



Towards optimization of functionalized single-walled carbon nanotubes adhering with poly(3-hexylthiophene) for highly efficient polymer solar cells

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ABSTRACT

In this paper, we present the optimization of single-walled carbon nanotubes (SWCNTs) by acid-treatment, solution ultrasonication time and dispersion in photoactive layer for efficient organic solar cells. After non-covalently adhering with poly(3-hexylthiophene) (P3HT), pre-functionalized SWCNTs were blended into the composites of P3HT and [6,6]-phenyl-C₆₁-butyric acid methyl ester (PCBM) as photoactive layer, and a maximum power conversion efficiency (PCE) of 3.02% with a short-circuit current density of 11.46 mA/cm² was obtained from photovoltaic cell indium-tin oxide (ITO)/poly(ethylene-dioxythiophene):poly(4-styrenesulfonate) (PEDOT:PSS)/P3HT:PCBM:SWCNTs/Al with an optimum 0.3 wt% SWCNTs in P3HT:PCBM:SWCNTs nanocomposite, the PCE can be enhanced by more than 10% as compared to the control device ITO/PEDOT:PSS/P3HT:PCBM/Al. The performance improvement by incorporating with functionalized SWCNTs is mainly attributed to the extension of excitons dissociation area and fastening charge carriers transfer across the active layer.

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1. Introduction

Organic solar cells (OSCs) are of great interest as potential renewable energy sources and have displayed significant potential for competition with conventional inorganic photovoltaic cells. These solar cells are fabricated from inexpensive organic materials, employ easy preparation methods, and can be deposited on large scale and low weight flexible substrates. Most current high-efficiency organic solar cells consist of a bulk heterojunction (BHJ) of semiconducting polymers and fullerene derivatives [1,2]. The enormous donor–acceptor interfacial area of the BHJ maximizes the opportunity for exciton dissociation, overcoming the short exciton diffusion lengths of organic materials [3]. The BHJ structure, however, is often considered less optimal for charge transport due to the lack of dedicated pathways for each type of carrier [4]. This morphological limitation of the BHJ, along with the intrinsic slow transport properties of organic semiconductors, makes it challenging to utilize the full potential of organic solar cells [5].

One straightforward way to address the retarded carrier transport in organic solar cells is to incorporate one-dimensional nanomaterials, such as nanorods [6–8] or nanotubes [9–13], within semiconducting materials. In this regard, carbon nanotubes (CNTs) are an ideal material, as they have excellent carrier mobility, mechanical flexibility, and compatibility with the solution process [14–16]. Despite these conceptual advantages, however, solar cells with CNTs incorporated in their semiconducting active layers have demonstrated significantly

poorer performance than those without CNTs [10,17]. Without charge selectivity, any small proportion of metallic CNTs present may build up undesired pathways for electron–hole recombination [9]. Furthermore, inhomogeneously dispersed CNT aggregates give rise to a fatal device short circuit.

Most recently, a highly efficient polymer–fullerene BHJ solar cells with a certified efficiency of 9.2% was reported [18], using an inverted structure which simultaneously offers ohmic contact for photogenerated charge-carrier collection and allows optimum photon harvest in the device. Usually, poly(3-hexylthiophene) (P3HT) and the fullerene soluble derivative [6,6]-phenyl-C₆₁-butyric acid methyl ester (PCBM) were used as electron donors and electron acceptors in OSCs, respectively, and efficient exciton dissociation and charge transport can be accomplished within P3HT:PCBM blend in a weight ratio of 1:0.8 [19]. Also, single-walled carbon nanotubes (SWCNTs), which are one-dimensional nanostructures with outstanding electron-transporting properties, high surface area, and chemical properties, have been successfully added in organic photovoltaic devices as the electron acceptor material [20,21]. Therefore, SWCNTs are a kind of ideal materials and they can provide effective carriers transport channels. However, it is a challenge to disperse SWCNTs in the polymer mixtures homogeneously, owing to their ability to form bundles. SWCNTs can be chemically modified, covalently or non-covalently, allowing a good dispersion in a polymer matrix. It has been demonstrated that covalently modified SWCNTs can improve the dispersity and result in a more homogenous photoactive layer [22–24]. However, one of the disadvantages is the negative effect of covalent functionalization on the electronic properties of the potential interfaces for charges transfer between SWCNTs and conjugated polymers. In

