



Influences of using a high mobility donor polymer on solar cell performance



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ARTICLE INFO

Article history:

Received 26 July 2013

Received in revised form 10 September 2013

Accepted 14 September 2013

Available online 25 September 2013

Keywords:

Organic photovoltaics

Organic solar cells

Polymer semiconductors

High mobility

ABSTRACT

We report a p-type polymer semiconductor, PDBFBT, which exhibits very high space charge limited current (SCLC) mobilities of up to $2.3 \times 10^{-2} \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$, which are among the highest reported so far. When the polymer is employed as a donor material in solution coated bulk heterojunction organic solar cells (OSCs), with PC₆₁BM as the acceptor, an efficiency of 4.53% and very high fill factors (>70% in some cases) are achieved. Furthermore, in the inverted device configuration, consistent power conversion efficiencies are demonstrated throughout a wide range of active layer thicknesses (~100 nm to ~800 nm). Our results demonstrate the benefits of using very high mobility donor polymers in solar cell applications and will be very useful for the development of new semiconductor materials, as well as the design of device structures for more feasible manufacturing of high efficiency, large area photovoltaic devices via high speed roll-to-roll printing processes.

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1. Introduction

Growing research efforts within the field of organic solar cells (OSCs) have led to rapid improvements in cell efficiency values over the last several years. The promise of lower manufacturing costs through roll-to-roll processes makes polymer-based solar cells particularly appealing [1], but a gap between the efficiency levels of organic and inorganic photovoltaic devices still remains. One factor that may contribute to the lower efficiency of OSCs is the poor charge carrier mobilities of polymers, which are typically several orders of magnitude lower than that of silicon and other inorganic semiconductors used for solar cells [2–4].

Recently a small number of polymer semiconductors for organic thin film transistor (OTFT) applications have shown hole mobility (μ_h) values on par with those of amorphous silicon [5–8]. Within diode configurations such as OSCs, however, polymers demonstrate much lower mobility due to the different device geometry and thus different charge transport characteristics [9]. Charge transport in the active layer of an OTFT device occurs parallel to the substrate surface between the source and drain electrodes, whereas in an OSC device, charge carriers (holes and electrons) traverse the active layer perpendicular to the substrate toward their respective electrodes (anode and cathode). Moreover, the presence of an acceptor material within the bulk heterojunction layer impacts the crystallinity, chain orientation, as well as the morphology of the polymer semiconductor, which often results in decreased mobility values [10]. Different techniques are therefore required for measuring the charge mobility of OTFT and OSC devices. For OTFTs, the field-effect transistor (FET) method [11] is generally employed, whereas methods such as space charge limited current (SCLC) [12,13] or carrier

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extraction by linearly increasing voltage (CELIV) [14] are used to characterize the vertical charge flow for OSCs.

The application of high mobility semiconductors in OSCs is expected to reduce charge recombination and thus contribute to improved efficiency through higher fill factors (FF) [15], as well as short-circuit current densities (J_{SC}). The influence of high mobility in OSCs on FF and J_{SC} has not been well established due to the limited number of high mobility polymers available for such studies. Poly(3-hexylthiophene) (P3HT), a commonly used polymer donor, is generally considered to possess one of the highest SCLC hole mobilities (μ_h), with values reported as high as $5 \times 10^{-3} \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ [16]. High SCLC μ_h values, on the order of $10^{-3} \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$, have also been reported for other donor polymers in neat films [17] and in blends with PCBM [18,19], which in some cases were associated with very high FF values (i.e. >65%) [18,19].

A diketopyrrolopyrrole (DPP)-based polymer, PDQT (Fig. 1a), was reported to show high hole mobility values of $\sim 1 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ in OTFT devices [20]. Recently we investigated the use of PDQT as a donor for OSCs [21] and found that this polymer showed very high SCLC hole mobility values, up to $2.0 \times 10^{-2} \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$, when blended with PC₆₁BM. The use of this high mobility polymer effectively suppressed charge recombination, leading to exceptionally high FF values ($\sim 70\%$). Moreover, the high mobility of PDQT allowed rather consistent efficiency values to be maintained over a wide range of active layer thicknesses (~ 100 – 800 nm) in the inverted device configuration. This overcomes the constraint that active layers consisting of commonly used donor and acceptor materials are required to be very thin ($\sim 100 \text{ nm}$) due to their poor charge carrier mobility [22–29].

