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Simulation of the Performance Parameters and Carrier Concentration Profile of Poly 3-Hexyl Thiophene / Phenyl-C61-Butyric Acid Methyl Ester Planar Hetero-junction Photovoltaic Cell

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P A P E R I N F O

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A B S T R A C T

In this research work, the performance parameters , such as fill factor (FF), external quantum efficiency (EQE) , maximum power density and carrier concentration profile of a planar hetero-junction poly 3-hexyl thiophene (P3HT) / phenyl-C61-butyric acid methyl ester (PCBM) photovoltaic cell has been simulated for different values of carrier mobility where the simulation has been performed under the consideration of incident solar radiation of 1 kW/m^2 irradiance, air mass of 1.5, ambient temperature of 300K and indium tin oxide (ITO) and aluminium (Al) has been considered as the anode and cathode of the P3HT/PCBM solar cell respectively. The performance parameters has been determined for electron mobility of 5×10^{-4} , 5×10^{-3} , 5×10^{-2} and 5×10^{-1} (cm^2/V.s) at the acceptor and hole mobility of 1 × 10-4 , 1 × 10-3 , 1 × 10-2 and 1 × 10-1 (cm2/V.s) at the donor layer. Carrier concentration profile has been studied for 0.4 and 0.5 V junction voltage and for different values of carrier mobility. Finally highest external quantum efficiency of 2.413% and maximum power density of 24.13 W/m2 has been obtained for hole mobility of 1×10^{-1} (cm^2/V.s) and electron mobility of 5×10^{-1} (cm^2/V.s).

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INTRODUCTION

Due to the shortage of Coals and other natural fuels, generation of electricity at thermal power stations may be hampered at near future. So the research on the Renewable Energy Technology at the field of electrical power generation has been increased in past few years. Photovoltaic devices with high efficiency will play a very important role in huge amount of electrical power generation by efficiently using the solar energy. Renewable energy technology is an example of clean energy which doesn't pollute the environment with heat and smoke like fuels in the power plant. So healthy environment can be ensured using renewable energy in electrical power generation system [1-4]. All energy sources may have some positive or negative impact on our environment. The cleanest and most sustainable techniques to generate electricity as it produces no toxic pollution or green house gas emission would be the technology used for photovoltaic (PV) solar cells. For efficient and cost effective use of the incident solar energy, high performance photovoltaic device is necessary. In this research work, several ways have been analyzed from the fabrication point of view to enhance the performance of organic solar cell and to generate large amount of electrical power from the cell.

During the past several years, research of organic solar cell has been developed due to the introduction of new organic materials, improved materials engineering, and more sophisticated device structures [5, 6]. Photovoltaic cell based on organic semiconductors are interesting for several reasons. For example, by modifying the chemical structure of the compounds the electrical properties of organic semiconductors can be tailored in endless combinations [7,8]. Basic structure of a planar hetero-junction junction poly 3-hexyl thiophene (P3HT)/ phenyl-C61-butyric acid methyl ester (PCBM) has been shown in Figure 1 [9]. In this figure ITO and Al is the anode and cathode respectively. In this PV cell, the incident solar radiation is absorbed at the active layer, creating bound electron-hole paiers, called excitons which diffuse to the interface of the donor and acceptor

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layer. The build in electrical field of the hetero-junction separates the exciton to free charge carriers, electron diffuses through the acceptor layer and hole diffuses through the donor layer and reach to the cathode and anode terminal respectively [10]. In organic semiconductors like P3HT and PCBM, the recombination mechanism of charge carriers is controlled by the mobility of the charge carriers. So, in organic solar cells both the carrier extraction and the losses via carrier recombination is simultaneously controlled by the mobility. Amount of light absorbed in the active layer governs the amount of excitons created in a solar cell [11, 12].