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addition, the complex process of covalent functionalization and the long time of preparation increase the production cost of solar cells. To wrap pre-functionalized CNTs with polymers is a common method to improve CNTs dispersion [25–27] in solution and to preserve the electronic properties of the unmodified molecules. The non-covalent π – π stacking interaction leads to efficient dispersion of the SWCNTs in the P3HT solution [28], and it was reported that P3HT adheres better to nanotubes than other conjugated polymers [29].

In the three-component SWCNT–fullerene–conjugated polymer system, fullerenes (or PCBM) are for efficient charge separation while SWCNTs are for high-mobility pathways for electron transport to improve organic photovoltaic properties. The efficiencies of the P3HT:C₆₀–SWCNT-based photovoltaic cells were reported to be relatively low as compared to the widely studied P3HT:PCBM cells [30]. Berson et al. [17] reported that the power conversion efficiency (PCE) of P3HT:PCBM:(0.1 wt%) CNT-based BHJ solar cell finally reached 2% with short circuit current density $J_{SC} = 9.3 \text{ mA/cm}^2$, open circuit voltage $V_{OC} = 0.57 \text{ V}$ and fill factor $FF = 0.38$. Kymakis et al. [31] reported that solar cells based on P3HT:PCBM (1:1) mixture with functionalized SWCNTs (0.5 wt%) showed a PCE of 1.4% at illumination of 100 mW/cm^2 . Recent studies have demonstrated that the incorporation of the covalently functionalized SWCNTs in P3HT:PCBM-based and PTB7:PC₇₁BM-based solar cells demonstrated a PCE of 3.6% [32] and 8.6% [23], respectively. However, the said reported preparations of covalently functionalized SWCNTs are complicated and usually they destroy the chemical structure of SWCNTs. Therefore, it is essential to explore novel methods of acid-treatment and retain their excellent mechanical and electrical properties. It is reasonable for someone to know how much it can improve the efficiency by this method.

Therefore, under the condition of trying to keep the chemical and electrical properties of SWCNTs, in this paper we present two acid-treatment methods to functionalize SWCNTs and compared them with each other, and we found that the original chemical structure of SWCNTs was not destroyed by these two methods. After decorating functionalized SWCNTs with P3HT, we fabricated and characterized P3HT:PCBM:SWCNTs-based solar cells. Our experimental data show that the optimum concentration of SWCNTs in P3HT:PCBM:SWCNTs nanocomposites is 0.3 wt% and the PCE of ITO/PEDOT:PSS/P3HT:PCBM:SWCNTs/Al can be enhanced by more than 10% as compared with that of the control device ITO/PEDOT:PSS/P3HT:PCBM/Al.

2. Experimental method

2.1. Materials preparation

Regioregular P3HT and PCBM were purchased from 1-Material Inc. and Sigma Aldrich Chemie GmbH, respectively. SWCNTs (90% nanotube purity, diameter <2 nm, length up to 15 μm) were purchased from Shenzhen Nanometer Harbor Co., Ltd. In order to know the effect of

acid treatment on the device performance, we used two methods of acid treatment to deal with pristine SWCNTs:

