

Efficient small molecule-based bulk heterojunction photovoltaic cells with reduced exciton quenching in fullerene



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ABSTRACT

Most highly efficient small molecule-based bulk heterojunction (BHJ) photovoltaic cells contain a large concentration of fullerene in their blend active layers. However, the excitons generated in fullerene can seriously quench at the surface of the commonly used MoO₃ buffer layer, becoming a key limitation to the photovoltaic performance of these cells. In this study, we've investigated various anode buffer layers in the thermally evaporated tetraphenyl-dibenzoperiflanthene (DBP) and C₇₀-based BHJ cells with high C₇₀ concentration. It's been found that obviously enhanced power conversion efficiency (PCE) of up to 6.26% can be obtained in DBP and C₇₀-based BHJ cells via simply replacing the MoO₃ buffer by poly(3,4-ethylenedioxythiophene): poly(styrenesulfonate) (PEDOT: PSS), which is also a commonly used anode buffer material in polymer-based BHJ cells. Photoluminescence spectra results have confirmed the suppression of exciton quenching at the anode interface by inserting this PEDOT: PSS buffer. Moreover, after adding a C₇₀ interlayer for better electron extraction and the further suppression of exciton quenching, the DBP and C₇₀-based M-i-n photovoltaic cells show a remarkable PCE of 7.04% under illumination with 100 mW/cm², AM 1.5G simulated solar light.

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1. Introduction

Small molecule-based organic photovoltaic (OPV) cells have attracted great research interest over many years due to their potential as lightweight, low-cost, and flexible energy sources, and significant efforts have been devoted to develop various donor materials and device architectures to enhance their photovoltaic performance. In recent years, high power conversion efficiencies (PCEs) have been achieved by developing bulk heterojunction (BHJ) small molecule-based OPV cells with low donor concentration in a fullerene matrix via either thermal evaporation or solution processes [1–7]. The bulk heterojunction structure comprising a uniformly distributed donor/acceptor (D/A) blend active layer is beneficial for efficient exciton dissociation at the D/A interface [1–3,8–11]. On the other hand, since the hole mobility of small molecule donors is usually much lower than the electron mobility of fullerene, employing a low donor ratio will give more balanced carrier transport in BHJ OPV cells, which can promote better charge extraction and reduce charge recombination in the blend active region [4,12,13]. In most small molecule-based BHJ OPV cells, especially the thermally evaporated ones, MoO₃ is employed as the

anode buffer layer due to its deep work function that is favorable for efficient hole-extraction [3,14]. However, as previously reported, excitons generated in the fullerene may easily quench at the MoO₃/fullerene interface [15], which becomes a key limitation to the photovoltaic performance in such BHJ OPV cells with a low donor ratio and high fullerene ratio.

In this study, we've demonstrated that largely improved photovoltaic performance of tetraphenyl-dibenzoperiflanthene (DBP) and C₇₀-based BHJ OPV cells with high C₇₀ concentration can be achieved through simply replacing the MoO₃ anode buffer by poly(3,4-ethylenedioxythiophene): poly(styrenesulfonate) (PEDOT: PSS), which is an anode buffer material extensively used in polymer-based BHJ OPV cells [10,11]. Photoluminescence (PL) spectra confirmed the suppression of exciton quenching at the interface of the C₇₀ and PEDOT: PSS layers. With a PEDOT: PSS anode buffer layer, a PCE of 6.26% can be obtained in DBP and C₇₀-based BHJ cells with enhanced external quantum efficiency (EQE) and short-circuit current density (J_{sc}) compared with those cells with a MoO₃ buffer. In addition, after adding a C₇₀ interlayer for further reduced exciton quenching in C₇₀ and better electron extraction, the so-called M-i-n OPV cells-based on DBP and C₇₀ present an even higher PCE of up to 7.04% with an open-circuit voltage (V_{oc}) of 0.88 V, a fill factor (FF) of 0.59, and a J_{sc} of 13.4 mA/cm² under illumination of 100 mW/cm², AM 1.5G simulated solar illumination.