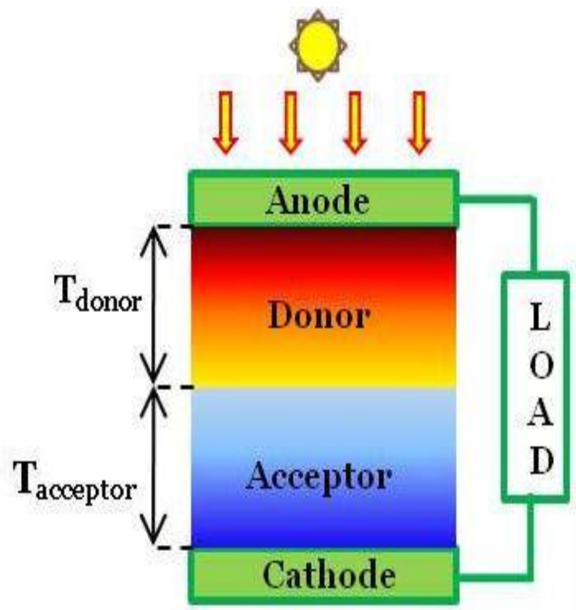


Figure 1. Basic structure of a Planar Hetero-junction Solar Cell

This is determined by the strength of the absorption, the overlap of the absorption spectrum with the solar spectrum, and the thickness of the absorbing layer. An increase in carrier mobility has a positive effect on carrier transport, enhancing carrier extraction, but on the other hand it will increase the bimolecular recombination strength as well. Disassociation of charge carriers at the hetero-junction region is also governed by the charge carrier mobility. For carrier mobility lower than a particular value decreases the dissociation [13]. As a result, at low mobility not only the increased recombination reduces the solar cell performance, but also many of the excitons will not dissociate into free carriers and recombine to their ground state [14]. These results indicate that a high charge carrier mobility is beneficial for the performance of organic-photovoltaic (OPV) cell. Diffusion of charge carriers at the active layer of organic cell can be studied from the carrier concentration profile. Diffusivity of charge carriers can also be analyzed from the carrier concentration profile via analyzing the gradient of the carrier concentration [15].

Simulation

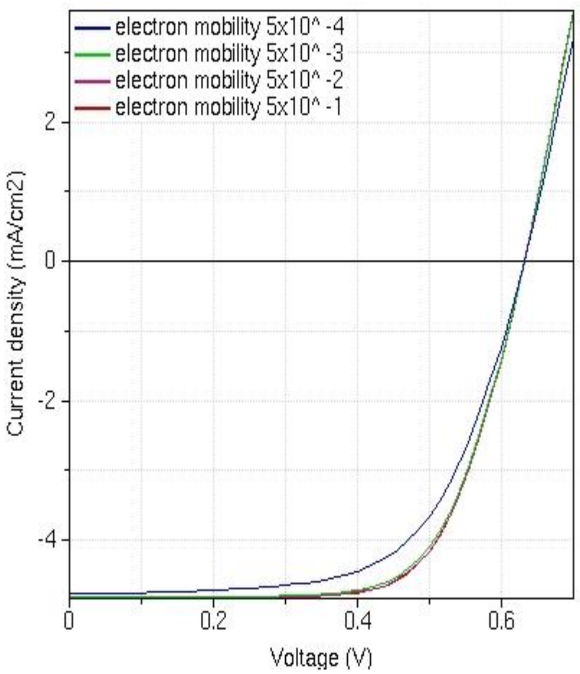
In this research , the simulation study of the electrical characteristics and carrier concentration profile of a P3HT/PCBM Planar Hetero-junction Solar Cell has been performed by considering P3HT and PCBM as the donor and acceptor layer of the cell respectively. Indium tin oxide (ITO) and aluminium has been considered as the anode and cathode material of the cell, respectively. The simulation is performed under the condition of 1 KW/m^2 incident solar radiation, 1.5 AM and 300K ambient temperature.

