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Research Article

Theoretical Performance Analysis of Inverted P3HT: PCBM Based Bulk Hetero-Junction Organic Solar Cells through Simulation

Murad Jemal Husen,[1] **Fekadu Gochole Aga**,[2] **and Solomon Tiruneh Dibaba**[1]

[1]*Department of Applied Physics, School of Applied Natural Science, Adama Science and Technology University, Adama, P.O. Box 1888, Ethiopia*
[2]*Department of Materials Science and Engineering, School of Mechanical, Chemical and Materials Engineering, Adama Science and Technology University, Adama, P.O. Box 1888, Ethiopia*

Correspondence should be addressed to Solomon Tiruneh Dibaba; solomondibaba27@gmail.com

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In this study, the role of active layer thickness, hole transport layer thickness, and electron mobility on the performance of P3HT: PCBM-based inverted organic solar cells has been investigated. The simulation has been done for device structure ITO/ZnO/P3HT: PCBM/MoO_3/Ag using the general-purpose photovoltaic device model (GPVDM) program tool. The short circuit current density (J_{sc}), open circuit voltage (V_{oc}), fill factor (FF), and power conversion efficiency (PCE) of the cell were determined by varying the thickness of the active layer from 140 nm to 260 nm, the hole transparent layer from 10 nm to 40 nm, and electron mobility from 0.5×10^{-3} cm^{2}V^{-1}s^{-1} to 6.5×10^{-3} cm^{2}V^{-1}s^{-1}. The PCE improvement was observed at 220 nm and 20 nm active layer and hole transporting layer thickness, respectively, for 4.5×10^{-3} cm^{2}V^{-1}s^{-1} electron mobility. The results confirmed that the thickness of the active layer, hole transport layer, and charge carrier mobility plays an important role in the performance improvement of organic solar cells.

1. Introduction

The high demand for energy consumption, the lack of conventional fossil fuel supplies, and its adverse effects on the environment are some of the driving factors for finding an alternative renewable energy supply [1]. The application of solar energy is among the renewable energy sources that have received great attention in addressing global energy demand [2, 3]. Solar energy can be converted directly into electricity using photovoltaic cells [4], through processes of photon absorption, electron-hole creation, separation, and transport of free charge carriers for collection at electrodes [5]. Polymer solar cells are one of the types of solar cells that use a blend of conjugate conducting polymers and fullerene derivatives [6] as the active layer for the conversion of light into electricity. The alternate double and single bonds in the materials help an effective transfer of electron in the cell [7]. Low production costs, easy fabrication methods, flexibility, and lightweight are some of the unique properties of polymer solar cells that make them the next generation solar cells [8–10]. One of the challenges in the polymer-based solar cells is their low power conversion efficiency. Several scientific research have been done to improve the performance of organic solar cells [11].

In this work, the effect of active layer thickness, hole transport layer thickness, and electron mobility on the performance of the inverted ITO/ZnO/P3HT: PCBM/MoO_3/Ag device structure were investigated using simulation. The P3HT: PCBM blend active layer, with high absorption in the visible region [12, 13], together with ZnO electron and MoO_3 hole transport layers, has been used to determine the optimum thickness of the layers for better performance of the cell [14].

The simulation computed using the general-purpose photovoltaic device model (GPVDM) program tool, and the physical mechanism of absorption explained extensively. ITO/ZnO/P3HT: PCBM/MoO_3/Ag is the device structure used for modelling purpose under AM1.5 solar radiation