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2. Experimental

The materials used in our devices, including MoO₃, 1,4,5,8,9,11-hexaazatriphenylene hexacarbonitrile (HAT-CN) [16], DBP [17], C₇₀, and bathocuproine (BCP) are commercially available. MoO₃ and BCP were used as received. C₇₀ and DBP were purified by multistep thermal sublimation. All the OPV devices were fabricated on indium-tin-oxide (ITO) coated glass substrates. The substrates were precleaned using deionized water, acetone and isopropanol under sonication and then treated with UV-ozone for 30 min prior to use. MoO₃, C₇₀, BCP, and the Al cathode were deposited via thermal evaporation under high vacuum at base pressure of $\sim 5 \times 10^{-5}$ Pa. PEDOT:PSS films of 30 nm thickness were prepared via spin coating. The Al cathode was deposited through a shadow mask, and the overlap between the ITO anode and the Al cathode defined an active area of 3×3 mm². After the deposition of the Al cathode, the devices were transferred directly to a nitrogen-filled glove box for encapsulation without exposure to air. The EQE and current density–voltage (*J*–*V*) characteristics were measured by an integrated characterization system for thin film solar cells, CEP-2000 by Bunkoukeiki Co. The PCE was measured under 100 mW/cm² illumination of AM 1.5G solar spectrum. A reference silicon diode with a KG-5 filter certified by the National Institute of Advanced Industrial Science and Technology in Japan was used to calibrate incident light intensity. Absorption spectra were measured by a SHIMADZU MPC-2200 UV–visible spectrophotometer. Surface roughness profiles were measured with AFM (Veeco). The HOMO levels of the fullerene materials were determined using Riken Keiki AC-3. The LUMO levels were then derived by subtracting the optical band gaps from the HOMO levels. The PL spectra were obtained using a commercial spectrophotometer equipped with a standard solid sample holder, and all of the samples were

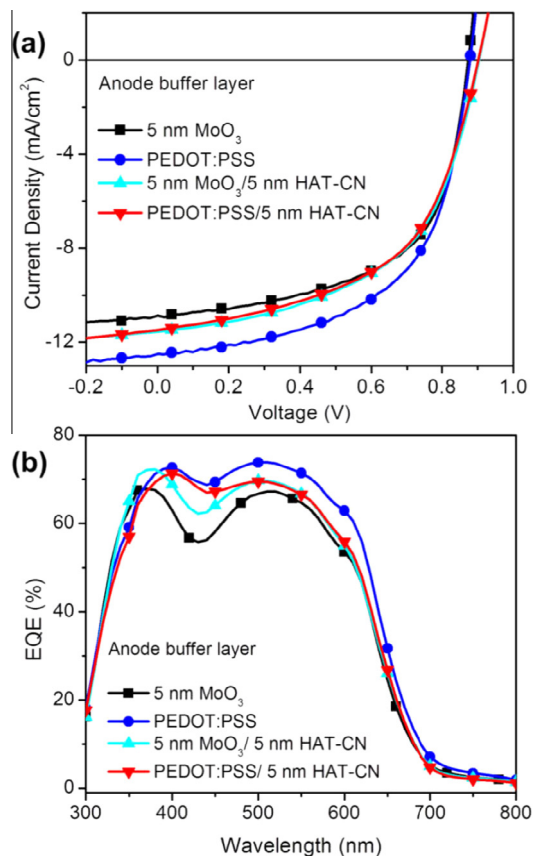


Fig. 2. (a) *J*–*V* curves of DBP and C₇₀-based BHJ cells using different anode buffer layers and (b) the corresponding EQE spectra.

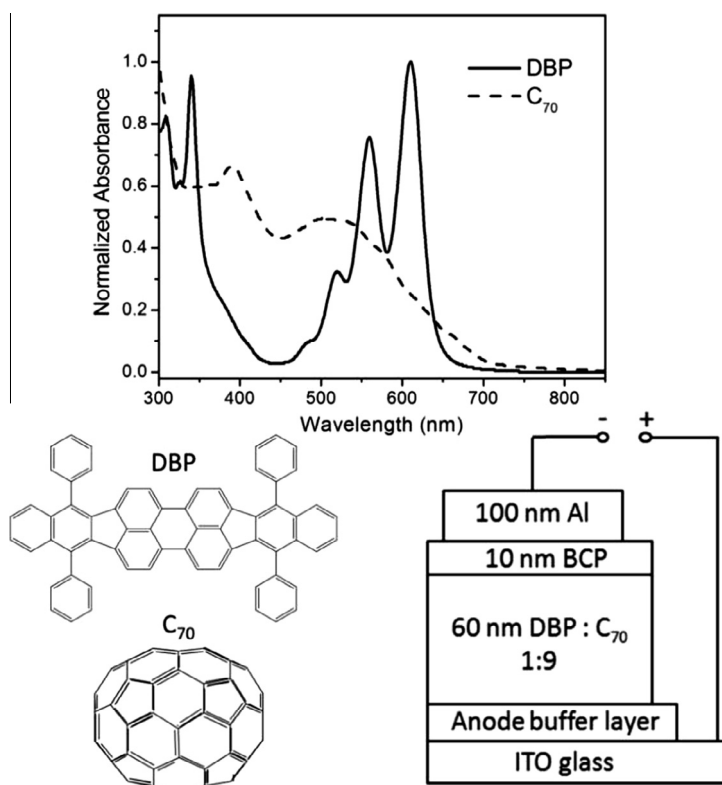


Fig. 1. The normalized absorption spectra of DBP and C₇₀, their chemical structures and the device architecture of DBP and C₇₀-based BHJ cells with various anode buffer layers.

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