

Enhancing the Absorption and Power Conversion Efficiency of Organic Solar Cells

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Abstract— Optimizing the thickness of organic solar cells (OSCs) is a potent way to enhance the power conversion efficiency (PCE). In the present work, we have investigated a novel structure in which poly (9, 9-dioctylindeno[1,2-b]fluorene-co-benzothiadiazole) (PIF8BT): *N'*-bis (1-ethylpropyl) -3, 4, 9, 10-perylene tetracarboxy diimide (PDI) is used as a photoactive absorber layer. The influence of window layer material such as Zinc oxide (ZnO) and titanium dioxide (TiO₂) with various electrode materials including Indium tin oxide (ITO), Fluorine tin oxide (FTO), aluminum (Al) Silver (Ag) and Gold (Au) with different combinations have been investigated with the objective to enhance the absorption and PCE of the cell. Extracted results shows that the proposed scheme of the structure with ITO/Al as top and bottom electrode holds the highest performance parameters including $J_{sc}=9.26$ (mA/m²), $V_{oc}=0.59$ (V), $FF=68.86\%$ and $\eta=3.86\%$ respectively as compared to different electrode combination and window layers with the same photoactive absorber material(PIF8BT:PDI). This indicates that the proposed structure can be a good choice for replacing less efficient in-organic cell.

Keywords— Organic solar cells, Bulk Heterojunction, PIF8BT:PDI, Buffer layer, Power Conversion Efficiency.

I. INTRODUCTION

Organic photovoltaic (OPV) continue to be the most emerging technology due to the rapid increase in the demand of sustainable clean energy. Today the depletion of fossil fuel and rapid increase in the population is of great concern. And to counter this problem with renewable sustainable energy source without effecting the environment is of main consideration by utilizing non-toxic material to fulfill the global energy demand and to minimize the energy crisis [1]. Conventional silicon (Si)-technology can be replaced by the OPV, as the OPV provide a striking potential for the replacement of non-organic former technology [2-4]. In order to penetrate in the market, the main seeking promise of OPV is reduced cost linked with its manufacturing. The incomparable properties of OPV materials provide a broad

pathway scope for more novel possibilities such as, solution process facile fabrication over larger area, tunable opto-electronic properties, high mechanical flexibility and chemical customization. [5-7]. In contrast to this, the limitations for OPV in order to commercialize for potential applications is its low efficiencies extracted so far[8]. The recent years reported an efficiency of 11%, [9] it is tacit that OPV need to be optimized with improved performance with high conversion efficiency in order to captivate industrial point of interest and ensure commercially reliable technology. Also, air and moisture de-stabilize the OPV based devices, which need to be stabilize under ambient conditions in order to obtain better performance[10].

For a typical OPV bulk heterojunction (BHJ), a photo absorber (active layer) is placed between two conductive electrodes in which the top electrode is mostly transparent conductive oxide(TCO) i.e., indium tin oxide (ITO) or Fluorine tin oxide (FTO) and bottom electrode is metal like Aluminum (Al), Magnesium (Mg) and calcium (Ca). The photons first incident on the anode side TCO, which give rise to exciton generation, and then propagate towards D/A in the absorber layer. As the number of photons is increases with the rise in sunlight intensity, the excitons get separated and collected at the top and bottom electrode [11-13].

Herein, we investigated a novel structure in which PIF8BT: PDI is used as an active absorber layer. The complete simulated structure consist of ITO/PEDOT: PSS/PIF8BT: PDI/Al. The influence of different electrode materials on the proposed structure is tested and scheme for best electrode selection on top and bottom surface is investigated.

II. DEVICE MODELLING

The proposed investigated OSC structure is depicted Figure 1. The structure consist of four effective layers in which indium tin oxide (ITO) is used as top electrode. After the ITO layer, buffer layer (BL), PEDOT: PSS is placed which is also known as Hole transporting layer (HTL) and electron blocking layer(EBL). PEDOT: PSS has excellent stability, mechanical flexibility and highly conductivity [14-16]. Below the (BL) layer, PIF8BT: PDI is introduced as a photoactive layer with variable thickness. Different window layers including zinc oxide (ZnO) and titanium dioxide

(TiO₂) is used as these window layers has high transparency, larger exciton binding energy and can enhance transmittance [17, 18].

