

Effect of shifting of aromatic rings on charge carrier mobility and photovoltaic response of anthracene and thiophene-containing MEH-PPE-PPVs

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ABSTRACT

We have investigated the charge carrier mobility and photovoltaic response of two thiophene-[**P1** (MEH-PPE₁-PThV₂) and **P2** (MEH-PThE₁-PPV₂)] as well as two anthracene-containing poly (phenylene-ethynylene) family of polymers [**P3** (MEH-PPE₁-PANV₂) and **P4** (MEH-PANe₁-PPV₂)], whereby the position of thiophene or anthracene has been shifted from between two double bonds (**P1** and **P3**) to the bridge between triple bond and double bond (**P2** and **P4**). **P2** shows better photovoltaic performance than **P1**, whereas similar photovoltaic characteristics were found for **P3** and **P4**. The devices using the blends of **P2** as donor and PCBM as acceptor (1:3 weight ratio) exhibited a short-circuit current density of $J_{SC}=5.2 \text{ mA/cm}^2$, an open-circuit voltage of $V_{OC}=800 \text{ mV}$, fill factor $FF=0.44$ and resulting power conversion efficiency $\eta_{AM\ 1.5}=1.8\%$.

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1. Introduction

Organic solar cell research has attracted worldwide attention during the last two decades. Organic semiconductors are easily processable, light weight, easy to integrate in a wide variety of devices and have chemically tunable properties.[1] These properties describe the advantages of organic “plastic” solar cells over that of conventional silicon solar cells.

Conjugated polymers, also known as semiconducting polymers, are distinguished by alternating single and double bonds between carbon atoms on the polymer backbone [2]. Polymeric organic solar cells mainly consist of an electron-donating conjugated polymeric material and an electron-accepting material, to make a mutually percolating structure with interpenetrating networks [3,4,5].

Among π -conjugated polymers, polythiophenes are promising candidates not only for organic solar cells but also for other optoelectronic devices such as light emitting diodes and field effect transistors (OFETs).[6] At present, the commonly used polythiophene derivatives, as the electron donor in polymer solar cells, are mainly poly(3-hexylthiophene) (P3HT) and poly(3-octylthiophene) (P3OT) [7,8,9]. Recently, Heeger et al. demon-

strated 6.1% bulk heterojunction solar cells with internal quantum efficiency reaching 100% [10]. Research on the subject of organic solar cells has focused on improving the power conversion efficiency of laboratory type organic solar cells and also focuses on the operational stability that can be achieved under ideal conditions [11–15]. The improvement in organic solar cells creates a demand for advanced materials with better absorption and transport properties. The main efforts for improvement are based on designing and developing new generation of materials among conjugated polymers [16].

In this study, we have investigated the hole mobility and the photovoltaic performance of two thiophene-containing polymers [poly{(1,4-(5-(2-ethylhexyl)oxy)-2-methoxy)-phenylene-ethynylene-1,4-(5-[(2-ethylhexyl)oxy]-2-methoxy)phenylene-vinylene-2,5-thiophenylene-vinylene)} (MEH-PPE₁-PThV₂) (**P1**) and poly{(1,4-(5-(2-ethylhexyl)oxy)-2-methoxy)-phenylene-ethynylene-2,5-thiophenylene-vinylene-1,4-(5-(2-ethylhexyl)oxy)-2-methoxy)-phenylene-vinylene} (MEH-PThE₁-PPV₂) (**P2**)] as well as two anthracene-containing polymers [poly{(1,4-(5-(2-ethylhexyl)oxy)-2-methoxy)-phenylene-ethynylene-1,4-(5-[(2-ethylhexyl)oxy]-2-methoxy)phenylene-vinylene-9,10-anthracenylene-vinylene)} (MEH-PPE₁-PANV₂) (**P3**) and poly{(1,4-(5-(2-ethylhexyl)oxy)-2-methoxy)-phenylene-ethynylene-9,10-anthracenylene-vinylene-1,4-[(5-(2-ethylhexyl)oxy)-2-methoxy]-phenylene-vinylene} (MEH-PANe₁-PPV₂) (**P4**)]. The difference between **P1** and **P2** as well as between **P3** and **P4** lies in the position of thiophene or anthracene in polymeric backbone.

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In this work, we have evaluated the photovoltaic performance of the **P1–P4** as donor materials with respect to (1) the position of either thiophene or anthracene within the conjugated backbone and (2) the density of the hydrophobic side chains around the conjugated backbone. The devices using the blends of **P2** and PCBM with 1:3 ratio showed J_{SC} of 5.2 mA/cm², a V_{OC} of 800 mV and fill factor of 0.44 which corresponds to the power conversion efficiency of 1.8%.

2. Experimental

The synthesis, molar masses thin film optical and electrochemical characteristics of the four polymers have been described elsewhere [17]. The chemical structures are depicted in Fig. 1 while Table 1 summarizes the SEC, optical and electrochemical data.

