SIMULATION OF ELECTRICAL PROPERTIES OF HETEROJUNCTION AND BILAYER ORGANIC SOLAR CELLS USING 'OGHMANANO' SOFTWARE

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ABSTRACT. This paper presents a comparison between heterojunction organic solar cells (HOSCs) and bilayer organic solar cells (BOSCs) in terms of the simulation of the fill factor (FF) and the power conversion efficiency (PCE). HOSCs are a competitive alternative source of electrical energy. BOSCs have gained a lot of interest because they are known to be environmentally friendly. Currently, the construction of the organic solar cells is motivated by the need for optimising the perfect material to generate greater electrical energy. Thus, the organic solar cell structures design and certain materials is of vital importance to develop and enhance the conversion efficiency and fill factor of organic solar cells. The simulation tools are 'OghmaNano' the method used in this study. HOSCs consist of the structure layer such as ITO/ZnO/P3HT:PCBM/PEDOT:PSS/Au. BOSCs consist of the structure layer which is ITO/ PEDOT:PSS/P3HT/Al. Thus, BOSCs at 0.5 W/m^2 light intensity achieved a FF of 0.761608 % and for the PCE realised 3.816099 % at 2.5 W/m^2 light intensity. HOSCs at 0.09 W/m^2 light intensity achieved a FF of 0.688035 % and the PCE realised 4.961236 % at 0.4 W/m^2 light intensity.

KEYWORDS: organic solar cells; heterojunction; bilayer; fill factor; power conversion efficiency

1 INTRODUCTION

Manufacturing solar cells is always high on the challenge list particularly in the nanotechnology field as it offers possible and trusty applications. Solar cells employ a light responsive material that can alter solar energy to be direct current electric energy. It is utilised because it has reduced to low maintenance and low resistance to obtain the electricity created when cells are revealed to sunlight (Bagher, 2014). Organic solar cells (OSC) are a third-generation energy resource technology. This is because of the profusion of their basic materials. OSC have attracted research because of their low cost and mechanical flexibility. This technology also has attained a maximum power conversion efficiency of 11 % but is restricted by its long term reliability (Ranjitha et al., 2019). A p-n junction is one of solar cell applications. A p-type material of the semiconductor is combined with an n-type material as well as a p-n junction, alongside it works as the basic unit of a diode. The p-type and the n-type material are both of the same semiconductor material, the junction is called as a homojunction. If the junction layers are created with different semiconductor materials, it is referred to as a heterojunction (Alhuda et al., 2017).

2 LITERATURE REVIEW

A heterojunction organic solar cell (HOSC) consists of polymer or small molecules or both. The electron concentration for the donor is higher than the acceptor. The donor is energised by light. Thus creating a positive charge in the donor and a negative charge in the acceptor. Both charges move in a HOSC. Charge transfer happens between molecules while electron hopping moves a positive charge and hole hopping moves a negative charge. Then, the charges will transfer into the electrodes. HOSCs contain an anode layer, hole transport layer (HTL), active layer, electron transport layer (ETL) and a cathode layer. The active layer consists of electron donors and electron acceptors. The HTL and ETL, as two interfacial layers can improve the interface electronic structure between the active layer and two

electrodes. Zinc oxide (ZnO) is a metal oxide as an interface layer as a semiconductor that has excellent transport properties and good electrical properties, in addition to operating as an inverted structure. Fabrication of ZnO films has great potential due to high potential applications in organic solar cells.

In parallel, increasing the charge extraction and transport. BOSCs can be as effective as bulk heterojunction equivalents. However, the photophysics of bilayer devices is basically different to bulk heterojunctions. The factor of the different performance is that the long-range interlayer energy transfer plays a significant role in increasing the efficiency of bilayer devices (Yang et al., 2012). BOSCs encompass two layers in between the conductive electrodes. The two layers contain a dissimilar amount of the electron affinities and ionisation energies, thus electrostatic forces are formed at the the two layers. This structure of layers is also known as a planar donor-acceptor heterojunction (Peng et al., 2013).