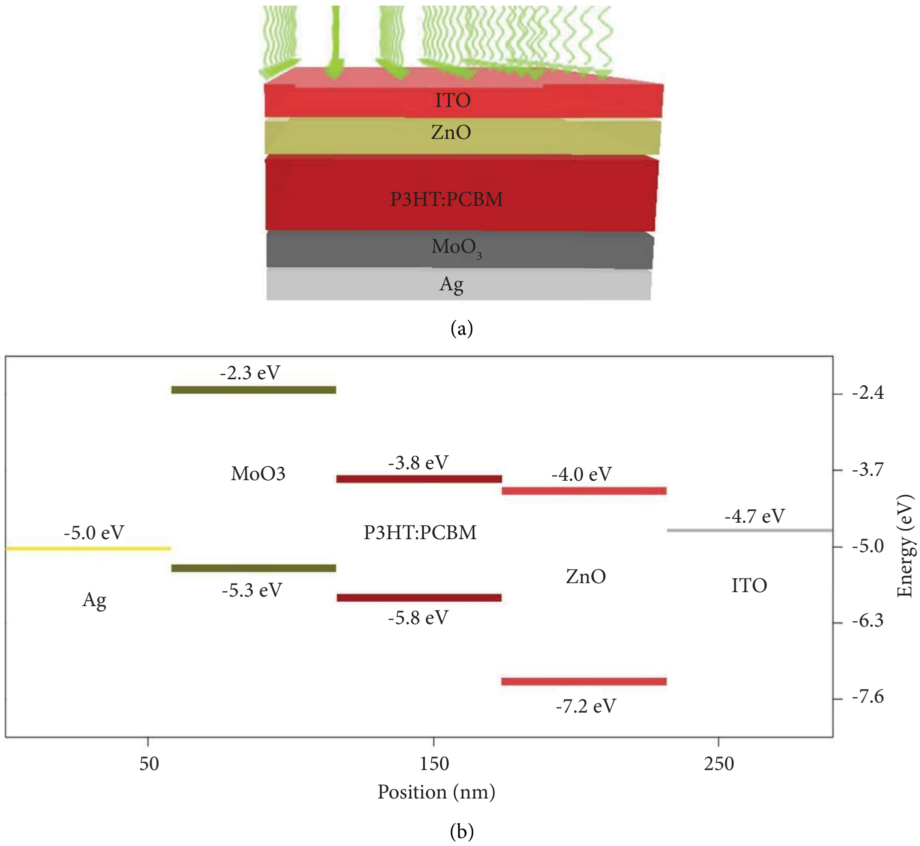

FIGURE 1: (a) ITO/ZnO/P3HT: PCBM/MoO3/Ag device structure. (b) The energy level diagram for each components of the cell.

from one sun. The device structure used to analyse the performance of the cell and the energy diagram of each component of the cell are shown in Figures 1(a) and 1(b), respectively. The GPVDM software for the electrical and optical models is governed by the Poisson's and continuity equations for electrons and holes, as given in equations (1)–(3), [15].

$$\frac{d}{dx}\varepsilon_o\varepsilon_r\frac{d\varphi}{dx} = q(n-p), \tag{1}$$

$$J_n = q\mu_e n\frac{dE}{dX} - qD_n\frac{dp}{dx}, \tag{2}$$

$$J_p = q\mu_p p\frac{dE}{dx} - qD_p\frac{dp}{dx}. \tag{3}$$

In this study, the performance of P3HT: PCBM-based inverted polymer solar cell is investigated for various thickness of active layer, hole transport layer, and value of electron mobility's. The parameters used for the simulation are shown in Table 1.

2. Result and Discussion

2.1. The Effect of Active Layer Thickness. The simulation was performed by varying the active layer, hole transport layer thickness, and the electron mobility by fixing two of them to understand the role of each parameter on the performance of the cell. We first varied P3HT: PCBM thickness for constant MoO_3 thickness and electron mobility, and then varied MoO_3 layer thickness for constant P3HT: PCBM thickness and electron mobility. Finally, electron mobility was varied for constant P3HT: PCBM and MoO_3 layer thickness. For each procedure, we investigated the performance of P3HT: PCBM-based inverted polymer solar cells in detail. Figure 2 shows the *J*-*V* characteristics of the solar cell by varying the active layer thickness from 140 nm to 260 nm for 40 nm steps. The demonstrated results for various thickness of the active layer are given in Table 2.

We notice that for 220 nm thickness of P3HT: PCBM, the highest PCE of 5.13% was obtained as given in Table 2. The PCE increases as active layer thickness increases from 140 nm to 220 nm and decreases with further increase in thickness which indicates the optimum thickness for better performance is 220 nm. The result is expected since the absorbed photons are directly proportional to the active layer thickness. However, further increasing the active layer thickness causes the free charge carrier recombination, which contribute to a reduction in PCE as reported in the literature [16] and our findings were consistent with reported literature on inverted and some conventional organic solar cells [16, 17].

2.2. Effect of Hole Transport Layer (HTL) Thickness. The selectively charged transport layer is used to decrease free charge carrier recombination and increase carrier collection

Table 1: Simulation parameter.