Performance Analysis of P3HT/PCBM Solar cell for varying donor layer Thickness :

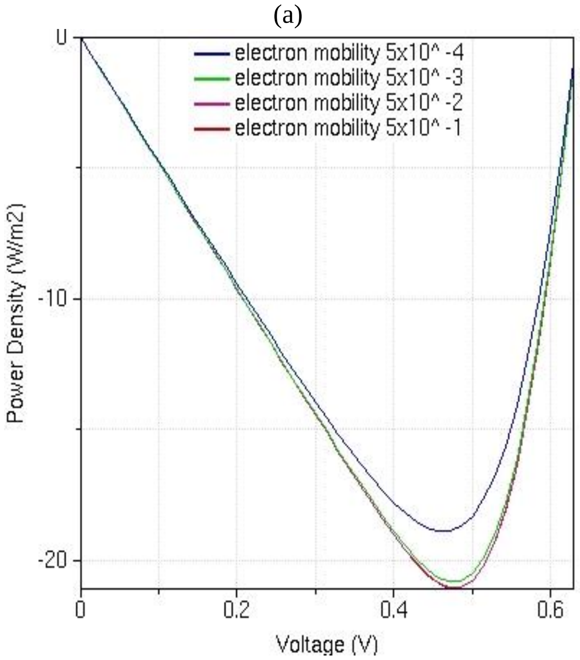
By varying the doping concentration in the active layer, work function and conductivity at the active layer of the organic solar cell can be tuned easily. So, mobility of the charge carriers, induced at the hetero-junction of the donor-acceptor interface layer, can be varied and controlled easily and efficiently. The performance parameters of the P3HT/PCBM Planar Hetero-junction solar cell are determined for varying the mobility of electrons and holes at active layer of the solar cell. Mobility of charge carriers in the organic semiconductors play important role in the performance of organic solar cell. Photo-generated excitons diffuse to the heterojunction interface of the organic active layer of the cell and separated to free charge carriers (electron and hole). In OPV cell, mobility of charge carriers is related to the charge extraction and recombination. An increase in carrier mobility has a positive effect on the transport of carriers, facilitating carrier extraction, but on the other hand it will increase the bimolecular recombination strength as well. Low mobility leads to a build-up of charge carriers in the solar cell, high mobility of charge carriers give rise to an efficient extraction and decreases the charge carrier density due to fast carrier extraction, which implicitly lowers the open-circuit voltage of the solar cell, affecting the performance of the solar cell. Besides, during the faster extraction of charge carriers, the probability of carrier recombination also increases. As a result, in case of large increase of carrier mobility in organic solar cell, the value of external quantum efficiency does not increase significantly, rather, a slight increase in EQE occurs in such case.

Here, the performance of the P3HT/PCBM planar heterojunction solar cell has been studied for different values of electron and hole mobility. The light IV characteristics of the organic solar cell for varying electron mobility is shown in Figure 2(a) and the power-voltage characteristics curve is shown in Figure 2(b).

Here, electron and hole mobility is considered as a optimum value of $5x10^{-4}$ and $1x10^{-4}$($cm^2/V.$ s) respectively. The thickness of both donor and acceptor layer in considered 50 nm. At this condition, the Fill Factor (FF) and EQE is obtained 0.6294 and 1.8863 % respectively.



(a)



(b)

Figure 2. (a) Light IV characteristics with varying electron mobility (b) Power-voltage characteristics with varying electron mobility

Maximum power transfer per unit area of the cell is found 18.86 W. After that, keeping the hole mobility fixed to that optimum value, the electron mobility is increased to the value $5x10^{-3}$, $5x10^{-2}$, $5x10^{-1}$ ($cm^2/V.$ s). The performance of the organic solar cell was studied. For the three increasing values of electron mobility, the FF has obtained 0.687, 694 and 0.695 and solar cell EQE 2.078, 2.102 and 2.104%, respectively. Also , Maximum output power is found 20.78 , 21.01 and 21.03 W/m^2, respectively. It is seen that, with the increase of electron mobility in the active region of the organic solar cell, the efficiency, FF and output power of the cell increases. But, it is also observed that, for large values of carrier mobility, i.e. $5x10^{-2}$ and $5x10^{-1}$ $cm^2/V.$ s, the increase in the efficiency and other performance parameters are very small. For high mobility, the increasing recombination of charge carriers and lowering open circuit voltage affects the performance parameters of the cell. As a result, it restricts the improvement of the efficiency, FF and maximum output of solar cell