The total of electricity created by the OSC via solar cell processes is still low paralleled to Silicon Solar Cells (SSC). This is because the OSC has a higher band gap that limits the absorption of the solar spectrum. The reduction in the charge mobility can be upgraded by using materials with high purity and a typical crystal. To improve FF and PCE in BOSCs, materials with near-ideal properties are essential for photovoltaic material design. Structural analysis of organic solar cell devices is required. Another strategy is to utilise molecular engineering to alter the HOMO and LUMO energy band levels of the photons. The HOMO level should be reduced to increase the Voc energy level and the LUMO should be compatible with the efficient electron transfer of the fullerene (Cornelius, 2014). Thus, the results improve the device execution parameters with open-circuit voltage (Voc), short-circuit current (Jsc), fill factor (FF) and PCE. These methods of developing new materials would be capable to greatly enhance the device performance of organic solar cells. The focus of this study is to compare the design and to simulate the HOSC and BOSC structure of organic solar cells using the 'OghmaNano' simulation tool to increase the FF and PCE.

3 METHODOLOGY

The design structure of HOSCs consists of five layers as ITO/ZnO/P3HT:PCBM/PEDOT:PSS/Au and is shown in Figure 1. Indium tin oxide (ITO) is used as a transparent conductive substrate that is sensitive to respond to light and is also known as a transparent conducting oxide. Zinc oxide (ZnO) is a metal oxide as an interfacial layer as a semiconductor that has very good transport properties and good electrical properties, alongside operation as an inverted structure. ZnO films fabrication has a great capability because of high potential application in organic solar cells.

Poly(3-hexylthiophene) (P3HT) is used as a p-type material as well as a donor layer. Phenyl-C60-butyric acid methyl ester (PCBM) is used as an n-type material as well as an acceptor layer. The acceptor layer accepts the electrons from the donor and the charge separation arises. These two materials are blended with better quality rather than being easy to synthesis and process. The most important acceptor layer is soluble in most organic solvents. Table 1 shows the parameters used in the simulation at T=300 K for P3HT:PCBM (Bagher, 2014).

PEDOT:PSS as the hole transport layer (HTL) is shown to be a main factor to increase the efficiency of the P3HT:PCBM bulk heterojunction (BHJ) solar cells. It is also known that the conductive polymers work as a hole transporting layer, because of its simple processing, and high transparency. Gold (Au) depends on the shape of its nanostructures like nanoparticles and nanorods which enhances the conductivity of organic solar cells (Lee et al., 2016).

The design structure of BOSC consists of four layers ITO/PEDOT:PSS/P3HT/Al as shown in Figure 2. P-type material is used as a donor layer of the BOSC. The light absorbing materials are presented as Poly(3-hexylthiophene) (P3HT). P3HT material is chosen because it is relatively easy to synthesise and process. Then, n-type material is used as an acceptor layer of the BOSC. The charge separation occurred when acceptor takes the electrons from the donor. The N-type material used is (,4-ethylenedioxythiophene):poly(styrenesulfonate) (PEDOT:PSS). Table 1 shows the parameters used in simulations.

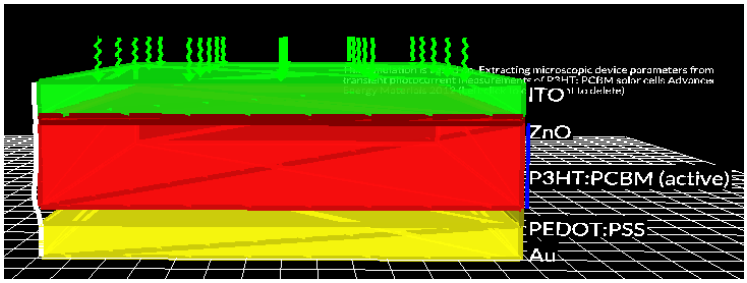

Figure 1: ITO/ZnO/P3HT:PCBM/PEDOT:PSS/Au layers

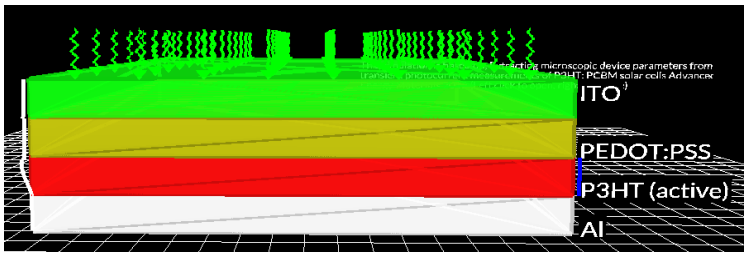

Figure 2: ITO/ PEDOT:PSS/P3HT/Al layers

Table 1: Parameters used in Simulations (Wu et al., 2017)