Layer name	Layers thickness (nm)
ITO	30
ZnO	20
P3HT: PCBM	Vary (140,180,220, 260)
MoO_3	Vary (10,20,30,40)
Ag	80
Electron mobility ($cm^2V^{-1}s^{-1}$)	Vary (0.5×10^{-3}, 2.5×10^{-3}, 4.5×10^{-3}, 6.5×10^{-3})

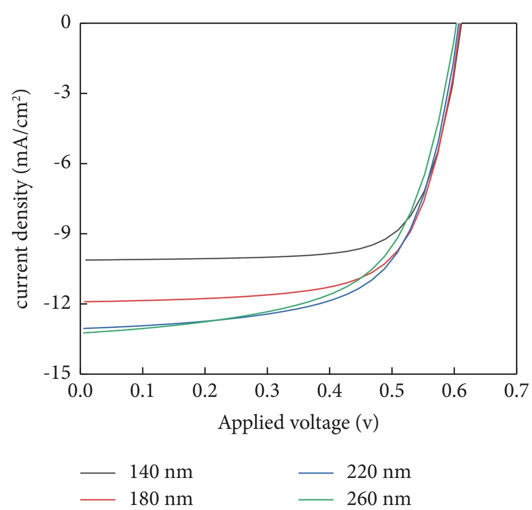

Figure 2: Current density vs applied voltage for various active layer thicknesses.

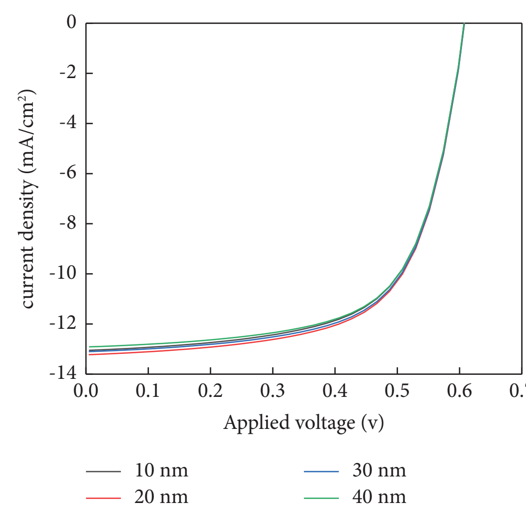

Figure 3: Current density vs applied voltage at different thickness of HTL.

Table 2: Evaluated parameters of the cells for various thickness of active layer.

Active layer thickness (nm)	J_{sc} (mA/cm^2)	V_{oc} (V)	FF (%)	PCE%
140	−10.122	0.61	72	4.50
180	−11.906	0.60	69	5.02
220	−13.049	0.607	64.8	5.13
260	−13.239	0.603	61.6	4.90

at the electrode in cells [18]. In this section, we demonstrated the role of hole transport layers thickness on the performance of inverted P3HT: PCBM-based PSC. Molybdenum oxide (MoO_3) is chosen as the hole transport layer due to its high conductivity and better transparency [19]. The MoO_3 thickness varied from 10 nm to 40 nm with a step of 10 nm.

As seen in Figure 3 and Table 3, the variation in hole transport layer thickness impacts the parameters of the inverted organic solar cell. Particularly, short circuit current density (J_{sc}) and power conversion efficiency (PCE) vary with variation in the thickness of the hole transport layer, and both parameters exhibit the optimum values at 20 nm, which are −13.223 mA/cm^2 and 5.22%, respectively. More increase in HTL thickness and decreases in J_{sc} and PCE are observed in Table 3.

Table 3: Evaluated parameters of the cells for various thickness of HTL.

HTL thickness (nm)	J_{sc} (mA/cm^2)	V_{oc} (V)	FF (%)	PCE (%)
10	−13.049	0.607	65.1	5.134
20	−13.223	0.608	65.3	5.222
30	−13.109	0.607	65.1	5.188
40	−12.912	0.606	65.3	5.122

2.3. Effect of Electron Mobility. The electron mobility is an essential parameter to enhance the performance of a polymer solar cell as it influences the charge recombination dynamics and extraction [20, 21]. Finally, the electron mobility effect was demonstrated at 220 nm and 20 nm active layer and HTL, respectively. For the demonstration, electron mobility varied from $0.50\times10^{-3}\,cm^2V^{-1}s^{-1}$ to $6.50\times10^{-3}\,cm^2\,V^{-1}s^{-1}$ with step of $2\times10^{-3}\,cm^2V^{-1}s^{-1}$as per reported procedures [14, 22]. Then after, the values of J_{sc}, V_{oc}, FF, and PCE were determined as a function of electron mobility (EM) as shown in Table 4. The current density vs. applied voltage at different electron mobility is shown in Figure 4(a). Fill factor vs. electron mobility and PCE vs. electron mobility results are summarized in Figures 4(b) and 4(c), respectively. Both parameters have been found to vary in a similar manner. PCE is found to increase with electron mobility up to $4.5\times10^{-3}\,cm^2V^{-1}s^{-1}$, and then it becomes constant at nearly 5.23%.