For power of the solar cell. Fig. 4.6 shows the Light IV characteristics curve of the P3HT/PCBM varying hole carrier mobility. Here, again the electron and hole mobility is considered as a optimum value of $5x10^{-4}$ and $1x10^{-4}$ ($cm^2/V.$ s), respectively. Then, keeping the electron mobility fixed to that optimum value, the hole mobility is increased to the value of $1x10^{-3}$, $1x10^{-2}$ and $1x10^{-1}$ ($cm^2/V.$ s). Here, the FF has obtained 0.768, 0.794 and 0.797, respectively. The EQE of 2.329, 2.406 and 2.413 % resulted maximum output power of 23.29 , 24.05 and 24.13 W/m^2, respectively. It is studied that, the increase in the performance parameter values of the solar cell with the increase of electron mobility is very little than that of varying hole mobility. As, the effective mass of electron is less than the hole, so with increasing the electron mobility, the probability of carrier recombination affect in case of electron is higher than that of the hole. So, the variation of the values of the efficiency, FF and maximum output power of the organic solar cell with increasing hole carrier mobility is of less significant. As, the mobility of hole carrier is increased, the value of the performance parameters of the cell rises slightly, shown in Figure 3.

Study of photo generated Carrier Concentration Profile at P3HT/PCBM Solar cell at certain junction electric field :

In the organic solar cell, the excitons are separated under the electric field at the planar hetero-junction of D-A interface of the active layer. Electric field potential is dependent on the work function of the donor and acceptor layers of the cell. The work function is also dependant on the donor and acceptor concentration. So, by varying the donor and acceptor concentration at the active layer of the solar cell, formed by P3HT and PCBM layer, the work function and hence, the electric field potential at the hetero-junction can be tuned easily and efficiently. In case of P3HT/PCBM organic solar cell, the maximum tunable junction voltage is 0.7 V.

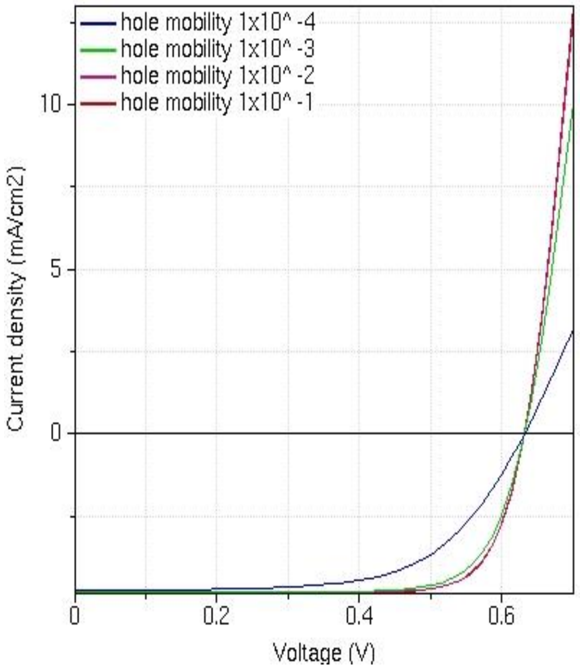


Figure 3. Light IV characteristic curve with varying hole mobility

Here, carrier concentration profile, showing both hole and electron carrier concentration, of the organic solar cell was studied at two different junction voltage 0.4 V and 0.5 V. If the junction electric potential is increased, more electrical energy will be faced by the excitons and carrier concentration at the junction will be increased. The carriers will be diffused to the anode and cathode terminal. At these terminals, the concentration of the carriers will be maximum. Here, the thickness of the active layer is considered 100 nm and mobility of electron in the acceptor layer and mobility of hole in donor layer is considered $5x10^{-4}$ and $1x10^{-4}$ (cm^2/V. s), respectively. The carrier concentration profile for junction voltage 0.4 and 0.5 V is shown on Figures 4.1 (a) and 4.1 (b). Then, the mobility of the electrons and holes in the active region is increased and the carrier concentration profile is studied. Keeping the hole mobility at the donor layer fixed at $1x10^{-4}$ cm^2/V. s, the electron mobility is increased to the value $9x10^{-2}$ cm^2/V. s. The simulation curve of carrier concentration profile at this condition is shown on Figures 4.2 (a) and 4.2 (b), for both junction voltage 0.4 and 0.5 V. Here, it is seen that, the carrier concentration profile for increased carrier mobility, becomes nearly linear and due to increased mobility of carriers, the concentration of electrons and holes at the junction region become large.