Parameter	Value
Electron mobility ($m^2V^{-1}s^{-1}$)	2.48e-07
Hole mobility ($m^2V^{-1}s^{-1}$)	2.48e-07
Effective Density of free electron states (m^{-3}) (@300 K)	1.28e27
Effective Density of free hole states (m^{-3}) (@300 K)	2.86e25
Relative permittivity (au)	3.8
Eg (eV)	1.1

Using 'OghmaNano' the value of light intensity is keyed in and 'Run' is clicked. The simulation then generates the electrical parameters. The software also calculates the internal electrostatic potential and is shown in the database terminal. Electrical and optical parameters are generated in this software. The way of characterising a solar cell is the measurement of current-voltage characteristics. The figures of merit are Isc, Voc and the FF. The PCE is determined by the short-circuit current density and the open circuit photo voltage, where, Pin is the incident power density, FF is the fill factor and Jsc is the short circuit current and Voc is open circuit voltage. The data could be obtained from different light intensities of the OSC. The performance of the OSC depends on the FF which is determined from measurement of the *I-V* curve and is defined as (Koole et al., 2014).

$$FF = \frac{Voptimal * IoptimaL}{Voc\ Isc} \quad (1)$$

Then, the power conversion efficiency (η) formula is as below:

$$\eta = \frac{(Pmax)}{Pin} = \frac{Voptimal * Ioptimal}{Pin} = \frac{FF * Voc * Isc}{Pin} \quad (2)$$

4 RESULTS AND DISCUSSION

HOSCs at 0.09 W/m^2 light intensity yielded a FF of 0.688035 % and the PCE achieved 4.961236 % at 0.4 W/m^2 light intensity as shown in Figure 3. The FF completely increased as the light intensity increased from 0 to 0.09 W/m^2. Nevertheless, the FF reduced when the light intensity was higher than 0.09 W/m^2 due to the FF values being completely connected to the loss in carrier transport at ETL but the PCE showed vice versa. This might be due to the PCE which are slightly connected with the microstructure and the surface roughness. The power efficiency would indicate a slight decrease when greater than 0.4 W/m^2 light intensity due to the recombination of the holes in P3HT with the electrons in the electrode. HOSCs consist of a structure layer such as ITO/ZnO/P3HT:PCBM/PEDOT:PSS/Au. ZnO metal oxide operates as an interfacial layer and as ETL on the top of ITO as an inverted organic solar cell. Besides that, the surface morphology of the metal oxide assists the light to be absorbed. This might be due to the nanostructure of the HOSCs as a nanorod. The ETL acts to block the reverse holes arising from HOSCs travelling to the cathode, by controlling the electron only collection on the ITO side. Therefore, the transport of carriers through the layers to the Au electrodes takes place while averting the chemical or physical property responses between the HOSCs and the cathode.