All the simulations are performed in the GPVDM a free source solar cell simulator. The advantage of this software compared to other [19, 20] is that it can calculate both the optical and electrical property of the cell more precisely. In our investigation, we investigated both the electrical and optical model on the proposed structure which include poisson equation (1), Drift diffusion model by equation (2, 3) and continuity equations (4, 5) for electron-hole. Whereas, for recombination of carrier Shockley-Read-Hall (SRH) is used in 1D- and time domain [21-23]

$$\frac{d}{dx} \epsilon_0 \epsilon_r \cdot \frac{d\phi}{dx} = q(n-p) \quad (1)$$

$$J_n = q\mu_c n \frac{\partial E_c}{\partial x} + qD_n \frac{\partial n}{\partial x} \quad (2)$$

$$J_p = q\mu_v p \frac{\partial E_v}{\partial x} - qD_p \frac{\partial p}{\partial x} \quad (3)$$

$$\frac{\partial J_n}{\partial x} = q \left(R_n - G + \frac{\partial n}{\partial t} \right) \quad (4)$$

$$\frac{\partial J_p}{\partial x} = q \left(R_p + G + \frac{\partial p}{\partial t} \right) \quad (5)$$

The more detail analysis on the above equations can be found in [24-27].

III. RESULTS AND DISCUSSION

In order to optimize the thickness of the absorber layer with special emphasis on improving the performance parameters with improved η is main consideration. We have investigated a structure in which PIF8BT: PDI is used as an absorber layers and effect of thickness on high temperature on the performance of the cell is studied. In our proposed structure PIF8BT: PDI is used as a main absorber material in which ITO and Al is used on top and bottom electrode respectively. For hole transport material, PEDOT: PSS layer is utilized. However, different window and electrode material is tested on the proposed structure and comparison of the performance parameters with different combination schemes is analyzed for better performance of the cell.

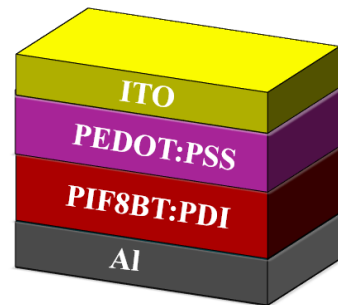


Figure 1. Schematic of proposed structure based on PIF8BT: PDI absorber material.

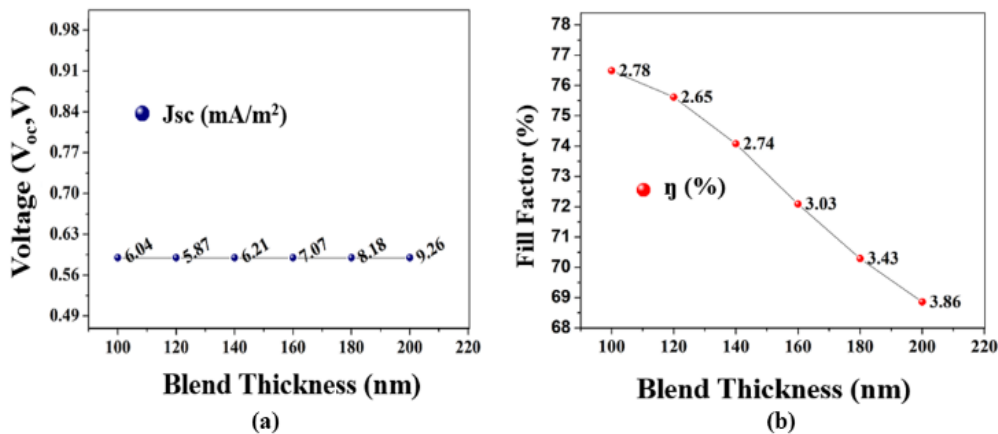


Figure 2. Influence of blend thickness on (a) V_{oc} and J_{sc} , (b) FF and η

To investigate proposed structure (illustrated in Fig. 1), we have first varied the thickness of the absorber layer (PIF8BT: PDI) and observed the influence of thickness on the V_{oc} , J_{sc} , FF and η . The reason for varying the absorber layer thickness is that this layer plays a key role in the overall cell performance [28, 29]. The photon is absorbed and electron-hole pair is generated in this absorber layer [30]. Fig. 2(a) shows the variation of V_{oc} and J_{sc} as the dependent of thickness. It is visible from the fig. 2(a) that when the thickness of the absorber layers increases the J_{sc} also increases. This rise in J_{sc} is due to the fact when the absorber

layer thickness is increases large amount of photon is absorbed which results in the greater value of J_{sc} [31]. The J_{sc} increases from 6.04 (mA/m²) to 9.26 (mA/m²) when thickness varied from 100 (nm) to 200 (nm). The fig. 2(a) also indicates that V_{oc} is not much effected with the increase in the thickness. Fig. 2(b) shows FF and η as a function of thickness, as the V_{oc} and J_{sc} has relation with FF and η [32] therefore, by increasing the thickness of the absorber layer the η also increases. This rise in η is due to the larger amount of photons absorption in the active region which results in the greater number of excitons which enhances the η . The best optimum thickness for extracting the highest η of the

investigated proposed structure is 200(nm). At 200(nm) the efficiency recorded to be 3.86%. However, different window layer materials is tested on the proposed structure and recorded parameters are summarized in table I.

