Proceedings of the
International Conference on Mechanical Engineering and Renewable Energy 2019
(ICMERE2019) 11 – 13 December, 2019, Chittagong, Bangladesh

ICMERE2019-PI-245

DESIGN, OPTIMIZATION AND PERFORMANCE ANALYSIS OF P3HT: PCBM BASED ORGANIC SOLAR CELLS

M. T. Ahsan, H. Ali and J. Chakrabartty

Department of Electrical and Electronic Engineering, Chittagong University of Engineering & Technology, Chittagong-4349, Bangladesh.

ahsanalvee01@gmail.com , mhossainali2425@gmail.com, joychakr@cuet.ac.bd

Abstract- *Organic solar cells have been identified as a potential candidate for solar energy harvesting over the past decades. The optimization of the thickness and the carrier mobility of each layer in the device is crucial for enhancing the device performances. In this manuscript, we present numerically simulated results enhanced photon to electricity conversion efficiency of the organic solar cells by virtue of thickness and mobility optimization approaches of the devices. We used GPVDM software for simulating the device structure: ITO/PEDOT:PSS/P3HT:PCBM/ZnO/Al. The results show that the 200 nm of the active absorber layer (P3HT:PCBM) of the device exhibited maximum efficiency of ~8.79% with fill factor (FF) of ~0.62. The efficiency increased further up to ~10.16% while optimized the mobility of the carrier (2.48x10 $^{-6}$cm^{2}v^{-1}s^{-1}) of the same layer. Keeping constant the thickness and the mobility of the active layer, the thickness optimization of PEDOT:PSS (20 nm), ITO (60 nm), and ZnO (40 nm) layers further increased the efficiency up to ~11.25%. These results exhibit a promising route to enhance the efficiency of the organic solar cells which could be useful for other researchers as well to fabricate the practical devices.*

Keywords: Heterojunction, organic solar cells, P3HT:PCBM, GPVDM Software, mobility, absorption.

1. INTRODUCTION

Solar to electricity conversion process is regarded as one of the most popular forms of clean energy generation approach. Among all other solar energy conversion devices, organic materials based solar cells have potentials to harness efficiently solar energy into electricity due to their enriched optoelectronic properties. Organic solar cells (OSC) have several advantages such as low cost, environment friendly, easy to installation etc. For these reasons, OSCs have attracted enormous research interests now a day. Among all other solar energy materials available to use in OSCs, P3HT:PCBM organic blend is so far the most widely used material for its high light absorption properties that leads to high energy conversion efficiency. An OSC is a device that generates current from sunlight through exciting electrons in a blend of organic materials from a nearly filled set of concentrations of energy to a basically empty set of concentrations of energy. As result, electron-hole pairs (EHP) are generated in the device [1]. These excited electrons are mobile charged species which are free to move around the polymers [2]. However, electrons and holes have a finite lifetime and need to be dissociated prior to recombine with each other which may decrease the device performances. The goal of designing an efficient solar cell is to find some way to force electrons to preferentially travel in one direction while the holes move in the opposite direction. Due to the movement of excitons, electron and holes eventually be accumulated across the electrodes results in a generation of voltage across the device, which is later used to operate the load at short circuit condition [3]. A schematic of a planar heterojunction (PHJ) of organic photovoltaic (OPV) device is shown in Fig. 1. The optoelectronic phenomena in Fig. 1 occurs basically in four-steps: (i) photon-induced exciton generation in organic semiconductor, (ii) exciton diffusion to the donor/acceptor (D/A) interface, (iii) formation of charge transfer (CT) state, and (iv) dissociation of CT state into free electrons and holes that are subsequently swept towards the respective electrodes with the effect of built-in electric field.

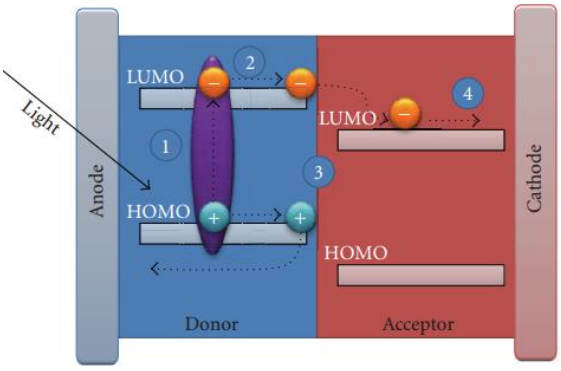

Fig. 1 Optical processes in organic solar cells.