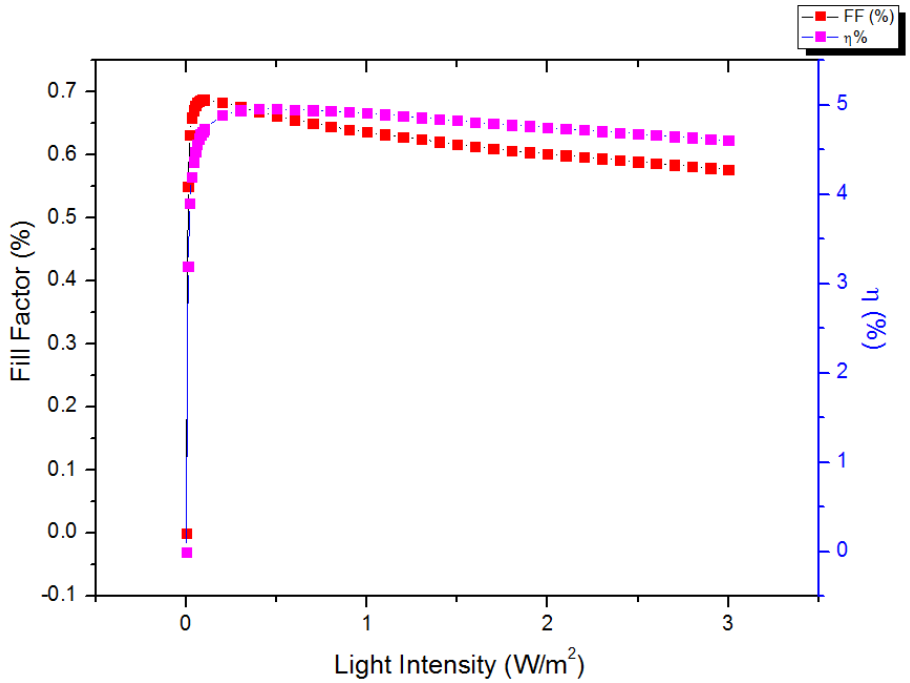

Figure 3: Fill factor and PCE vs light intensity of ITO/ZnO/P3HT:PCBM/PEDOT:PSS/Au

A semiconductor lifetime is based on the rate of recombination that is related with the concentration of minority carriers and the efficiency of the HOSCs. The quantity of minority carriers was raised above equilibrium by several transients by external excitation and additional minority carriers that could possibly degenerate back to that equilibrium carrier concentration via the process of recombination. This means, the recombination rate is correlated to the minority carrier lifetime and the minority carrier diffusion length. In the meantime, a large significant decrease in the short circuit current density could be also observed as shown in Figure 4. This characteristic occurs when beaming a solar-like light onto the cell, where the power of such a beam is from 0.01 W/m^2 to 3 W/m^2. Starting approximately with Voc= 0.638212 and the shortcut current density slowly decreasing until it achieved Jsc= -374.9339 A/m^2. Furthermore, the charge transfers of the carrier of ZnO imply the reason for increasing the short circuit current density. An increase in Voc of the OSC with the increasing of light intensity is due to the surface morphology effects of the HOSC. The Voc increased with the increase in light intensity and Jsc showed a contrary trend. The Fill Factor (FF) is the ratio of the real maximum reachable power to the product of the open circuit voltage and short circuit current. So, the fill factor influences the value of Jsc and Voc. In order to enhance the power efficiency of organic solar cells, the main critical issue is to obtain a high FF for better implication (Guo et al., 2018).

