

Solvent-resistant small molecule solar cells by roll-to-roll fabrication via introduction of azide cross-linkable group



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ABSTRACT

A novel cross-linkable azide-functionalized diketopyrrolopyrrole based compound DPP(BT-N₃)₂ was designed and synthesized via Stille coupling. Cross-linking of such molecule could help us fabricate insoluble film which could be used to fabricate heterostructures through solution processing, without dissolving the pre-patterned layers. In order to investigate the photovoltaic performances of the newly synthesized compound, large area solar cells were produced by roll coating technique. Two set of devices were fabricated by employing DPP(BT-N₃)₂ as either an electron donor or acceptor. A best power conversion efficiency of 0.067%, combined with an open circuit voltage of 0.53 V, and a fill factor of 37.6% were obtained for the device with DPP(BT-N₃)₂ as an electron acceptor. In addition, we could prove that the large area small molecule based organic solar cells could be fabricated using roll coating, which could be used in the industries for large-scale of production.

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1. Introduction

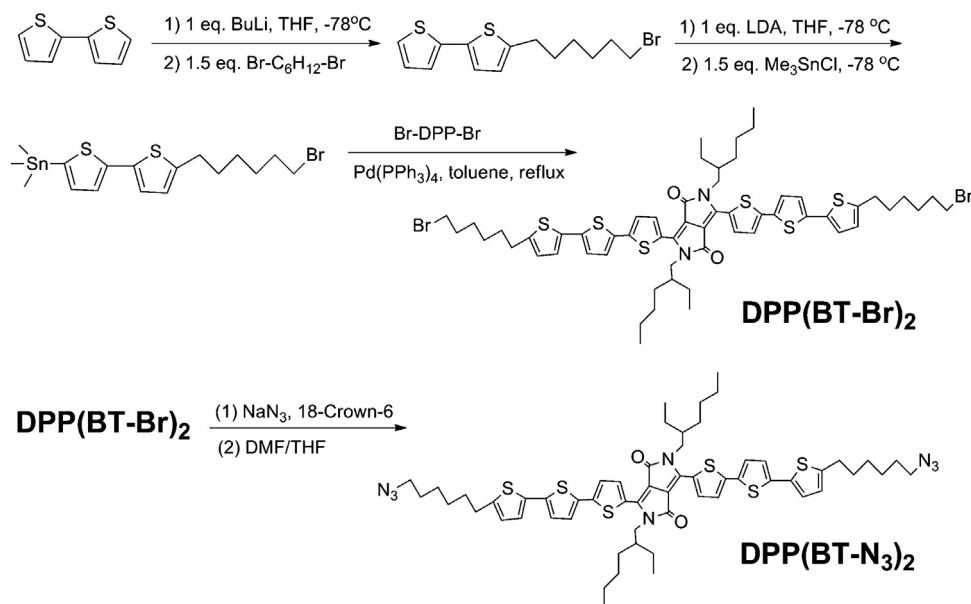
Since few decades intense research has been conducted in the area of organic photovoltaic (OPV) because it is believed to be a potential renewable energy source [1–3]. Mostly the conjugated polymers are widely used to fabricate organic electronic devices such as organic field-effect transistors, organic light-emitting diodes and organic solar cells (OSCs). But the researchers have diverted their attention toward organic small molecules because of ease of synthesis, purification, ease of tuning the bandgap by grafting various electron donating or withdrawing moieties, possibility of synthesizing donors and acceptors, etc. [4–7]. Moreover, small molecules are advantageous over the polymers because of their molecule regularity, high charge carrier transport, and less batch-to-batch variation in properties (reproducibility), crystallinity, and enhanced solubility [8–13].

In contrast to the vacuum-deposited small molecule based organic photovoltaic (SM-OPV) devices, the solution processed SM-OPV has shown great progress with increased power conversion efficiency (PCE). Especially, large area of active layers can be fabricated using solution processing techniques such as, spin coating, printing and doctor blading. Though a lot of small molecule based organic solar cells were fabricated and reported, most of them were processed at the laboratory level using a spin coater. But spin coating is difficult to integrate with roll-to-roll thin film fabrication techniques. Roll-to-roll (R2R) technique is widely used in the industries, which is capable of producing large-scale devices and it can be operated in a normal environment. This R2R device fabrication technique is normally used to fabricate polymer based organic electronic devices [14–16]. According the best of our knowledge, fabrication of SM-OPV by roll-to-roll coating has not been fulfilled. This is most likely due to the easier diffusion of active layers from the above-coated layers, especially for the inverted structure. Moreover, highly viscous liquids are necessary to pattern the uniform thin films [17,18]. The viscosity of the coating solution was increased by adding polystyrene to the solution. It has been reported that the addition of isotactic semicrystalline polystyrene to poly(3-hexylthiophene) (P3HT) had very little influence on the

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Scheme 1. Synthesis of DPP(BT-N₃)₂.

performance of organic field effect transistors and a decrease of mobility was observed only when the concentration of P3HT was reduced below 3 wt% [19]. Generally the conjugated molecules are unstable when they are exposed to air or solvent, which limits their practical application. Therefore, it is mandatory to design and synthesize new materials for the fabrication of stable OPVs. In order to overcome the lack of solvent resistance, a cross-linkable molecule can be used for securing a stable morphology, as was reported elsewhere [20–24]. So, it remains a great challenge for the researchers to identify a unique roll-to-roll thin film fabrication technique, which is capable of fabricating large scale small molecules based organic solar cells as well as the synthesis of new stable conjugated molecules.