Both free electrons and holes are involved in producing the photocurrents [4, 5]. The efficacy of collecting charged particles depends mainly on three factors:

mobility of the charge carriers, internal electric field that sweeps the carriers to the respective contacts, and the carrier recombination rate. Since the carrier mobility in the organic semiconductors is poor (10^{-5}–10^{-3} $cm^2V^{-1}s^{-1}$), the charge carriers tend to pile up at the donor-acceptor (D–A) interfaces [8]. The efficiency of the devices is calculated by the following equation:

$$\eta = (FF*I_{SC}*V_{OC})/P \quad (1)$$

where *FF*, *Isc*, *Voc*, and *P* indicates fill factor, short circuit current, open circuit voltage, and incident power of the photon flux. The short circuit current depends largely on the photon absorption and the internal quantum efficiency of the device. The photon absorption could be increased by increasing the thickness of active layers [6]. However, the possibility of carrier recombination increases with increasing the thickness of active layers because of its low charge carrier mobility. This recombination losses decrease the FF. In principle, the mobility of the organic semiconductors can be improved in several ways such as introducing a charge transfer layer in the device, thermal annealing, and a high conjugated crystal structure that may contribute to the efficiency as well [7, 8].

In practice, the power conversion efficiency (PCE) of P3HT:PCBM bulk heterojunction based OPVs is reported in general in the range of from 5% to 10% as they have a good absorption coefficient, suitable cell morphology, and charge carrier mobility [9, 12]. The basic device structure of P3HT:PCBM based OPVs can be found as ITO/HTL/P3HT:PCBM/Al [12]. In order to further enhance the efficiency of that device, it is necessary to modify the device structure along with obtaining a detailed understanding of the processed leading from the absorption of photons to the extraction of charge carriers. The fundamental requirement for achieving high PCE in the OPV cells is to minimize the interfacial recombination [16]. One approach for lowering the recombination loss is the enhancement of the carrier mobility in the OSC [10]. In 2012, B. Ray et al. [8] introduced a fixed-charged layer at the D-A interfaces in order to reduce carrier recombination and thus increasing the FF (>0.80) which results in an increase of PCE. The fixed charged layer at the interface creates an interfacial field that depletes the interface of free carriers and thus reduces the carrier recombination. Another vital aspect in OPV is the optimization of layer thickness. Y. Min et al. [11] investigated the effect of layer thickness along with morphology on the performance of OPV. They concluded that the photocurrent is highly dependent on the thickness of the active layers and the optimized thickness is proposed to be 80 nm [11]. J. Mullerova et al. [13] studied optical absorptions of P3HT:PCBM blend where they studied the absorbance spectra of P3HT:PCBM based OPVs. They found that the absence of the illumination led to ~ 6% decrease of PCE within 60 min [13]. Other researchers investigated the same devices as well on the thickness optimization and on the carrier mobility optimization in order to study their impact on the absorbance spectra. For example, S. Babiker et al. [14] analyzed the effect of thickness optimization of P3HT:PCBM layers (simulation) and observed that 120 nm of P3HT:PCBM layers led the efficiency up to ~6%. M. Ulum et al. [15] proposed the optimized thickness of 100 nm with an efficiency of ~7.61% and found that the PCE decreased due to lowering of short circuit current above 100 nm. N. Karim et al. [17] reported the PCE enhancement from 3.08% to 6.65% by virtue of carrier mobility optimization ($5x10^{-3}$ $cm^2v^{-1}s^{-1}$) when the thickness of organic blend was 230 nm. These leads an interesting fact that there is a possibility to optimize both thickness and carrier mobility to get efficient OPV devices. In addition, since the layer thickness of OPV devices increases, more incident photons are absorbed leading to more exciton generation. However, the generated carriers decay exponentially over the time with the distance traveled. A larger distance leads to an increase in probability of recombination of carriers. However, if the device is thicker, efficiency will be lower as it can't absorb more photons results in poor generation of excitons. These two opposite criteria must be balanced by finding the optimized thickness of absorber layer. In the other hand, carrier mobility plays a crucial role to determine the performance of OPV devices. Increasing carrier mobility decreases carrier recombination and thus increase the PCE. Due to the carrier scattering effect, the carrier mobility however may not be increased further beyond a certain carrier concentration limit. Therefore, there must be a balance between these two opposite conditions.

