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Fabrication and Characteristics of Fullerene–Perylene Dyad Based Organic Photovoltaic Cell

Byoung Min So¹, Chan Moon Chung², and Se Young Oh^{1,*}

¹Department of Chemical & Biomolecular Engineering, Sogang University, Seoul 121-742, Korea ²Department of Chemistry, Yonsei University, Wonju, Kangwon-do 220-710, Korea

Fullerene is an acceptor material which is used most usually in organic photovoltaic cell. By the way, the reduction of electron mobility and the phase separation of conducting polymer and fullerene in the actual bulk heterojunction photovoltaic cell limit further improvement of device performance. In order to overcome the problems, fabrication of hybrid planar mixed heterojunction cells and synthesis of donor–acceptor dyad have been studied. In the present work, we have synthesized fullerene–perylene dyad to improve the fullerene based photovoltaic cell. In order to explore the properties of the synthesized material, the measurements of absorption spectrum and energy level were carried out. We have investigated the energy conversion efficiency of organic photovoltaic cell consisting of ITO/PEDOT-PSS/MEH-PPV:fullerene–perylene dyad/AI.

Keywords: Photovoltaic Cell, MEH-PPV, Fullerene–Perylene Dyad, Energy Conversion Efficiency.

1. INTRODUCTION

Organic photovoltaic cells have attracted considerable attention due to their potential for low cost solar energy conversion.¹⁻⁶ Since donor-acceptor (D-A) heterojunction organic photovoltaic cell having 0.95% efficiency using copper phthalocyanine and perylene tetracarboxylic derivative was reported by Tang et al., the power conversion efficiency has steadily improved through the development of new materials and device structures.^{7,8} The discovery of ultrafast photoinduced charge transfer from conducting polymer to Buckminsterfullerene C₆₀ has promoted research towards high efficiency organic photovoltaic cells.9-11 Actually, the structure of fullerene is favorable to serve as a strong electron acceptor in both ground and excited states. However, the low solubility in most solvent, the reduction of electron mobility and the phase separation formed in the bulk heterojunction photovoltaic devices using conducting polymer and fullerene limited further improvement of energy conversion efficiency.

The synthesis of fullerene derivatives and the control of photovoltaic cell structures have been widely studied to improve the energy conversion efficiency of photovoltaic cell. Methanofullerene [6,6]-phenyl C_{61} -butyric acid methyl ester (PCBM) is the representative fullerene

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derivative material that solubility and electron mobility was improved. Also, synthesis of donor–acceptor dyad based on fullerene has been carried out.¹² Reduction of electron mobility in bulk heterojunction structure was confirmed by Förrest et al.^{13, 14} Planar mixed hetero junction of D/D + A/A structure has designed to overcome the reduction problem.

In the present work, we have synthesized fullerene derivative (FP) containing perylene moiety that has high electron mobility, electron acceptor property and optical activity. And then, physical and electrical properties of synthesized FP were investigated with UV-Visible, cyclic-voltammetry and current–voltage source meters. We have investigated the energy conversion efficiency of organic photovoltaic cells consisting of ITO/PEDOT-PSS/MEH-PPV:FP/Al under various FP contents.

2. EXPERIMENTAL DETAILS

2.1. Reagents and Materials

Fullerene (C_{60}), sarcosine, perylene and poly(2-methoxy-5-(2-ethylhexyloxy)-1,4-phenylenevinylene (MEH-PPV) were purchased from Aldrich Co. Ltd. Poly(3,4ethylenedioxythiophene):poly(styrenesulfonate) complex (PEDOT-PSS) was purchased from Bayer Co. Ltd. Other chemicals were used as a reagent grade. Synthesis of

^{*}Author to whom correspondence should be addressed.

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Scheme 1. Synthetic route of fullerene-perylene derivative (FP).

fullerene-perylene derivative (FP) was carried out following the synthetic routes as shown in Scheme 1.

2.2. Synthesis of Fullerene–Perylene Derivative (FP)

2.2.1. 3-Fomylperylene

Perylene (3.9 mmol) in 1,2-dichlorobenzene (100 mL) was stirred under N₂ atmosphere. 1,1-Dichloromethyl methyl ether (5.1 mmol) and TiCl₄ (5.9 mmol) were subsequently added, and the mixture was stirred for 1 h, then allowed 5 to warm to room temperature. The reaction mixture was poured onto ice (100 g) and concd. HCl (5 mL). The organic layer was diluted with chloroform (100 mL), washed with 5% HCl (100 mL), water (300 mL), dried over Na₂SO₄ and evaporated. The residue was purified by column chromatography on silica gel in CHCl₃ to give a desired compound as orange crystal (57 mg, 50.9%).¹⁵

2.2.2. Fullerene-Perylene Derivative (FP)

A mixture of C_{60} (0.3 mmol), 3-formyl perylene (0.32 mmol) and sarcosine (1.2 mmol) in dried toluene was refluxed for 24 h under N₂ atmosphere. The resulting mixture was concentrated and separated on a silica gel column using toluene/petroleum ether (8:1) to give a FP (176 mg, 56.7%). Anal. Calc. C: 96.97%, H: 1.67%, N: 1.36%; Found C: 96.82%, H: 1.83%, N: 1.31%.

