRACT

We synthesized PP-TPD, based on a phenanthro[1,10,9,8-cdefg]carbazole unit as a donor and a thieno [3,4-c]pyrrole-4,6-dione (TPD) unit as an acceptor for efficient bulk heterojunction photovoltaic cells. The copolymer achieves a relatively low bandgap (1.6 eV) by its internal charge-transfer, which concurs with the results of density functional theory (DFT) calculation for the distribution of HOMO and LUMO levels. In addition, we fabricated the bulk-heterojunction (BHJ) photovoltaic cells as a function of the blend ratio of the donor (PP-TPD) and acceptor (PC₇₀BM), and applied a solvent additive and an interlayer to the device, with the optimized ratio used in this study. To comprehend the relationships between the device performance and the synergetic effects of 1,8-diiodooctane (DIO) and titanium oxide (TiO_x) within the PP-TPD: PC₇₀BM blends, we investigated the hole mobility related to the charge carrier transport, the charge generation, and the charge transport resistance using space-charge limited current (SCLC) measurement, photocurrent analysis, and impedance spectroscopy, respectively. Especially, we implemented fluorescence imaging by Raman spectroscopy, which related to the charge generation and recombination dynamics within the surface of photoactive areas.

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1. Introduction

Organic photovoltaic cells (OPVs) have attracted increasing interest owing to their potential as light weight, flexible, large area devices in the production of renewable energy [1,2]. Of the total OPVs produced, their performance has reached over 10%, coinciding with the breakthrough of the development of new conjugated polymers as electron donors [3,4]. To improve the device performance of OPVs, studies have been performed on increasing the photovoltaic parameters, including the open circuit voltage (V_{oc}), the short circuit current (J_{sc}), and the fill factor (FF) [5,6]. Each factor can be affected by the intrinsic properties of a new donor-

acceptor copolymer, which is involved in an energy level arrangement and charge carrier mobility, etc. [7,8] Thus, the molecular structure of a donor-acceptor (D-A) copolymer must be designed correctly.

For the efficient molecular design of a D-A copolymer, we focused on the thieno [3,4-c]pyrrole-4,6-dione (TPD) unit. In recent studies, polymers based on a TPD unit have presented a relatively low band gap, which is related to their effective optical absorption, good hole mobility, and well-arranged energy level for efficient charge transport [9,10]. Also, in order to exploit these advantages of the polymer, the solubility and molecular packing, and the interaction between the donor and acceptor molecules can be considered when designing the polymer [11].

The device performance of an OPV based on any new copolymer is closely related to the nano-morphology of the active layer and the insertion of the interlayer. The nano-morphology of the polymer and acceptor blend plays an important role in the device performance when a new polymer is synthesized and applied in an

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OPV. Therefore, among the methods to control the morphology of the polymer and acceptor blend, the application of a solvent additive has been suggested by recent research groups, which has led to the improved efficiency of BHJ OPVs [12,13]. Also, the proper application of an interlayer that has a well-aligned energy level and good charge carrier affinities results in efficient charge transport and generation [14–16].

Therefore, we synthesized donor-acceptor copolymer, which is composed of phenanthro[1,10,9,8-cdefg]carbazole as the donor unit and a TPD unit as the acceptor. The polycyclic aromatic structured phenanthro[1,10,9,8-cdefg]carbazole is one of most attractive electron rich building blocks for organic electronics because of its planar and extended π conjugated structure [17,18], which leads to enhanced intermolecular interaction and charge-carrier mobilities [19]. TPD is a strong acceptor, and induces strong intra- and inter-chain interactions along and between the chain backbones as a result of good electron delocalization due to its relatively compact, symmetrical, and planar structure. In addition, for PP-TPD: PC₇₀BM OPV, we induced 1,8-diiodooctane (DIO) as a solvent additive and titanium oxide (TiO_x) as an electron transport layer in order to enhance the photovoltaic parameters of the device. To clarify the effects of DIO and TiO_x on the PP-TPD: PC₇₀BM system, the morphological change of the blends was demonstrated by scanning electron microscopy (SEM) and atomic force microscopy (AFM), the results of which corresponded to the charge transport and generation properties investigated in the electrical analysis and impedance spectroscopy. It has recently been discovered that the new low bandgap polymer containing polycyclic aromatic phenanthro[1,10,9,8-cdefg]carbazole and TPD is one of the candidates for high-performance organic solar cells, and that the application of a solvent additive and an interlayer contributes to the charge transport and generation in the devices, as obtained by electrical analysis and fluorescence imaging analysis [9]. Therefore, it is expected that the results of this work will facilitate study on the optimization of a copolymer system.

2. Experimental

2.1. Materials

All chemicals were purchased from Aldrich and Alfa: 1,3-bis(5-bromo-thiophen-2-yl)-5-octyl-thieno [3,4-c]pyrrole-4,6-dione, isopropoxyboronic acid pinacol ester, dimethylformamide (DMF), Tetrahydrofuran (THF), and n-bromosuccinimide (NBS) were used without further purification.