Table 4: Evaluated parameters of the cells for various thickness of EM.

EM (cm^2 V–^{1}s^{-1})	J_{sc} (mA/cm^2)	V_{oc} (V)	FF (%)	PCE (%)
0.5×10^{-3}	−13.174	0.61	57	4.74
2.5×10^{-3}	−13.223	0.60	64	5.09
4.5×10^{-3}	−13.190	0.60	65	5.23
6.5×10^{-3}	−13.105	6.58	62	5.21

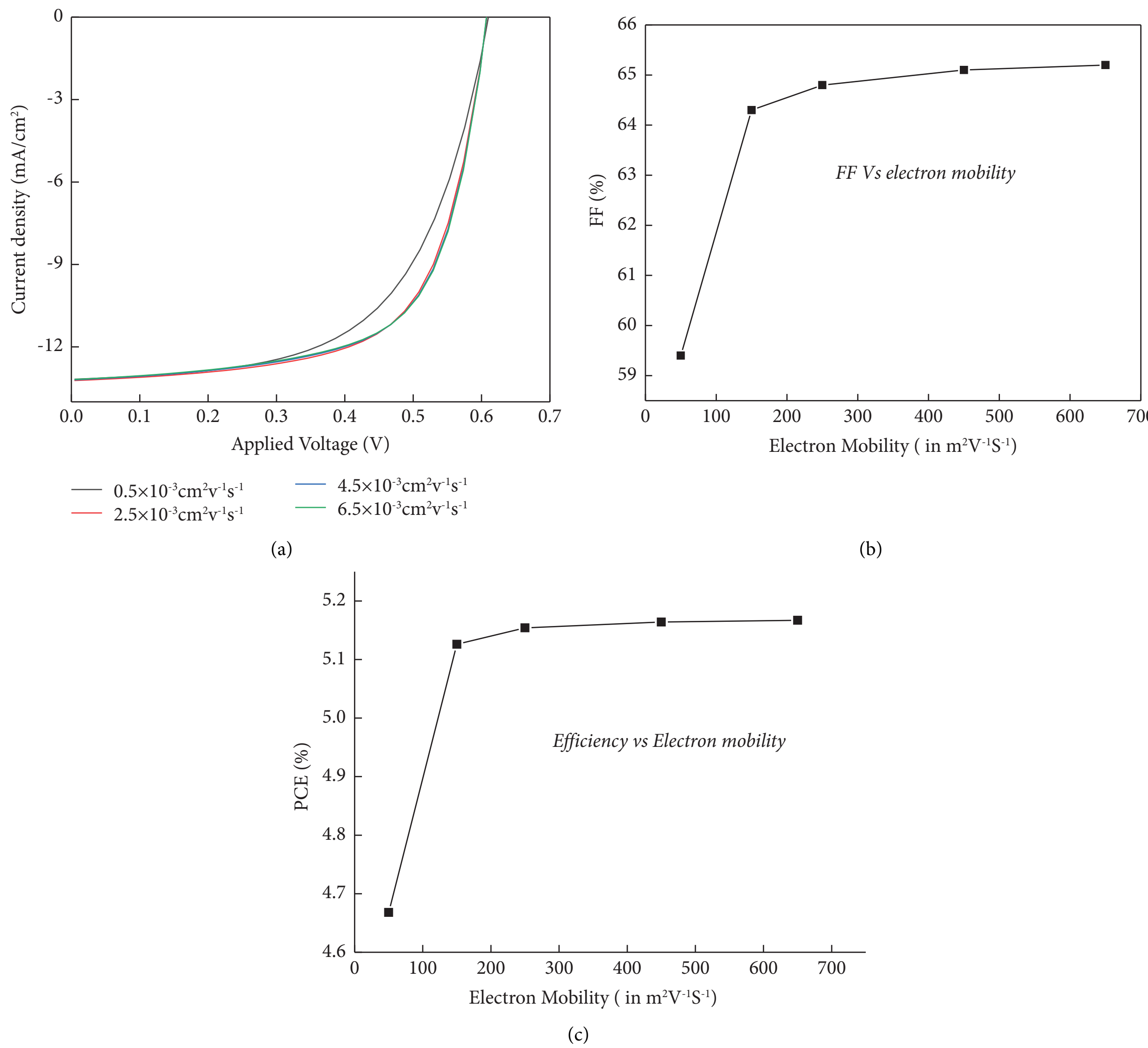

Figure 4: (a) Current density vs. applied voltage at different electron mobility. (b) FF vs electron mobility. (c) Efficiency vs electron mobility.