After that, the mobility of hole at the active region of the solar cell is increased to $4x10^{-2}$ and almost linear carrier concentration profile has been studied, shown in Figures 4.3(a) and 4.3 (b).

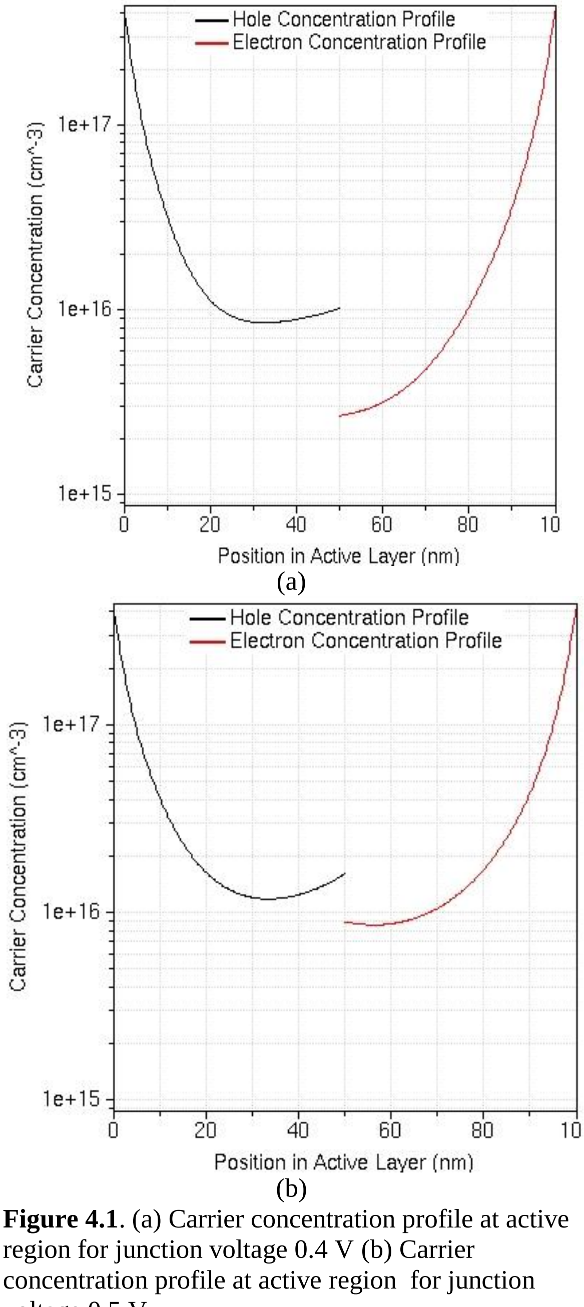
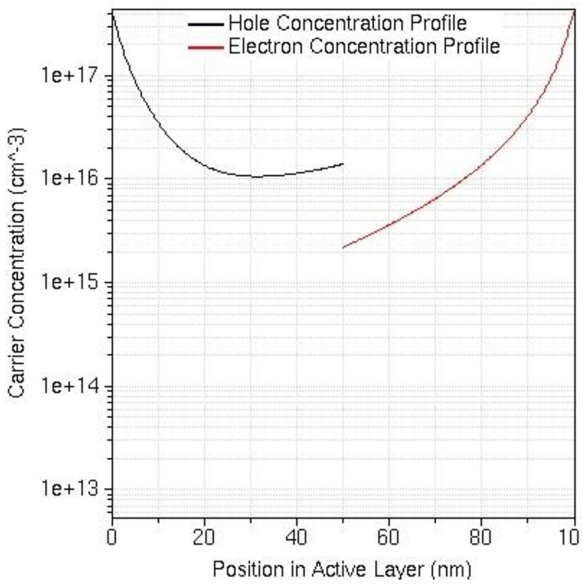
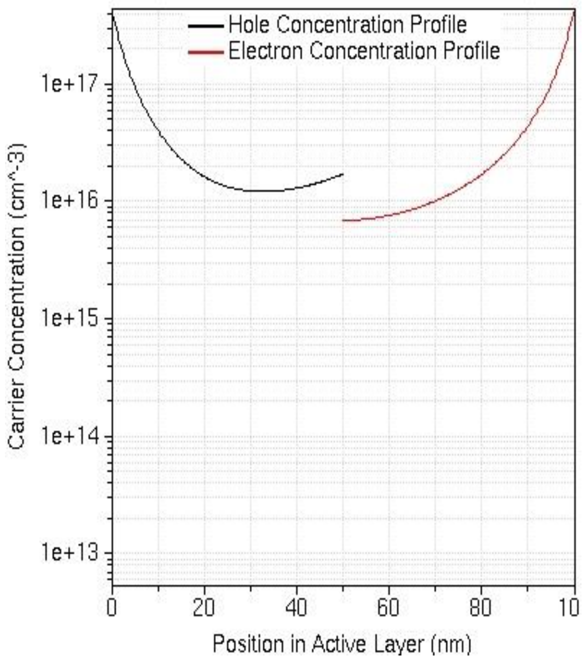