2.2. Instrumentation

The characterization of polymer was followed by literature methods [20]. Density functional theory (DFT) calculations were carried out at the B3LYP/6-31G^{*} level of theory using the Spartan 08 computational programs.

2.3. 1-(2-Decyltetradecyl)-3,10-bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1H-phenanthro[1,10,9,8-cdefg]carbazole (M1)

The synthesis of monomer was followed by literature method [20]. (Yield: 0.6g, 27.3%) ¹H NMR (CDCl₃, 300 MHz): δ (ppm) 8.99–9.02 (d, 2 H), 8.70–8.73 (d, 2 H), 8.46 (s, 2 H), 7.86–7.92 (t, 2 H), 4.66–4.68 (d, 2 H), 2.37 (m, 1 H), 1.52 (m, 24 H), 1.10–1.42 (m, 40 H), 0.85–0.91 (m, 6 H).

2.4. Polymerization of PP-TPD

The synthesis of polymer was followed by literature method

[20]. The crude polymer was collected by filtration and purified by Soxhlet extraction with methanol, acetone, hexane, toluene, tetrahydrofuran, and chloroform, successively. The PP-TPD was obtained by precipitation of the chloroform solution in methanol. (Yield: 0.36 g, 75%) ¹H NMR (500 MHz, CDCl₃) δ (ppm): δ 8.53 (br, 2H), 8.09 (br, 2H), 7.66 (br, 2H), 7.39 (br, 4H), 6.98 (br, 2H), 5.23 (s, 2H), 3.74 (s, 2H), 2.1 (s, 1H), 1.97 (s, 2H), 1.1 (br, 50), 0.77 (br, 9). (Mn = 33,000 g/mol, Mw = 50,400 g/mol).

2.5. Device fabrication and characterization

Organic photovoltaic cells (OPVs) based on PP-TPD:PC₇₀BM bulk heterojunction were fabricated on the indium tin oxide (ITO) coated glass substrates. The substrates were cleaned with detergent and then sonicated with water, acetone, and isopropyl alcohol for 20 min each. The ITO was treated with UV-ozone treatment to convert the surface property of the ITO from hydrophobic surface to hydrophilic surface. A hole transport layer of PEDOT:PSS (Al4083) was then spin-coated on top of the ITO (thickness of ~40 nm). The substrate was annealed at 140 °C for 10 min in air. The PP-TPD:PC₇₀BM solution was prepared at a concentration of 20 mg/mL as a function of a donor: acceptor ratio (1:1, 1:2, and 1:4 w/w) in dichlorobenzene without DIO and with DIO 3 vol.%. This solution was then spin-casted on top of the PEDOT:PSS layer. Then, a ~10 nm TiO_x layer as an electron transfer layer was formed on the photo-active layer by spin-coating. A ca. 100 nm aluminum (Al) layer as a cathode electrode was then deposited under a pressure of 2.0×10^{-6} Torr through thermal evaporation.

The current density-voltage (*J*-*V*) characteristics and impedance spectroscopy of the OPVs were measured using a ZIVE SP1 and a solar simulator with AM 1.5 Global conditions at an intensity of 100 mW/cm² and an illuminated cell area of 0.15 cm². After power calibration (ABET technologies, Inc., LS150, USA) with a monochromator (DONGWOO OPTRON Co., Ltd., MonoRa-500i, Korea), the incident photon-to-current efficiency (IPCE) spectra of the solar cells were determined in order to demonstrate that the short-circuit current of *J*_{sc} related to the *J*-*V* curves. The surface morphology of the blend of PP-TPD:PC₇₀BM without and with DIO 3 vol.% was observed by AFM (Park NX10) using non-contact mode and SEM.

For the charge carrier mobility measurements, hole-only devices were fabricated with the structure of ITO/PEDOT:PSS/PP-TPD:PC₇₀BM without and with DIO/Al. The Al layer was deposited at a speed of 1 Å/s to minimize the penetration of Al atoms (which created a noise) into the BHJ layer. The *J*-*V* characteristics of the single charge carrier devices were measured by modeling the current in a dark condition under an applied forward bias. The characteristics were then analyzed in the space charge limited region. The mobility was determined from the modified Mott-Gurney equation:

$$J = \frac{9}{8} \epsilon_0 \epsilon_r \mu \frac{V^2}{L^3} \exp\left(\frac{0.89\beta}{\sqrt{L}} \sqrt{V}\right)$$

where *J* is the current density, *L* is the thickness of the active layer, μ is the hole carrier mobility, ϵ_0 and ϵ_r are the electric permittivity of free space and the relative dielectric constant of the active layer, respectively, and β is the electric field-activation factor.

$$V = V_{appl} - V_r - V_{bi}$$

where *V*_{appl} is the applied voltage, *V*_r is the voltage drop due to contact resistance and series resistance across the electrodes, and *V*_{bi} is the built-in voltage.

Raman spectroscopy was performed using a Raman microscope

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