In this work, we report the effect of different layer thickness and mobility of active layer on the PCE of OPV devices. The work deals with two aspects: the thickness and the carrier mobility of the active absorber layer. The results show the optimized thickness of the active absorber layer of 200 nm, HTL layer of 20 nm, ITO layer of 60 nm, and ETL layer of 40 nm. The optimized carrier mobility has found to be $2.48x10^{-7}$ $cm^2v^{-1}s^{-1}$. The maximum efficiency of the proposed device is simulated that is up to ~11.25%. This work may bring new ideas in the OPV fields and hopefully would be a fruitful concept for practical device fabrication purposes.

2. DEVICE SIMULATION PARAMETERS

General-Purpose Photovoltaic Device Model (GPVDM) is a free general purpose software for numerically simulate the OPVs which performs on the basis of solving Poisson equation, the bipolar drift diffusion equations, and the carrier continuity equations in 1D and time domain [19], as presented in eq. (2), eq. (3) and (4), and eq. (5) and (6) respectively.

$$\frac{d}{dx} = \varepsilon_0 \varepsilon_r \frac{d\phi}{dx} = q(n - p) \quad (2)$$

$$J_n = q\mu_c n \frac{\partial E_c}{\partial x} + qD_n \frac{\partial n}{\partial x} \quad (3)$$

$$J_p = q\mu_h p \frac{\partial v}{\partial x} - qD_p \frac{\partial p}{\partial x} \quad (4)$$

$$\frac{\partial J_n}{\partial x} = q(R_n - G + \frac{\partial n}{\partial t}) \quad (5)$$

$$\frac{\partial J_p}{\partial x} = -q(R_p - G + \frac{\partial p}{\partial t}) \quad (6)$$

We have used bulk heterojunction architecture of a P3HT:PCBM based OPV device architecture as shown in Fig. 2. The layer configuration adopted in this simulation is ITO/PEDOT:PSS/P3HT:PCBM/ZnO/AL, where ITO used (Indium Tin Oxide) as an anode layer, PEDOT:PSS (Poly3,4-ethylene dioxythiophene thiophene polystyrene sulfonate) as hole transporting layer (HTL) or buffer layer, P3HT:PCBM (a blend of P3HT (3-hexylthiophene) and PCBM ((6,6)-phenyl-C61 butyric acid methyl ester) as active layer, ZnO as electron transporting layer (ETL), and Al as cathode layer respectively. The parameters used for the simulation are summarized in Table 1.

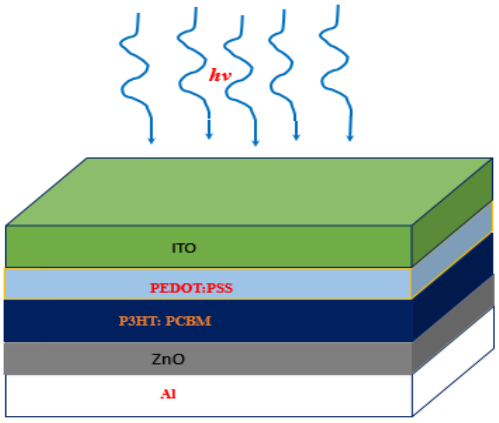

Fig. 2 P3HT:PCBM based organic solar cell.

Table 1 Electrical parameters of active layer.

Parameters	Value	units
Electron trap density	$3.8e^{26}$	$m^{-3}eV^{-1}$
Hole trap density	$1.4e^{-3}$	$m^{-3}eV^{-1}$
Electron mobility	$2.48e^{-6}$	$m^2V^{-1}S^{-1}$
Hole mobility	$2.48e^{-6}$	$m^2V^{-1}S^{-1}$
Relative permittivity	3.8	au
Number of traps	20	bands
Free electron to trapped electron	$2.5e^{-20}$	m^{-2}
Free hole to trapped hole	$4.86e^{-22}$	m^{-2}
Effective densities of free electron states	$1.28e^{27}$	m^{-3}
Effective densities of free hole states	$2.86e^{25}$	m^{-3}
Xi	3.8	eV
Eg	1.1	m^3S^{-1}

3. RESULTS AND DISCUSSIONS

The number of electron-hole pair (EHP) generation rate in the active layer as a function of wavelength is obtained for P3HT:PCBM (Fig. 3).