Figure 4.1. (a) Carrier concentration profile at active region for junction voltage 0.4 V (b) Carrier concentration profile at active region for junction voltage 0.5 V

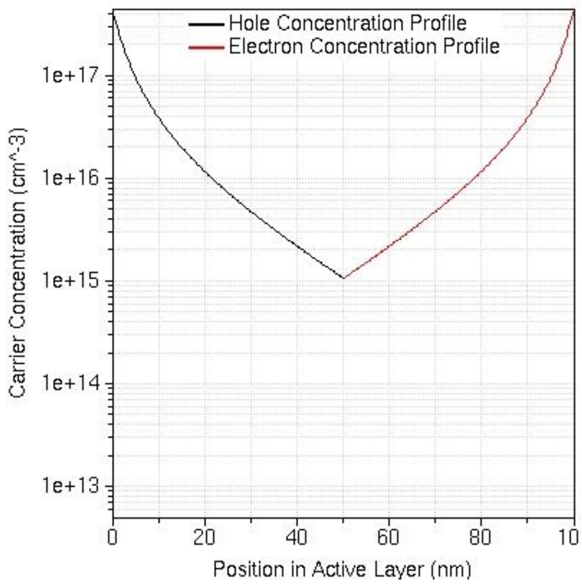


(a)

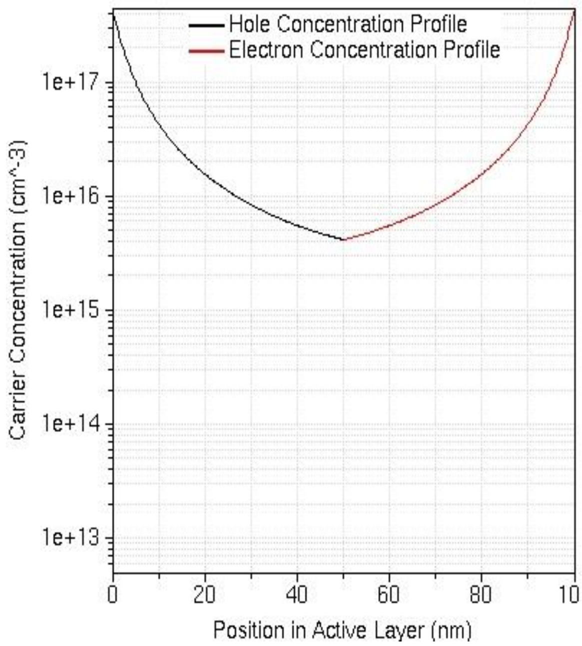


(b)