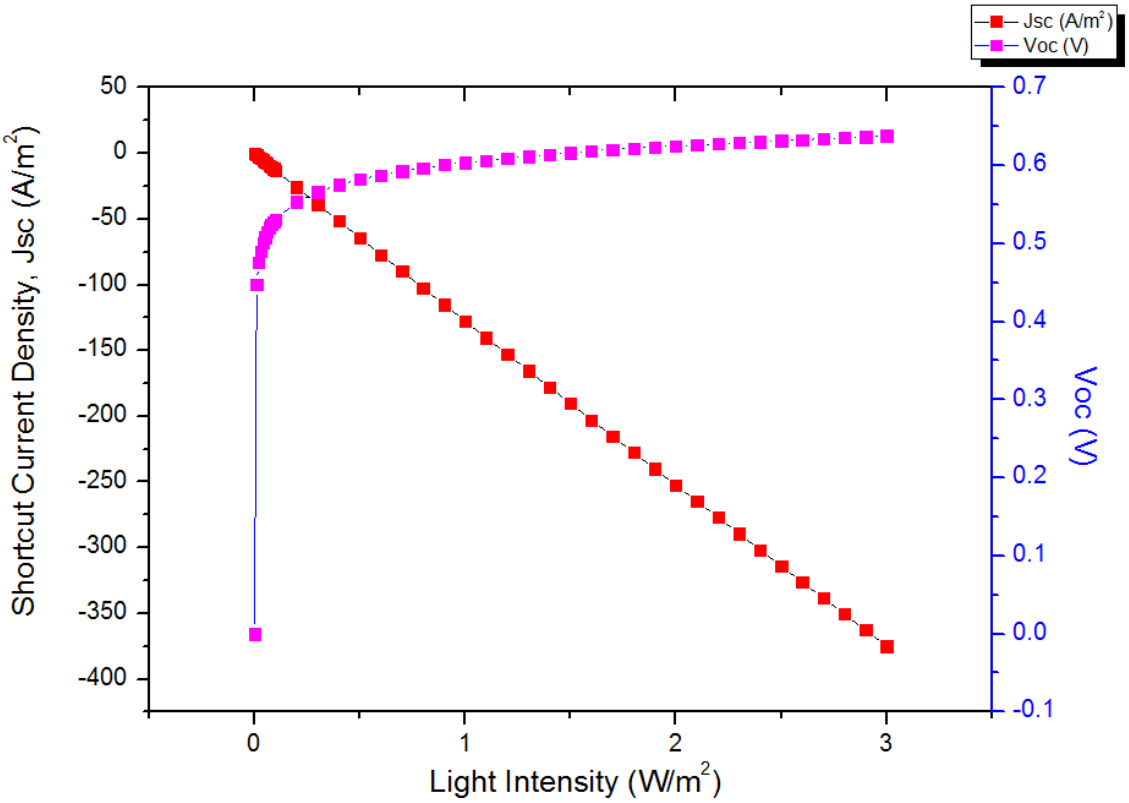

Figure 4: Shortcut current density and Voc vs light intensity of ITO/ZnO/P3HT:PCBM/PEDOT:PSS/Au

A BOSC at 0.5 W/m^2 light intensity revealed that the FF was 0.761608 % and the PCE achieved 3.816099 % at 2.5 W/m^2 light intensity. The BOSC was supplied with an inverted bias so that it worked as a diode. In Figure 5, it can be seen that the FF completely increased at a light intensity from 0 to 0.5 W/m^2. Nevertheless, the fill factor slowly reduced when the light intensity was higher than 0.5 W/m^2 due to the FF values being directly correlated to the loss in carrier transport at the interface, but the efficiency indicated vice versa. This might be due to the PCE slowly increasing which connects well with the microstructure of the P3HT.The P3HT acted as an electron donor layer and the PEDOT:PSS as an electron acceptor layer. PEDOT: PSS operated to block the flow of electrons and excitons towards the high work function metal electrodes.

