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Research Paper

Authigenic buffer layer: Tuning surface work function in all polymer blend solar cells

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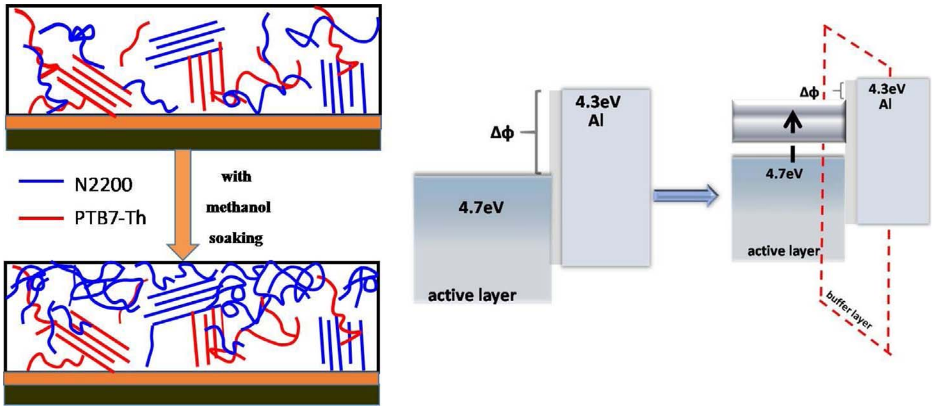
GRAPHICAL ABSTRACT



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ABSTRACT

Controlling interfacial composition between the electrodes and the photoactive layer is significant for adjusting the work function and improving the device performance of organic solar cells. Herein, an authigenic buffer layer is generated at the polymer blends surface of poly[4,8-bis(5-(2-ethylhexyl)thiophen-2-yl)benzo[1,2-b:4,5-b′]dithiophe-ne-alt-3-flu- orothieno[3,4-b]thiophene-2-carboxy-late] (PTB7-Th) as donor, poly[[*N*,*N*-bis(2-octyldodecyl)-napthalene-1,4,5,8-bis(dicarboximide)-2,6-diyl]-alt-5, 5′-(2,2′-bithiophene)] (N2200) as acceptor by soaking in poor solvent methanol. The authigenic buffer layer is mainly composed of N2200 molecule since it migrates out from the bulk phase more effectively than PTB7-Th molecule because of the difference of interaction between methanol and N2200, PTB7-Th (strong molecular polarity between N2200 and methanol). X-ray photoelectron spectroscopy (XPS) shows the content of N element increases. X-ray reflectivity (XRR) shows the thickness of neat N2200 film and the blend films were increased but the thickness of PTB7-Th film not with the increasing of methanol solvent soaking time. On the contrary, Kelvin probe force microscopy (KPFM) results show that the surface work function of blend film changes from 4.70 eV to 4.51 eV when soak into methanol for 40 s compared with pristine film, which suggests the energy barrier of the metal/organic interface decreased

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from 0.40 eV to 0.21 eV correspondingly. As a result, the power conversion efficiency (PCE) of all polymer solar cells based on the authigenic buffer layer was almost 20% higher than that pristine blends.

1. Introduction

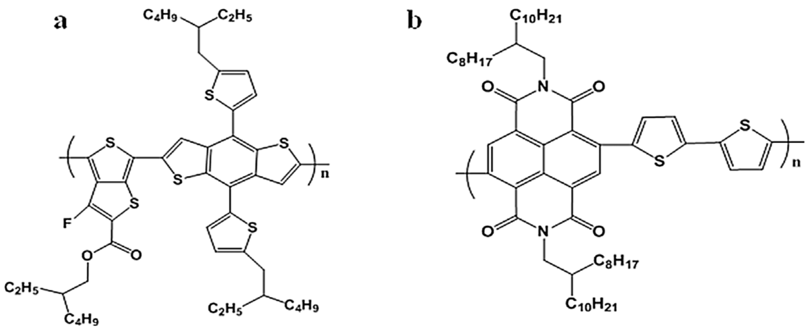
Over the past decades, much attention has been paid to organic solar cells (OSCs) for their unique merits such as plentiful material, well-defined molecular structures, flexibility, large area fabrication and low cost manufactured devices [1–6]. In order to realize large-scale commercial production as soon as possible, many techniques have been applied to improve the power conversion efficiency (PCE) of organic solar cells. Indeed, since Tang introduced the concept of donor-acceptor (D-A) heterojunctions in 1986 [7], with continuous efforts, the PCE have over 12% for single junction bulk heterojunction (BHJ) organic solar cells [8]. Considering the power conversion processes include light absorption, exciton generation and diffusion, carriers transport and collection [9–12], generally, the efforts on improving the performance of OSCs are mainly been focused on two feasible strategies. One is the application of new materials with special properties such as narrow band gap and high optical absorbing materials [13–15]. The other is the optimize the device engineering, for example, the explore of operation mechanism, manufacturing techniques, and device structures [16,17].