Figure 4.2. (a) : Carrier concentration profile at active region for junction voltage 0.4 V and increased value of electron mobility (b) : Carrier concentration profile at active region for junction voltage 0.5 V and increased value of electron mobility



(a)



(b)

Figure 4.3. (a) Carrier concentration profile at active region for junction voltage 0.4 V and increased value of both electron and hole mobility (b) : Carrier concentration profile at active region for junction voltage 0.5 V and increased value of both electron and hole mobility

RESULTS AND DISCUSSION

In this research work, the current-voltage characteristics of the P3HT/PCBM cell was studied with varying the carrier mobility and the fill factor (FF) , external quantum efficiency (EQE) and maximum output power per unit area of the cell (maximum output power density) of the cell has been determined. Results of these simulations are summarized in Tables 1 and 2. The carrier concentration gradient of the OPV cell has been observed from the carrier concentration profile with varying the junction voltage and carrier mobility and the diffusivity of the free chare carriers at the active layer has been analyzed. After analyzing, it has been obtained that, gradient of the charge carriers increases with increasing the electron and hole mobility at the P3HT/PCBM active layer, so diffusivity of the charge carriers from the donor-acceptor interface of the cell to the electrodes increase with minimum amount of loss.

CONCLUSION

It can be concluded from the simulations that, efficient P3HT/PCBM PHJ solar cell can be produced if the active layer is properly fabricated enhanced carrier mobility, particularly hole mobility at the donor layer of the cell. After studying the carrier concentration profile, it is concluded that, for great diffusion of charge carriers at the active layer of the cell, enhanced charge carrier mobility is necessary, which can be done by tuning the doping concentration at the active layer. The enhanced charge carrier mobility also provides low amount of losses of carriers at active layer and high electrical power at output.

TABLE 1. Performance of P3HT/PCBM Planar Hetero-junction Cell (PHJ) for varying Electron Mobility at Acceptor Layer

Mobility of electron (cm^2/V. s)	FF	EQE (%)	Maximum power density (W/m^2)
$5x10^{-4}$	0.629	1.886	18.86
$5x10^{-3}$	0.687	2.078	20.78
$5x10^{-2}$	0.694	2.102	21.01
$5x10^{-1}$	0.695	2.104	21.03

TABLE 2. Performance of P3HT/PCBM Planar Hetero-junction Cell (PHJ) for varying Hole Mobility at Donor Layer

Mobility of hole (cm^2/V. s)	FF	EQE (%)	Maximum power density (W/m^2)
$1x10^{-4}$	0.629	1.886	18.86
$1x10^{-3}$	0.768	2.329	23.29
$1x10^{-2}$	0.794	2.406	24.06
$1x10^{-1}$	0.797	2.413	24.13

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Persian Abstract

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چکیده

در این مطالعه، پارامترهای عملکردی همچون ضریب پرکردن، بازدهی کوانتومی خارجی، حداکثر چگالی توان و پروفایل غلظت حامل در یک سلول فتوولتاییک مورد بررسی قرار گرفته است. شبیه سازی انجام گرفته با در نظر گرفتن تابش ۱ کیلووات بر متر مربع، حجم هوای ۱،۵، دمای ۳۰۰ کلوین و آند و کاتد ایندیوم تین اکساید و آلومینیوم انجام شده است. پارامترهای عملکردی در جابه جایی الکترون در شرایط مختلف و در پذیرنده و لایه دهنده مورد بررسی قرار گرفته است. غلظت حامل برای مقادیر مختلف ولتاژ مورد بررسی قرار گرفته است. بیشترین بازده کوانتوم خارجی برابر با ۲/۴۱۳ ٪ و حداکثر چگالی قدرت ۲۴/۱۳ وات بر متر مربع بدست آمده است.