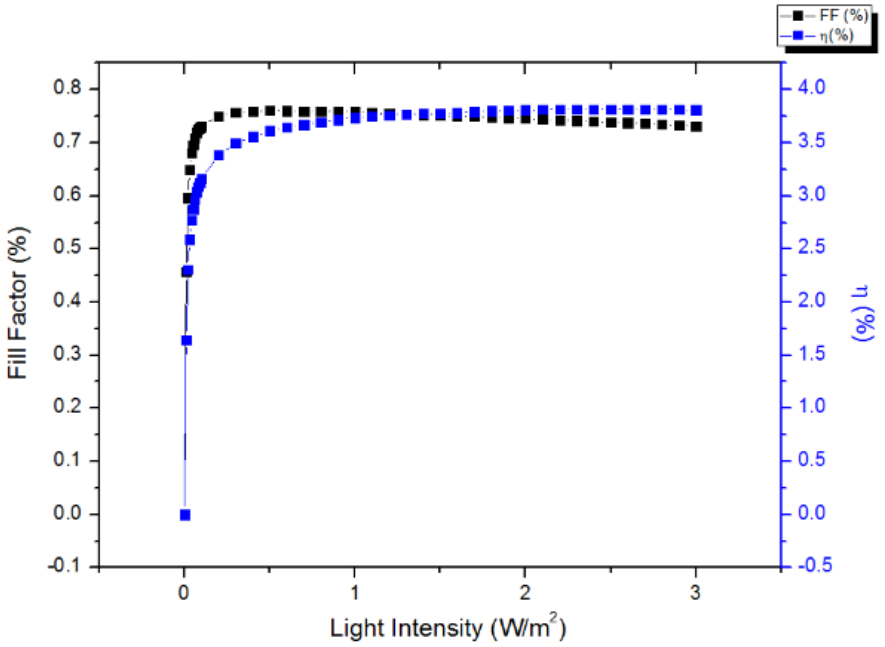

Figure 5: Fill factor and PCE vs light intensity of f ITO/PEDOT:PSS/P3HT/Al

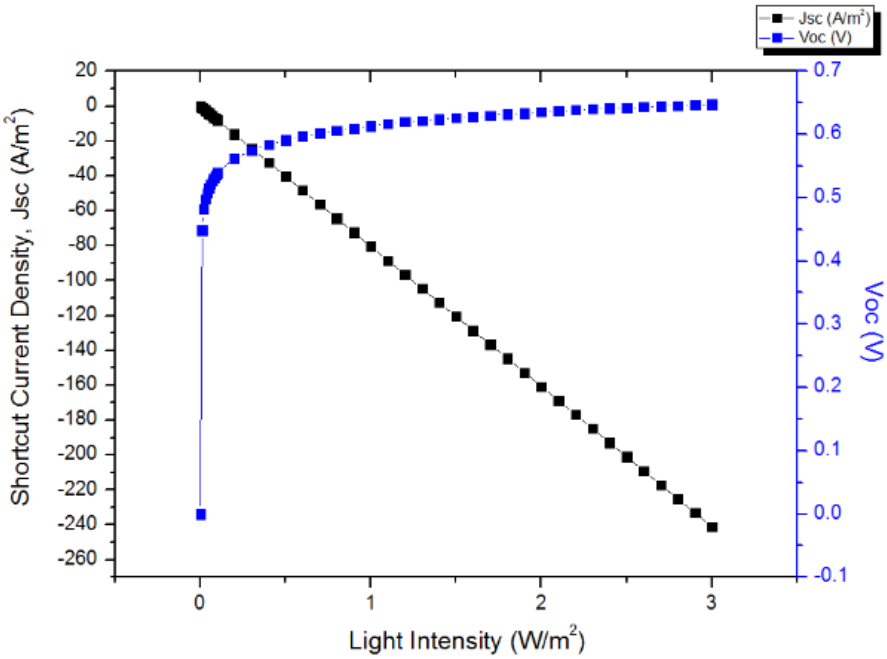

Figure 6: Shortcut current density and Voc vs light intensity of ITO/PEDOT:PSS/P3HT/Al

This characteristic occurs when beaming a solar-like light onto the cell, when the power of such a beam is from 0.01 W/m^2 to 3 W/m^2. Starting with approximately Voc= 0.647884 and the shortcut current density slowly decreasing until it achieved Jsc=-241.02 A/m^2. The light J-V measurement served to determine the main characteristic of the solar cell in Figure 6. In the meantime, a large significant decrease in the shortcut current density could also be observed as in Figure 6. Furthermore, the charge transfers of the carrier of PEDOT:PSS material may imply the reason for the decrease in the short circuit current density. An increase in the Voc of the OSC with increasing light intensity was due to the surface morphology effects of the HOSCs.

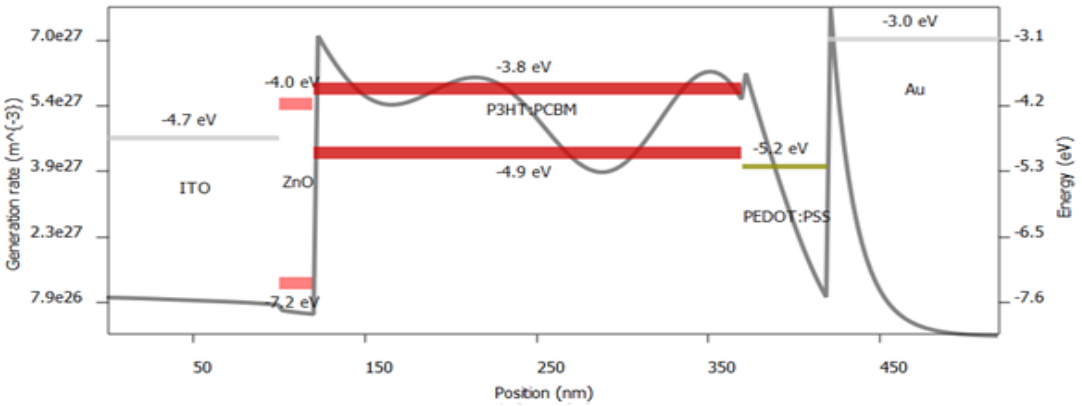

Figure 7: Generation rate and energy vs position of ITO/ZnO/P3HT:PCBM/PEDOT:PSS/Au