As a first time, we have demonstrated that the diketopyrrolopyrrole (DPP) based cross-linkable organic small molecule solar cells can be fabricated by roll coating [25–29]. The cross-linkable DPP derivative was used as either the electron donor or acceptor component in a bulk heterojunction solar cell with [6,6]-phenyl-C61-butyric acid methyl ester (PCBM) as acceptor or P3HT as donor. The device performance was investigated to verify the feasibility of SM OPV by R2R processing. Solvent-resistant tests were also carried out to verify that cross-linking could indeed improve the morphological stability.

2. Experiments

2.1. Synthesis

All the chemicals were purchased from Aldrich or Acros and used without any further purification unless otherwise stated. Bithiophene and 1,6-dibromohexane were purchased from Aldrich Chemical Co, and used without any further purification. 3,6-bis(5-bromothiophen-2-yl)-2,5-bis(2-ethylhexyl)pyrrolo[3,4-c]pyrrole-1,4(2H, 5H)-dione was synthesized using the procedure published elsewhere [30]. ¹H and ¹³C NMR spectra were collected using a Bruker Avance II 500 (500 MHz) nuclear magnetic resonance spectroscope. UV–vis absorption spectra were recorded using a Shimadzu UV-1700 spectrophotometer.

The synthetic route of the targeted molecule was shown in Scheme 1. The detailed synthetic process was as follows.

2.1.1. 5-(6-Bromohexyl)-2,2'-bithiophene (Compound 1)

Bithiophene (6.1 g, 36.09 mmol) was thoroughly dissolved in 100 mL of anhydrous tetrahydrofuran (THF) under argon atmosphere in a three-neck round bottom flask. In addition, 1.6 M n-butyllithium in hexane (22.5 mL, 36.09 mmol) was added drop wise to the stirring bithiophene solution at -78°C . The reaction mixture was thermalized to room temperature after the successful completion of reaction. Subsequently, one portion of 1,6-dibromohexane (8.1 mL, 52.49 mmol) was added to that reaction mixture and stirred overnight. The reaction was quenched with deionized water (50 mL) and stirred for another 30 min. The mixture was poured into the water and extracted twice with diethylether. The crude product was purified using column chromatography (hexane as eluent) to afford the product as a white solid (4.3 g, yield 35.6%). ¹H NMR (500 MHz, CDCl₃), δ (ppm): 7.19 (dd, 1H, $J=5.1$ Hz, 1.0 Hz), 7.12 (dd, 1H, $J=3.5$ Hz, 1.0 Hz), 7.07–6.93 (m, 2H), 6.70 (d, 1H, $J=3.5$ Hz), 3.43 (t, 2H, $J=6.8$ Hz), 2.82 (t, 2H, $J=7.5$ Hz), 1.96–1.83 (m, 2H), 1.79–1.64 (m, 2H), 1.55–1.47 (m, 2H), 1.47–1.39 (m, 2H). ¹³C NMR (125 MHz, CDCl₃), δ (ppm): 144.90, 137.91, 134.92, 127.68, 124.84, 123.79, 123.42, 123.06, 33.84, 32.68, 31.35, 30.00, 28.14, 27.89.

2.1.2.

5'-(6-Bromohexyl)-[2,2'-bithiophen]-5-yl)trimethylstannane (Compound 2)

1.5 mL diisopropylamine and 24 mL of anhydrous THF were taken into a round bottom flask and mixed thoroughly under Ar ambient. The solution was cooled down to -78°C and 1.6 M n-butyllithium in hexane (6.6 mL, 10.63 mmol) was added drop wise to that mixture. The reaction mixture was allowed to warm to -15°C and stirred for 2 h. The freshly prepared solution of lithium diisopropylamine was added drop wise to the cooled (-78°C) solution of the compound 1 (3.5 g, 10.63 mmol). The reaction mixture was thermalized to -20°C for 3 h. Again that mixture was cooled down to -78°C and one portion of trimethyltin chloride (1.86 M, dissolved in THF) was added. Then the reaction mixture was stirred at room temperature for 12 h. It was quenched with 20 mL of deionized water and stirred for another 30 min. The mixture was poured into water and extracted with hexane twice to afford the product as a citrine solid (4.5 g, yield 86.0%), which was used without further purification. ¹H NMR (500 MHz, CDCl₃), δ (ppm): 7.24–7.21 (m, 2H),

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