Maximum PCE which is 5.23% was obtained at optimized parameters of 220 nm, 20 nm, and 4.5×10^{-3} cm^2 V^{-1}s^{-1} of active layer thickness, hole transport layer, and electron mobility, respectively; the EQE of the device was evaluated as shown in Figure 5.

Absorbed photon density in different components of the device architecture of ITO/ZnO/P3HT: PCBM/MoO_3/Ag is shown in Figure 6. It is visible from the graph that the absorption increases from 0 nm to 300 nm in which absorber material is positioned.

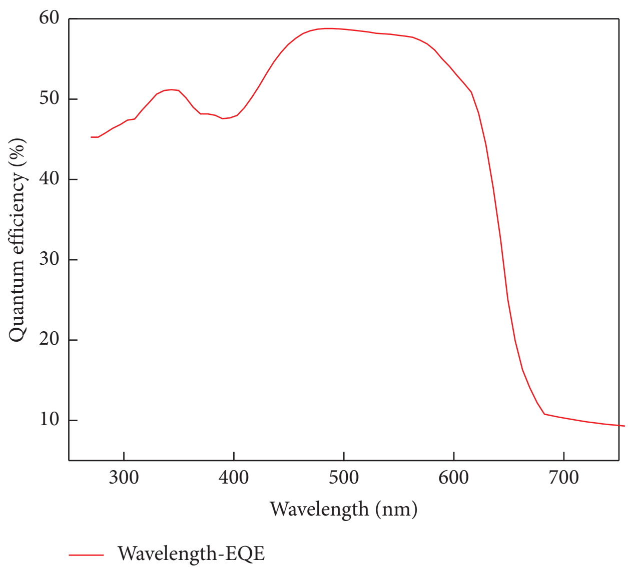

Figure 5: EQE the cell as the function wavelength.

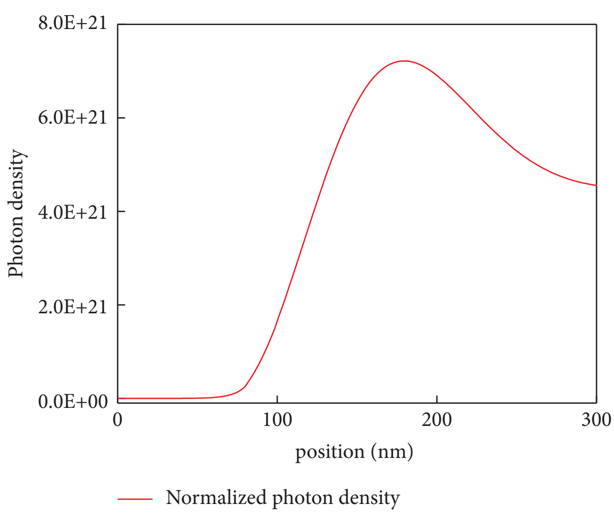

Figure 6: Normalized photon density.

3. Conclusion

The performance of the inverted P3HT: PCBM-based organic solar cell with device structures of ITO/ZnO/P3HT: PCBM/MoO_3/Ag was successfully studied via simulation using the GPVDM software. The investigation results showed that thickness of active layer, hole transport layer, and electron mobility plays a vital role in boosting the performance of the P3HT: PCBM-based bulk heterojunction organic solar cell. Accordingly, we optimized the thickness of the layers and the electron mobility of the device. The optimum performances of the cell were obtained at 220 nm, 20 nm, and $4.5 \times 10^{-3}\,cm^2/Vs$ for active layer thickness, hole transport layer thickness, and electron mobility, respectively. Thus, to enhance the performance of an inverted organic solar, the thickness of the active layer, the hole transport layer, and electron mobility have to be optimized.

Data Availability

The datasets generated during the study are available from the corresponding author upon reasonable request.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

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