In Figure 7, for the ITO and Au electrodes, every has a work function value of ~4.7 eV and 3.0 eV, respectively. The current density of the HOSC is greater than the ITO until it decrease fully by the end to the Au electrode due to a high surface to bulk surface ratio of morphology in which the particle size was sufficient to reach an effective contact in OSC. For the transparent ITO substrate, the generate rate was low. As the energy of the photons increased and overcame the bandgap energy of the material, the photons were absorbed and transfer the energy to the corresponding electrons, which in turn, excited the electrons into the conduction band. Then, ZnO as ETL absorbed photons was also low because of the conductivity of the metal oxide. In this case, ZnO as buffer layer had a conduction band energy less than that of the LUMO energy level of the P3HT:PCBM polymer. The generate rate was high when P3HT: PCBM absorbed the light. The electrons at the highest occupied molecular orbital (HOMO) of the material were absorbed at the conduction band of the LUMO. This then created an exciton in both donor and acceptor parts. This was the product of photons being absorbed to generate the minority and majority carriers. Absorbed photons of the design were higher for the P3HT: PCBM, but it decreased over time. Then, the excitons diffused to the donor-acceptor interface (at the ETL and HTL). At that moment, the dissociation of excitons could occur due to the driving forces by the change in free energy. This means the electrons jumped from PCBM (LUMO) of the active layer towards to the lower of the ITO electrode and holes jumped onto higher Au electrode. These indicated the charge separation occurred. Further, ZnO as a buffer layer was used as well as to avoid the P3HT after contacting with ITO substrates. In parallel, to reduce the recombination process of the electrons in the gathering electrode the ZnO as ETL could effectively work as hole-blocking layers to prevent the leakage current. The exciton was dissociated into electrons and holes or separated at the interface. HTL is a favourable material which has good conductivity and surface morphology. The charge transport consisted of positive charges and negative charges collected at the anode (holes) and cathode (electrons) (Yang et al., 2012).

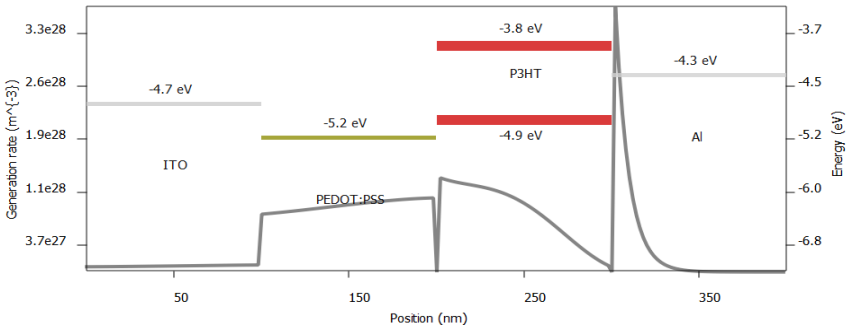

Figure 8: Generation rate and energy vs position of ITO/PEDOT:PSS/P3HT/Al

In contrast, for the ITO and Al electrodes had a work function value of ~4.7 eV and ~4.3 eV respectively as shown in Figure 8. When the photon energy was greater than the band gap of the BOSC material, the photons were absorbed by the material and the excited electrons jumped to the conduction band. After that, the minority and majority carriers were produced when the photons were absorbed. Absorbed photons of the design were higher for the P3HT but it decreased over time. At the

PEDOT:PSS acceptor layer, the absorbed photons were low due to the photovoltaic process. Photons generate charge carriers to produce photovoltaic energy. This means the electrons jump from the LUMO of the active layer towards the bottom of the ITO electrode. Then, the holes formed in the HOMO move to the anode. The reflection and transmission were normally measured as loss mechanisms as photons. Therefore, only if the photons had sufficient energy would the electrons be excited into the conduction band from the valence band. The performance would be normally influenced by a surface defect which is an oxygen vacancy defect created in the thin film. (Bagher, 2014)

5 CONCLUSION

Thus, the BOSCs at 0.5 W/m^2 light intensity indicated that the FF was 0.761608 %. The PCE achieved 3.816099 % at 2.5 W/m^2 light intensity. HOSCs at 0.09 W/m^2 light intensity revealed that the FF was 0.688035 % and the PCE achieved 4.961236 % at 0.4 W/m^2 light intensity. This means that the simulation and analysis of HOSCs with BOSCs using a simulation tool is successful. There is need for more design work to analyse to obtain the optimum material. These two types of OSCs can be used in solar cell applications.

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