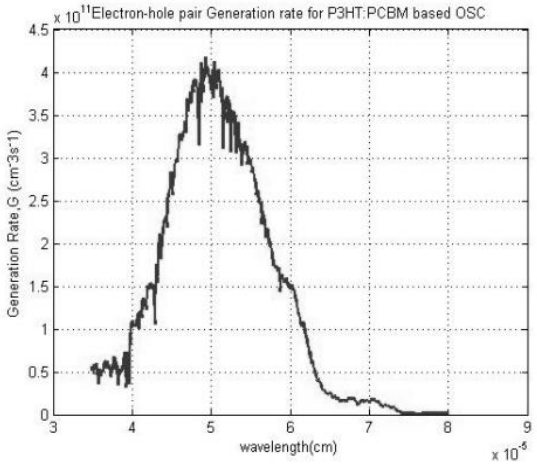

Fig. 3 Electron-hole pair generation rate for P3HT:PCBM based OSC as function of wavelength [17].

As observed from Fig. 3, the generation rate is higher in the wavelengths between 450 to 550 nm [17]. This is because the absorption coefficients for P3HT:PCBM based OSC is higher in that range [13, 20].

3.1 Effect of active layer thickness on the cell performance

Generally, as the layer thickness of the OPVs increase, more incident photons are absorbed. However, the incident photons decay exponentially with the distance travelled to the absorber layer [6]. Solar to electrical energy conversion efficiency will be low if the device is very thin since it cannot absorb sufficient number of incident photons [21]. On the other hand, the efficiency decreases with increasing the active layer thickness in the device structure. Since the carriers have to travel a large distance from their generation to extraction, the probability of carrier recombination increases [22]. Therefore, an optimized thickness is necessary to fulfil these opposite criteria. The optimum thickness of the active layer corresponds to maximum efficiency. In our simulation, the device performance has been varied over a range of thicknesses of active layer i.e. 50 nm to 600 nm. The best efficiency of 8.79% is observed for the thickness of active layer of 200 nm wherein the carrier mobility is of $2.48x10^{-7}$ $cm^2v^{-1}s^{-1}$.

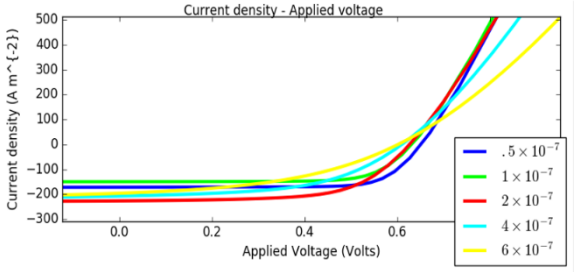

Fig. 4. J-V curves for different thicknesses of active layer (thickness unit: in meter).

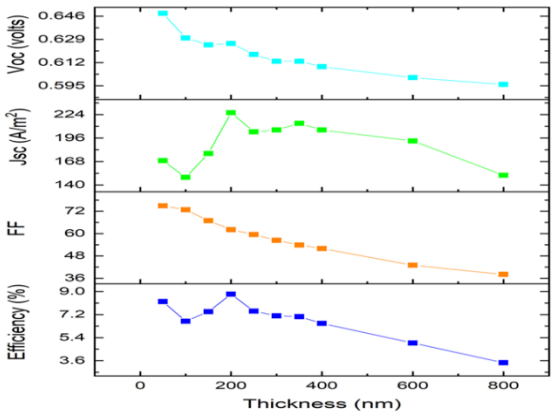

Fig. 5 Effect of thickness variation of active layer (P3HT: PCBM).

Table 2 Simulation parameters of absorber layer (P3HT:PCBM).

Thickness(nm)	J_{sc}	V_{oc}	FF	PCE
50	169.1	0.648	74.9	8.22
100	141.9	0.63	72.8	6.68
200	226.27	0.625	62.1	8.79
400	205.62	0.609	51.9	6.51
600	192.53	0.601	42.9	4.98
800	151.56	0.596	38.1	3.44

3.2 Effect of mobility of absorber layer on the cell performance

We have varied carrier mobility of active layer. As mobility increases, less recombination happens [23]. As a result, fill factor will be improved that leads to an increase in efficiency. Electron mobility has greater impact than hole mobility. If the difference of the mobility of these two carriers is large, then chances of recombination increases [24]. Moreover, after a certain limit, further increasing the mobility decreases the average speed of the carriers due to the increased collision between charged carriers and scattering effect [25]. The PCE was found to be 10.16% at the optimized of 2.48×10^{-6} $cm^2v^{-1}s^{-1}$.