A furan-based polymer, PDBFBT (Fig. 1b), which is a structural analogue of PDQT, was found to possess even higher hole mobility, up to $1.54 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$, in OTFTs [30]. PDBFBT is a rather attractive donor material for OSCs due to its optimum band gap ($\sim 1.4 \text{ eV}$) and its highly com-

patible energy levels with common acceptor materials such as PC₆₁BM (Fig. 1e). Several other furan-containing DPP polymers have been reported to demonstrate good OSC performance [31–36]. DPP-polymers comprising furan have greater solubility than their thiophene counterparts [32,35], which can lead to improved morphology in the active layer.

In this study, we found that neat PDBFBT films possess similar SCLC mobility values ($2.3 \times 10^{-2} \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$) to those of neat PDQT ($2.1 \times 10^{-2} \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$), which are among the highest SCLC mobility values for polymer semiconductors reported so far. We carried out systematic investigations on OSCs prepared with PDBFBT and PC₆₁BM using various donor/acceptor (D/A) ratios and active layer thicknesses in both standard and inverted configurations. Power conversion efficiencies (PCEs) as high as 4.53% were achieved in OSCs prepared with PDBFBT:PC₆₁BM, which are higher efficiencies than those achieved using PDQT as the donor. The inverted device configuration allows efficiency to be maintained throughout a wide range of active layer thicknesses ($\sim 100 \text{ nm}$ to $\sim 800 \text{ nm}$) and devices still show photovoltaic performance in layers as thick as $\sim 2 \mu\text{m}$. These results are attributed to the high SCLC μ_h of the donor material, PDBFBT.

2. Materials and methods

2.1. Materials

PDBFBT [30] and PDQT [20] were synthesized according to the literature. The number average molecular weight (M_n) and the polydispersity index (PDI) were measured by using a high-temperature gel-permeation chromatography (HT-GPC) at $140 \text{ }^\circ\text{C}$ with 1,2,4-trichlorobenzene as eluent and polystyrene as standards. The M_n and PDI of PDBFBT are 35, 300 and 2.60, respectively, while the M_n and PDI of PDQT are 21,100 and 2.72, respectively.

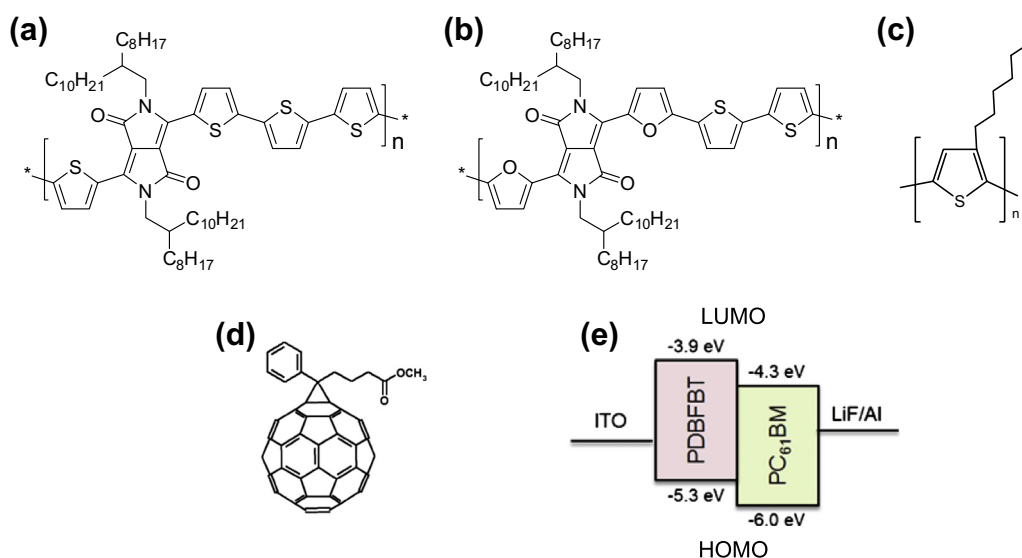


Fig. 1. Chemical structures of (a) PDQT, (b) PDBFBT, (c) P3HT and (d) PC₆₁BM. (e) Energy band diagram of PDBFBT:PC₆₁BM solar cell. Highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) values were taken from [30] and [48].

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