- (1) First, 1 g pristine SWCNTs were dispersed into a 1:3 mixture of nitric acid (HNO₃, 98%) and sulfuric acid (H₂SO₄, 98%) and then ultrasonicated for 1 h at 60 °C to eliminate impurities and to modify SWCNTs with terminal hydroxyl groups (–COOH) [33]. The resulting solution was diluted with deionized water and centrifuged at 8000 rpm for several times to remove any large aggregates and remaining acid, and then to dry them in an oven at 100 °C. The resulting solid sample of functionalized SWCNTs was dispersed in 1,2-dichlorobenzene (DCB) with sonicating for 1 h to be ready for further processing.
- (2) First, 1 g pristine SWCNTs were dispersed into 100 mL mixture of H₂SO₄ (98%) and HNO₃ (98%) in a volume ratio of 3:1, and then ultrasonicated it, stirring the mixture for 4 h at 60 °C. In this way, carboxylic acid groups or hydroxyl groups will be adhered on the SWCNTs surfaces. The mixture was diluted by 1 L deionized water and was preserved for 12 h to remove metal impurities. Acid purification and oxidation were performed to remove the amorphous carbon catalyst such as Fe and Ni, and to adhere terminal hydroxyl groups on the SWCNTs [34]. Then, the functionalized SWCNTs were washed with deionized water until the pH value was close to 7. After being sufficiently dried at 100 °C, the resulting solid sample of functionalized SWCNTs was dispersed in DCB with sonicating for 1 h to be ready for further processing.

Then, regioregular P3HT and PCBM in a weight ratio of 1:0.8 were dissolved in DCB and stirred for 24 h at room temperature. A different concentration of above-obtained functionalized SWCNTs solution was then added into the P3HT:PCBM solution; the blends were ultrasonicated for 1 h to decorate SWCNTs with P3HT.

2.2. Device fabrication and characterization

The photovoltaic devices (effective area of $2 \times 2 \text{ mm}^2$) were fabricated on precleaned indium–tin oxide (ITO) glass substrate, and poly (ethylene-dioxythiophene) doped with poly(4-styrenesulfonate) (PEDOT:PSS) was spin-coated on the ITO substrate as hole-transporting layer at 1000 rpm for 60 s, followed by 30 min of baking at 150 °C. Then, the above resulting P3HT:PCBM:(*x* wt%) SWCNTs nanocomposites in DCB solution were spin-coated over the PEDOT:PSS layer at a speed of 800 rpm. Finally, aluminum (Al) cathode was thermally evaporated to complete the devices. A post-annealing was performed at 150 °C for 20 min in nitrogen. The current–voltage (*I*–*V*) characteristics of all these devices were measured in air immediately after completing the devices, using a Keithley-4200 semiconductor characterization system and a solar simulator with a standard illuminating intensity (i.e. 100 mW/cm^2).

The PCE is defined by $\eta = \frac{V_{OC} J_{SC} FF}{P_{IN}}$, where FF is the fill factor, J_{SC} is the short-circuit current density, V_{OC} is the open-circuit voltage and P_{IN} is the incident light power.

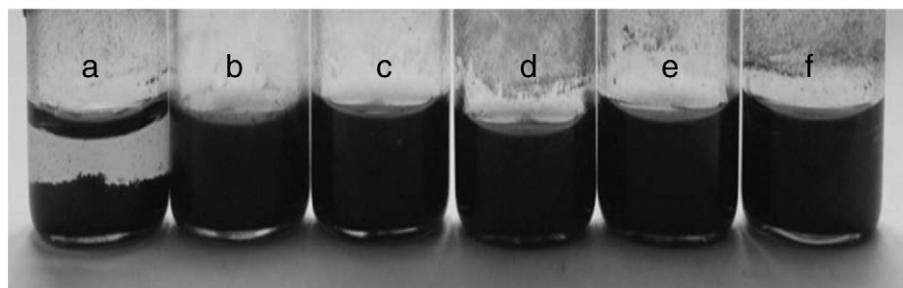


Fig. 1. After standing for 12 h. Solutions with ultrasonication time of 20 min (a), 30 min (b), 40 min (c), 50 min (d), 60 min (e) and 70 min (f).

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