Table I. Extracted performance parameter of PIF8BT: PDI with different windows layers.

Window Layers	V_{oc} (V)	J_{sc} (mA/m ²)	FF %	η %
ZnO	0.59	8.68	69.16	3.58
TiO ₂	0.59	8.37	69.31	3.45

The recorded parameters in table I. are less compared with our extracted results and its observed that windows layers has not much contributed to the conversion efficiency and shows a decrease in the performance parameters as compared to our proposed reference cell extracted results.

The same structure is tested with different top and bottom electrode to check the best compatibility with our proposed investigated cell in order to enhance η .

Table II. Extracted performance parameter of PIF8BT: PDI with different top and bottom electrode.

ELECTRODES	V_{oc} (V)	J_{sc} (mA/m ²)	FF %	η %
ITO/Ag	0.59	9.45	68.71	3.89
FTO/Al	0.59	8.70	69.09	3.50
FTO/Au	0.59	8.68	69.31	3.59
FTO/Ag	0.59	9.42	68.74	3.80

From table II. We can observed that recorded η is almost equivalent to the reference proposed structure and ITO/Ag has the closest value of η in comparison with the ITO/Al (proposed scheme). The reason for selecting ITO/Al is that it gives us almost the same η i.e., 3.86 % as that with ITO/Ag (3.89%) and FTO/Ag (3.80%). Also the price of (Al) is less compared to (Ag) so opting the ITO/Al for top and bottom electrode will be the best option in order to enhance η with making the cost of manufacturing less.

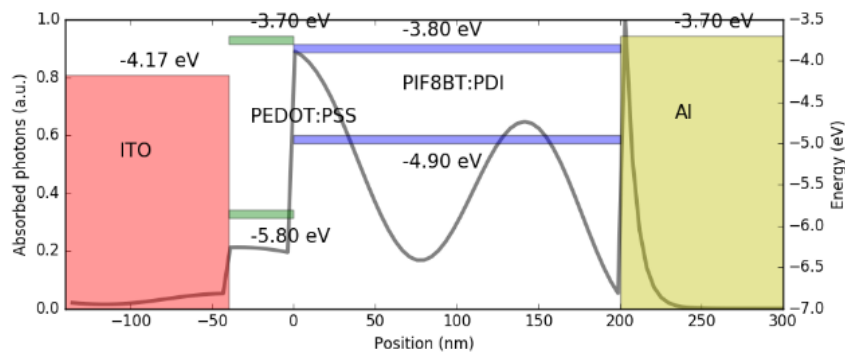


Figure 3. Photon absorption-localization energy variance of investigated OSC

Fig. 4 Shows the peaks for the absorption of photons in each material. It is visible from the graph that the peak is increases from 0(nm) to 200(nm) in which absorber material

is positioned. The rise in the aluminum (Al) layer indicates that some amount of photons are also absorbed in the Al layer.

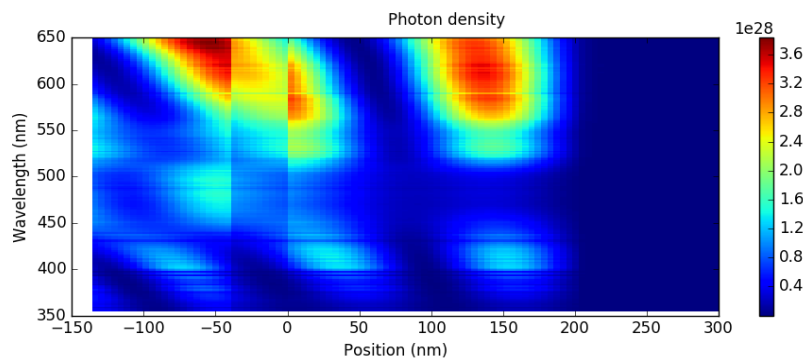


Figure 4. Photons distribution-localization energy variance of investigated OSC

The Fig. 4 Shows distribution of photons in the different material of the cell, and its visible from the figure that the photons are distributed randomly from 350 (nm) wavelength to 650 (nm) wavelength.

CONFLICT OF INTEREST

The authors hold no conflict of interest.

CONCUSLION

In summary, we investigated a novel organic material in which PIF8BT: PDI is used as active material. Our extracted results provide a new pathway for exploring new electrode materials incorporating with the novel organic material for η enhancement in the OSCs. Moreover, our work also highlighted the influence of window layer on the cell performance with different electrode combinations. Our recorded results shows a brand new avenue for improving the absorption and power conversion efficiency of OSCs which can be prefer for future applications.

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