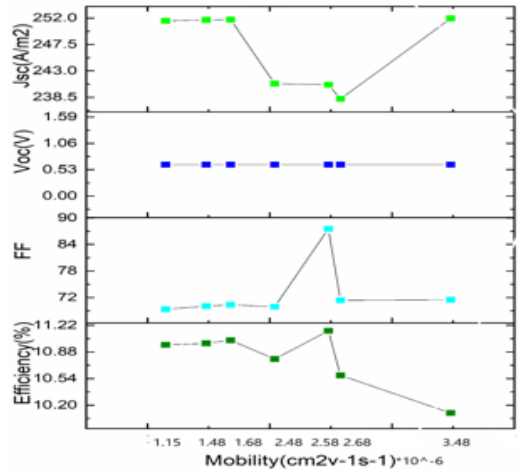

Fig. 6 Effect of carrier mobility of active layer.

3.3 Effect of HTL layer thickness on cell performances

We have then varied the thickness of PEDOT:PSS layer by keeping the thickness of active layer (P3HT:PCBM) at 200 nm and mobility at 2.48×10^{-6} $cm^2v^{-1}s^{-1}$. As it is a buffer layer, it smooths up the energy levels between ITO and active layer. In other word, it improves transportation of charges [26, 27]. In the software, we put a range of thickness (10 nm to 100 nm) in order to obtain the best PCE (10.82%) for an optimized PEDOT:PSS layer thickness that is 20 nm.

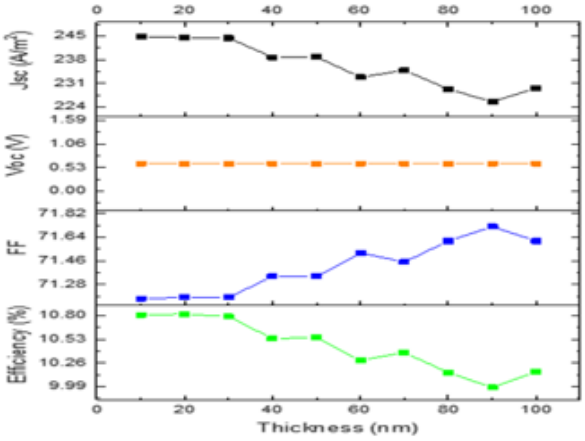

Fig. 7 Effect of thickness variation of PEDOT: PSS layer.

3.4 Effect of ITO layer thickness on cell performance

Likewise, the thickness of ITO layer was varied from 50 nm to 110 nm in the simulation tools. After optimizing layer thickness (60 nm), the efficiency further enhanced to 11.1%.

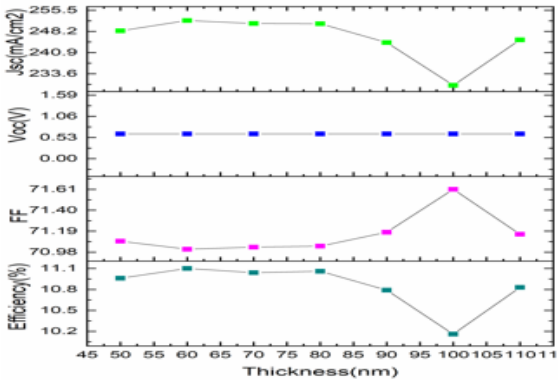

Fig. 8 Effect of thickness variation of ITO layer

3.5 Effect of ETL layer thickness on cell performances

We choose ZnO as ETL layer since it makes electron transportation smoother to cathode (Al) from absorber layer by decreasing the barrier height [28, 29]. As a result, efficiency will increase. The optimized thickness of ETL was found to be 40 nm and the efficiency at this thickness was 11.25%.

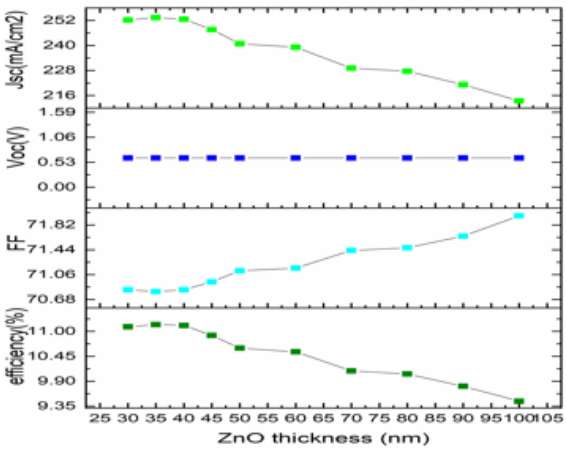

Fig. 9 Effect of thickness variation of ZnO layer on cell performances.