Recently, much more efforts have been dedicated to buffer layer, which is between active layer and electrode, because the properties of buffer layer are crucial to the device performance [18]. The performances of organic semiconductor solar calls are often limited by two aspects: One is the work function unaligned between active layer and electrode, which can cause non-ohmic contact leading to a low photovoltaic parameters mainly about open circuit voltage(Voc) [19]. The other is the positive and negative carries can't efficiently generate, diffuse and transport toward their respective electrode through build-in voltage generated by the electrodes work function difference [20]. However, investigators have confirmed the buffer layers have multiple functions such as tuning the energy level alignment [21–24], enhancing the light absorption [11], adjusting the molecular orientation and the crystalline structure of the active layer [25,26], expediting charges transport and collection [27], improving the selectivity toward holes or electrons [28], perfecting the device stability [29], etc. For these reasons, buffer layer between electrode and active layer become very necessary now.

Since buffer layer was introduction into organic solar cells by Shaheen et al. [30] there is a sharp improvement in material or making process. It can be classified into two categories according to adding the buffer layer between anode electrode and active layer or cathode electrode and active layer: anode buffer layer and cathode buffer layer. The principle of selecting buffer layer materials is mainly based on their energy levels and charge transport properties. Fortunately, the materials meet the conditions are lavish. For example, PEDOT:PSS [31] and various transition metal oxides, such as molybdenum oxide (MoO3) [32], vanadium oxide (V2O5) [33], nickel oxide (NiO) [34], are all common materials of anode buffer layer. Zinc oxide (ZnO) [35], fullerene derivative [36] and poly [(9,9-bis(30-(*N*,*N*-dimethylamino) propyl)-2,7-fluorene)-alt-2,7-(9,9–dioctylfluorene)] (PFN) [37] are usually reported to be cathode buffer layer. Among them zinc oxide (ZnO) is one of the most common inorganic materials of cathode buffer layer because it is transparency to whole visible region that is the integral absorption spectra of solar cells [38], and has a high electron mobility [39]. Furthermore, it has the advantages of solution process ability, electron selective properties, easy deposition, these features make ZnO is an ideal materials of buffer layer [40–42].

However, in the process of manufacture, mostly inorganic materials accompanied by thermal deposition in a high vacuum condition, or a high temperature annealing treatment to the solution processing, both of them are disadvantageous to realize large-area devices. Besides metal oxide, there are a large number of reports about conjugated polyelectrolytes and nonconjugated polyelectrolytes (NPEs), both of them are efficient electron-collecting (EC) interfacial layer. Although high efficiency could be achieved by this way, they still have many blemishes. Firstly, most polymer are p-type which is unfavorable to increase electron extraction unless using ultrathin film to prevent the possible increased electron extraction barrier [43]. Second, for some other polymer buffer layer such as PFN, the thickness of the PFN layer is sometimes difficult to control by spin coating process which is sensitive for PCE of polymer solar cells [44,45]. Apart from trying different materials, there are another useful processing to active layers such as thermal annealing, solvent vapor treatment and high boiling-point additives [46,47], however, these methods need accurately control the experimental conditions. The method of methanol treatment has been used in polymer/fullerene solar cells. Zhou et al. [48] reported that it was the most favorable strategy to remove the residual additions such as DIO. It was also attributed to an increased built-in voltage, a decreased series resistance and a reduced charge recombination. Moreover, Ye et al. [49] claimed that the vacuum level on the metal side of the device is lifted by the methanol treatment, thereby reducing the electron injection barrier at the organic/metal interface and resulting in a better device performance. Müller-Buschbaum et al. [50,51] reported a potential restructuring of the morphology inside the active layer induced by the solvent treatment. In short, all of these materials or methods present above could realize the goal to improve the PCE of solar cells, but we can also notice the defects are also existence that limits its application under certain conditions.

In this work we found that poor-solvents have a remarkable function to improve the PCE of all polymer organic solar cells when processing active layers. An authigenic buffer layer can be induced by soaking into methanol at the surface of all polymer blend system and have a remarkable function to adjust the surface work function in active layer.



Scheme 1. Molecular structure of a) donor polymer (PTB7-Th) and b) acceptor polymer (N2200).