For solar cell preparation, as substrates, glass sheets of 1.5 cm × 1.5 cm covered with ITO, from Merck KG Darmstadt, were used with an ITO (indium tin oxide) and sheet resistance < 15 Ωcm⁻². The ITO was patterned by etching with an acid mixture of HCl:HNO₃:H₂O (4.6: 0.4: 5) for 30 min. The part of the substrate which forms the contact is covered with a scotch tape to prevent etching. The tape was removed after etching and the substrate was then cleaned using acetone and isopropanol in an ultrasonic bath.

Poly(3,4-ethylenedioxythiophene)–poly(styrenesulfonate) (PEDOT:PSS) was spin coated on the glass–ITO substrate, and dried under a dynamic vacuum.

The blends for the active layer with 1:1, 1:2, 1:3 or 1:4 (w:w) ratios of **PX**/PCBM (**X** stands for **1**, **2**, **3** and **4**), prepared by dissolving 6 mg of polymer and 12 mg of PCBM (in the case of 1:2) in 1 ml of chlorobenzene (CB) and stirring at 50 °C overnight. For the top electrodes, 0.6 nm of lithium fluoride (LiF) and 100 nm of Aluminum (Al) were thermally evaporated.

All current–voltage (*I–V*) characteristics of the PV devices were measured using a Keithley SMU 236 under nitrogen in a dry glove box. A Steuernagel solar simulator for AM1.5 conditions was used as the excitation source with an input power of 100 mW/cm² white-light illumination which was calibrated using a standard

crystalline silicon diode. The solar cells were illuminated through the ITO side.

The evaluation of the solar cells was carried out by using the power conversion efficiency.

$$\eta_{AM1.5}(\%) = \left(\frac{P_{out}}{P_{in}} \right) \times 100 = \frac{FF \times V_{oc} \times J_{sc}}{P_{in}} \times 100.$$

The percentage efficiency, $\eta_{AM1.5}$, is given by the ratio of the power output (P_{out}), to the power input from the solar simulator (P_{in} , 100 mW/cm²). The output power of a solar cell under illumination is the product of the fill factor FF, the open-circuit voltage V_{oc} (V) and the current density under short-circuit conditions J_{sc} (mA/cm²). The fill factor is obtained using the following equation:

$$FF = \frac{V_{mpp} \times J_{mpp}}{V_{oc} \times J_{sc}},$$

where maximum power point of the product of the voltage and the current density (V_{mpp} and J_{mpp}) is divided by the product of the open-circuit voltage and the short-circuit current.

The spectrally resolved photocurrent was measured with an EG&G Instruments 7260 lock-in amplifier. The samples were illuminated with monochromatic light of a Xenon lamp. The incident photon to current efficiency (% IPCE) was calculated according to the following equation:

$$IPCE(\%) = \frac{I_{sc} \times 1240}{P_{in} \times \lambda_{incident}},$$

Table 1
SEC thin film optical and electrochemical data of **P1–P4**. [17].

Code	M_n [g/mol]	M_w/M_n	P_n	λ_a [nm]	$E_{gt}^{opt\ b}$ [eV]	HOMO [eV]	LUMO [eV]	E_g^{elec} [eV]
P1	16 600	1.9	26	508	2.11	5.17	3.23	1.94
P2	32 500	2.3	52	499	2.11	5.15	3.15	2.00
P3	33 000	2.4	46	453	2.22	5.21	3.23	1.98
P4	31 000	2.5	43	506	2.05	5.23	3.35	1.88

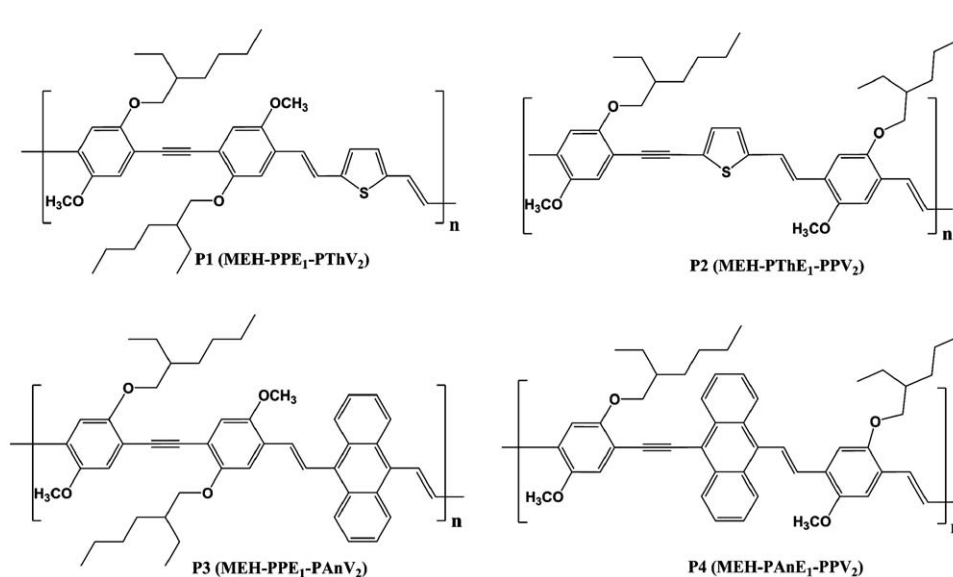


Fig. 1. Chemical structures of the polymers.

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