2.3. Spectroscopic Measurements

UV-Visible absorption spectrum was performed using UV/VIS/NIR spectrophotometer (Jasco V-570, Japan). The redox behavior of FP was studied through the measurement of cyclic voltammetry (CV) (IM6 system, Zahner Elektrik Co., Germany). The photovoltaic cell configuration used in the present study was ITO/PEDOT-PSS/MEH-PPV:FP/A1. All layers were fabricated on patterned ITO ($\leq 15 \Omega/\Box$) glass substrate using vacuum evaporation technique (ULVAC VTR-300M/1ERH evaporator, Japan) under 10⁻⁶ Torr. Before film fabrication, the patterned ITO substrate was immersed into ultrasonic bath of deionized water, acetone and methanol for 60 min, subsequently. Then cleaned ITO glass substrate was rinsed in deionized

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water and blown by N_2 gas. Current–voltage characteristics were measured using source meters (KEITHLEY-2400, 237).

3. RESULTS AND DISCUSSION

Figure 1 showed the UV-Visible absorption spectra of perylene, fullerene and FP compounds in 1,2-Dichlorobenzene solution. As shown in Figure 1, the absorption spectrum of the FP compound is similar to the sum of absorption spectra of two individual compounds of perylene and fullerene. This result suggests that there is no ground-state interaction between the two chromophores, perylene and fullerene. If the charge transfer of ground-state occurs between fullerene and perylene compounds, charge transfer absorption band appears in the 450~650 nm region. The absence of any characteristic charge transfer band in the absorption spectrum of FP implies that any charge separation occurs only after localized excitation on the perylene moiety.16 The redox behavior of FP was investigated with a CV. The cyclic voltammograms are shown in Figure 2, and the data are listed in Table I. We obtained the value of highest occupied molecular orbital (HOMO) level and lowest unoccupied molecular orbital (LOMO) level of FP using the cyclic voltammogram curve. LUMO level of FP was higher than



Fig. 1. UV-Visible absorption spectra of fullerene, perylene and fullerene–perylene derivative in 1,2-dichlorobenzene.

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10 8

6

_4

-8

-10

-1.5

-1.0

-0.5

0.0

Fig. 2. Cyclicvoltammogram of fullerene-perylene derivative.

Potential / V vs Ag/AgCl

Current (µA) 2 0 -2

0.5

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1.0

2.0

1.5

fullerene because of the effect of perylene moiety containing electron donating property. In general, it has been by Ir found that the addition of the electron donating group to the fullerene is expected to the increase of LUMO level. 95. Figure 3 showed current-voltage characteristics for Sthe 201 devices consisting of ITO/PEDOT-PSS/MEH-PPV:C₆₀ or FP/Al. In the case of MEH-PPV:C₆₀, measured open circuit voltage (Voc) is 0.57 V, short circuit current density (Isc) is 2.0 mA/cm², fill factor is 0.13, and power conversion efficiency is 0.18%. In the case of MEH-PPV:FP, Voc and Isc are increased to 0.73 V and 3.25 mA/cm², respectively. Fill factor is 0.12 and power conversion efficiency is 0.30%. Thus, it should be noted that efficiency of photovoltaic cell was improved using fullereneperylene derivative which is mainly due to the increase of LUMO level compared to the LUMO level of C₆₀ and exciton generation according to the introduction of perylene moiety containing optical activity. In order to explore the current-voltage characteristics, spin-cast bulk heterojunction organic photovoltaic cells were fabricated under various weight ratios of MEH-PPV and FP. Figure 4 showed the result of current-voltage characteristics. Voc is 0.65~0.73 V and fill factor is 0.13~0.16, which are almost constant independent of FP contents. However, the Isc was increased with increasing FP content up to 50 wt%owing to the increase of electron mobility. In the case of FP over 50 wt%, Isc was decreased, which is caused to the aggregation of bulky FP molecules.

Table I. The redox potentials and energy level of fullerene-perylene derivative.

E_1 (V)			E_2 (V)			Energy level (eV)		
E _{pc}	$E_{\rm pa}$	$E_{1/2 \text{ox}}$	$E_{\rm pc}$	E_{pa}	$E_{1/2 \mathrm{ox}}$	E _{HOMO}	$E_{\rm LUMO}$	$E_{\rm g}$
1.13	1.17	1.15	-0.71	-0.46	-0.59	5.40	3.65	1.74



Fig. 3. Current-voltage characteristics for ITO/PEDOT-PSS/MEH-PPV:C₆₀/Al (solid line), ITO/PEDOT-PSS/MEH-PPV:FP/Al (dash line).



Fig. 4. Current-voltage characteristics of phohtovoltaic cells consisting of ITO/PEDOT-PSS/MEH-PPV:FP/Al under various ratios.

4. CONCLUSIONS

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A novel fullerene-perylene dyad compound was successfully synthesized. And then, organic photovoltaic cell consisting of ITO/PEDOT-PSS/MEH-PPV:FP/Al was fabricated. Open circuit voltage and short circuit current of the prepared device using fullerene-perylene dyad was increased compared to the case of C₆₀, which is mainly due to the increase of LUMO level and electron carriers. Especially, it can be concluded that the photovoltaic cell using FP exhibited high energy conversion efficiency of 0.30%.

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