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Organic thin-film solar cell employing a novel electron-donor material

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1. Introduction

Organic materials have long attracted widespread attention in the field of electronics. For example, organic LEDs have been commercialized as a next-generation flat-panel display. In the field of solar cells, organic materials have also been attractive for next-generation solar cells because they have a high potential to become an alternative to the widely used Si. In particular, thin-film organic photovoltaic (OPV) cells employing organic small-molecule materials [1] have led to a significant reduction in production costs, and are targeted for Si-free and low-cost PV cells.

However, one of the significant shortcomings in present OPVs compared to Si-based PVs is that the conversion efficiency is much lower. The following four factors are necessary to obtain high-efficiency OPVs: (i) effective light absorption, (ii) a long exciton diffusion length, (iii) efficient charge separation, and (iv) efficient charge collection. Considerable research efforts spent for high-efficiency OPVs are predominantly aimed at developing the device structure, such as the insertion of an exciton-blocking (EB) layer [2,3], a bulk heterojunction interface structure [6–9]. In particular, using a bulk heterojunction interface structure is very effective for achieving high efficiency.

Meanwhile, the development of new materials, which originally exceed inorganic-based PVs in variety, is making slow progress. Especially, for an electron-donor (ED) material, copper phthalocyanine (CuPc) has been used ever since a classical device

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ABSTRACT

A highly efficient organic thin-film solar cell based on a heterojunction structure employing a novel electron-donor (ED) material, tetraphenyldibenzoperiflanthene (DBP), has been demonstrated for the first time. An organic photovoltaic (OPV) cell with 0.033-cm² active area, comprising DBP as an ED layer, fullerene C₆₀ as an electron-acceptor (EA) layer, and 2,9-dimethyl-4,7-diphenyl-1,10-phenanthroline as an exciton-blocking (EB) layer, has exhibited an open-circuit voltage (V_{oc}) of 0.92 V, a short-circuit current density (J_{sc}) of 6.3 mA/cm² and a conversion efficiency of 3.6% at 100-mW/cm² simulated AM1.5G sunlight. Meanwhile, those of a conventional cell employing copper phthalocyanine (CuPc) for an ED layer are 0.51 V, 4.3 mA/cm², and 1.4%, respectively. The high V_{oc} and J_{sc} of the DBP-based cell is attributed to the DBP's highest occupied molecular orbital (HOMO) level 5.5 eV and the effective light absorption, respectively.

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consisting of a heterojunction between donor and acceptor organics was reported [1–3,7]. Hence, developing a new organic material is a significant matter since it may greatly enhance the cell performance.

We have demonstrated a high-efficiency OPV cell employing a novel ED material, tetraphenyldibenzoperiflanthene (DBP) [10], for the first time. Here, the performance of the cell is compared with that of a conventional OPV comprising CuPc as an ED material, with other aspects being the same as in the present device.

2. Experimental method

Fig. 1 shows the fabricated device structure and the function of each layer. Fig. 2 shows the molecular structure of each organic material. As shown in Fig. 2(a), DBP has no negative environmental impact because its molecule is composed of only carbon and hydrogen. DBP and CuPc were used as the ED layer. Moreover, fullerene C₆₀ and 2,9-dimethyl-4,7-diphenyl-1,10-phenanthroline (BCP) were used as an electron-acceptor (EA) layer and as an EB layer, respectively. The optimized thicknesses of the ED material, C_{60} , and BCP in the present and cells are 200, 500, and 100 Å, and in the conventional cells are 500, 400, and 100 Å, respectively. Each organic layer was intentionally not mixed in the heterointerface region. A mixed heterointerface structure is known to be effective for achieving high-efficiency OPVs. However, we used a planar heterointerface structure because our main purpose in this study was to compare the potential of the ED materials. From this standpoint, we did not use an annealing process after the device fabrication.

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Fig. 1. The fabricated device structure and the function of each layer.



Fig. 2. Molecular structure of organic materials: (a) tetraphenyldibenzoperiflanthene, (b) copper phthalocyanine, (c) fullerene C_{60} , and (d) 2,9-dimethyl-4,7diphenyl-1,10-phenanthroline.

All devices were fabricated on 800-Å-thick layers of indiumtin-oxide (ITO) pre-coated onto glass substrates with a sheet resistance of 50 Ω /sq. The ITO surface cleaned by isopropyl alcohol was treated in ultraviolet/O₃ for 5 min immediately before loading the substrates into a high-vacuum chamber with a base pressure of 3×10^{-7} Torr, where each organic layer and a 2000-Å-thick Al cathode were deposited via thermal evaporation. Prior to deposition, the organic materials were purified by a recrystallization method and by repeated vacuum thermal gradient sublimation. The Al cathode was evaporated through a shadow mask to define a small cell area of 0.033 cm² and a large cell area of 1.6 cm². The fabricated cells were sealed using glass cap with desiccant in a N₂ atmosphere.

Absorption coefficient spectra of DBP and CuPc films on quartz glass substrates were measured using a HITACHI U4000 UV–vis spectrophotometer. The highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO) energies of organic materials were estimated from their oxidation and reduction levels as measured using cyclic voltammetry. The current density versus voltage (*J–V*) characteristics were measured in the dark and under AM1.5G simulated solar illumination of 100 mW/cm² (1 sun) at 25 °C in the air. Illumination intensity measurements were conducted using standard methods employing a National Institute of Advanced Industrial Science and Technology (AIST) traceable calibrated Si detector. External quantum efficiencies (EQE) were measured with a spectral sensitivity analysis system that utilized a 500-W Xe lamp for monochromatic light, calibrated against a calibrated Si photodiode.

3. Results and discussion

Fig. 3 shows the absorption coefficient spectra of DBP and CuPc films on quartz glass substrates. It is very important for solar cells that the absorption coefficient of the active layer is high because the device thickness to obtain sufficient light absorption can be relatively thin. In particular, it is difficult to fabricate OPVs with a

thickness that obtains sufficient light absorption since the exciton diffusion length is too short. One of the factors of the short exciton diffusion length is that the exciton lifetime of organic materials is very short, i.e. from a few nanoseconds to hundreds of nanoseconds. Therefore, an organic material with high light absorption has a high potential to be able to supplement the loss by the short exciton diffusion length. As shown in Fig. 3, the absorption coefficient of DBP film significantly exceeds that of CuPc in the visible wavelength region. In particular, DBP has shown high absorption in the range 550–600 nm, where the sun's spectrum strength is strong. This means that DBP offers effective light absorption for a solar cell. Therefore, this result suggests that the J_{sc} can be improved using DBP instead of CuPc for the ED layer.

Fig. 4 shows the energy diagram of EA and ED materials estimated from their oxidation and reduction levels as measured using cyclic voltammetry in (a) a DBP-based cell, and (b) a CuPc-based cell. The theoretical maximum V_{oc} is determined by the energy gap between the HOMO energy of an ED material and the LUMO energy of an EA material [11]. For improving the V_{oc} , it is necessary to increase the HOMO energy of the ED material or lower the LUMO energy of the EA material, so that V_{oc} depends on the combination of the ED and EA materials, and not on the device structure. This means that an ED material with high HOMO energy or an EA material with low LUMO energy has a high potential to



Fig. 3. The absorption coefficient spectra of DBP and CuPc films on quartz glass substrates.



Fig. 4. An energy diagram of EA and ED materials estimated from their oxidation and reduction levels as measured using cyclic voltametry in (a) a DBP-based cell, and (b) a CuPc-based cell.

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