4. CONCLUSIONS

In summary, we designed an OPV device structure (ITO/PEDOT:PSS/P3HT:PCBM/ZnO/Al) based on P3HT:PCBM organic blend. In P3HT:PCBM blend, P3HT acts as electron donor and PCBM acts as the electron acceptor, whereas PEDOT:PSS, ZnO ITO, and Al acts as HTL layer, ETL layer, transparent conducting layer and cathode layer respectively. The thickness, of each layer along with the carrier mobility of P3HT:PCBM was optimized to obtain champion device efficiency using GPVDM software. The champion device efficiency of ~11.25% was obtained for the thickness of P3HT:PCBM layer, ETL, HTL, ITO, and Al layer of ~200 nm, ~40 nm, ~20 nm, ~60 nm, and ~100 nm respectively. In addition, the carrier mobility of P3HT:PCBM was optimized to be 2.48×10^{-6} $cm^2v^{-1}s^{-1}$. The study of operating temperature and the photo stability is an important aspect for OPV devices which could be incorporated urther in future to assess the device performance. In order to make the OPVs much more stable, reliable, and interesting among the researchers, the focus should be on enhancing the PCE as well as on photo-degradation effect of the device.

5. ACKOWLEDGEMENT

We acknowledge Dr. Md. Mohi Uddin, Department of Physics, Chittagong University of Engineering & Technology (CUET), Chittagong for providing GPVDM software for our research.

6. REFERENCES

[1] Few, S., Frost, J.M. and Nelson, J., 2015. Models of charge pair generation in organic solar cells. *Physical Chemistry Chemical Physics*, *17*(4), pp.2311-2325.

[2] Hiramoto, M., Fukusumi, H. and Yokoyama, M., 1992. Organic solar cell based on multistep charge separation system. *Applied Physics Letters*, *61*(21), pp.2580-2582.

[3] Brabec, C.J., Dyakonov, V., Parisi, J. and Sariciftci, N.S. eds., 2013. *Organic photovoltaics: concepts and realization* (Vol. 60). Springer Science & Business Media.

[4] Gregg, B.A., 2005. The photoconversion mechanism of excitonic solar cells. *MRS bulletin*, *30*(1), pp.20-22.

[5] Vandewal, K., Gadisa, A., Oosterbaan, W.D., Bertho, S., Banishoeib, F., Van Severen, I., Lutsen, L., Cleij, T.J., Vanderzande, D. and Manca, J.V., 2008. The relation between open-circuit voltage and the onset of photocurrent generation by charge-transfer absorption in polymer: fullerene bulk heterojunction solar cells. *Advanced Functional Materials*, *18*(14), pp.2064-2070.

[6] Moulé, A.J., Bonekamp, J.B. and Meerholz, K., 2006. The effect of active layer thickness and composition on the performance of bulk-heterojunction solar cells. *Journal of applied physics*, *100*(9), p.094503.

[7] Chu, C.W., Yang, H., Hou, W.J., Huang, J., Li, G. and Yang, Y., 2008. Control of the nanoscale crystallinity and phase separation in polymer solar cells. *Applied Physics Letters*, *92*(10), p.86.

[8] Ray, B. and Alam, M.A., 2012, June. Achieving fill factor above 80% in organic solar cells by charged interface. In *2012 IEEE 38th Photovoltaic Specialists Conference (PVSC) PART 2* (pp. 1-8). IEEE.

[9] Chen, M.C., Liaw, D.J., Chen, W.H., Huang, Y.C., Sharma, J. and Tai, Y., 2011. Improving the efficiency of an organic solar cell by a polymer additive to optimize the charge carriers mobility. *Applied Physics Letters*, *99*(22), p.262.

[10] Proctor, C.M., Kuik, M. and Nguyen, T.Q., 2013. Charge carrier recombination in organic solar cells. *Progress in Polymer Science*, *38*(12), pp.1941-1960.

[11] Nam, Y.M., Huh, J. and Jo, W.H., 2010. Optimization of thickness and morphology of active layer for high performance of bulk-heterojunction organic solar cells. *Solar Energy Materials and Solar Cells*, *94*(6), pp.1118-1124.

[12] Vijay, P. and Sumaria, V., Advancement in P3HT PCBM solar cells, the most efficient Polymer Photovoltaic cell.

[13] Müllerová, J., Kaiser, M., Nádaždy, V., Šiffalovič, P. and Majková, E., 2016. Optical absorption study of P3HT: PCBM blend photo-oxidation for bulk heterojunction solar cells. *Solar Energy*, *134*, pp.294-301.

[14] Babiker, S.G. and Shuai, Y., 2012. Simulation of organic solar cells using AMPS-1D program.

[15] Ulum, M.S., Sesa, E. and Belcher, W., 2019, June. The effect of active layer thickness on P3HT: PCBM nanoparticulate organic photovoltaic device performance. In *Journal of Physics: Conference Series* (Vol. 1242, No. 1, p. 012025). IOP Publishing.

[16] Chiew, E.K., Yahaya, M. and Othman, A.P., 2013. Investigation of Recombination Process

of P3HT: PCBM Organic Solar Cell. In *Advanced Materials Research* (Vol. 622, pp. 1147-1151). Trans Tech Publications.

[17] Karim, N., Mime, F.I., Islam, M.R. and Mehedi, I.M., 2017, February. Performance analysis of P3HT: PCBM based organic solar cell. In *2017 International Conference on Electrical, Computer and Communication Engineering (ECCE)* (pp. 826-830). IEEE.

[18] Baek, S.W., Noh, J., Lee, C.H., Kim, B., Seo, M.K. and Lee, J.Y., 2013. Plasmonic forward scattering effect in organic solar cells: a powerful optical engineering method. *Scientific reports*, *3*, p.1726.

[19] Williams, J. and Walker, A.B., 2008. Two-dimensional simulations of bulk heterojunction solar cell characteristics. *Nanotechnology*, *19*(42), p.424011.

[20] Lee, W.H., Chuang, S.Y., Chen, H.L., Su, W.F. and Lin, C.H., 2010. Exploiting optical properties of P3HT: PCBM films for organic solar cells with semitransparent anode. *Thin Solid Films*, *518*(24), pp.7450-7454.

[21] Takeuchi, S., Kim, J., Yamamoto, Y. and Hogue, H.H., 1999. Development of a high-quantum-efficiency single-photon counting system. *Applied Physics Letters*, *74*(8), pp.1063-1065.

[22] Proctor, C.M., Kuik, M. and Nguyen, T.Q., 2013. Charge carrier recombination in organic solar cells. *Progress in Polymer Science*, *38*(12), pp.1941-1960.

[23] Mandoc, M.M., Koster, L.J.A. and Blom, P.W., 2007. Optimum charge carrier mobility in organic solar cells. *Applied physics letters*, *90*(13), p.133504.

[24] Mandoc, M.M., Koster, L.J.A. and Blom, P.W., 2007. Optimum charge carrier mobility in organic solar cells. *Applied physics letters*, *90*(13), p.133504.

[25] Etampawala, T., Ratnaweera, D., Morgan, B., Diallo, S., Mamontov, E. and Dadmun, M., 2015. Monitoring the dynamics of miscible P3HT: PCBM blends: A quasi elastic neutron scattering study of organic photovoltaic active layers. *Polymer*, *61*, pp.155-162.

[26] Ochiai, S., Kumar, P., Santhakumar, K. and Shin, P.K., 2013. Examining the effect of additives and thicknesses of hole transport layer for efficient organic solar cell devices. *Electronic Materials Letters*, *9*(4), pp.399-403.

[27] Lim, F.J., Ananthanarayanan, K., Luther, J. and Ho, G.W., 2012. Influence of a novel fluorosurfactant modified PEDOT: PSS hole transport layer on the performance of inverted organic solar cells. Journal of Materials Chemistry, 22(48), pp.25057-25064.

[28] Park, S., Tark, S.J., Lee, J.S., Lim, H. and Kim, D., 2009. Effects of intrinsic ZnO buffer layer based on P3HT/PCBM organic solar cells with Al-doped ZnO electrode. *Solar Energy Materials and Solar Cells*, *93*(6-7), pp.1020-1023.

[29] Manor, A., Katz, E.A., Tromholt, T. and Krebs, F.C., 2012. Enhancing functionality of ZnO hole blocking layer in organic photovoltaics. *Solar Energy Materials and Solar Cells*, *98*, pp.491-493.