AMPS-1D Simulation of P3HT Solar Cells: Impact of HOMO-LUMO Offset, Thickness, Temperature, and Optical Bandgap on Performance

Hadab Al-Otaibi
Department of Physics, College of Science, Northern Border University, Arar, Saudi Arabia
hadab1417@gmail.com

Omer I. Eid
Department of Physics, College of Science, Northern Border University, Arar, Saudi Arabia | Department of Physics, Faculty of Science, University of Khartoum, Khartoum, Sudan
Omer.Hassin@nbu.edu.sa, omereid@gmail.com. (corresponding author)

M. E. M. Eisa
Department of Physics, College of Science, Northern Border University, Arar, Saudi Arabia
memeisa@gmail.com

Amwaj N. Alzahrani
Physics Department, Taif University, Taif, Saudi Arabia
anzahrani@tu.edu.sa

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ABSTRACT

This study employed the AMPS-1D software to investigate the relationship between the open-circuit voltage (V_{oc}) and the energy difference between the Highest Occupied Molecular Orbital (HOMO) of the donor and the Lowest Unoccupied Molecular Orbital (LUMO) of the acceptor in P3HT:PCBM bulk heterojunction organic solar cells. The findings indicate a correlation between V_{oc} and the HOMO-LUMO offset up to 1.1 eV, after which V_{oc} remains constant. This behavior is further elucidated using a theorem based on the quasi-Fermi level, which predicts a V_{oc} of 0.64 V, in good agreement with our simulation result of 0.68 V. The Power Conversion Efficiency (PCE) of the solar cell was studied with respect to the active layer thickness, demonstrating an increase in PCE up to 0.40 μm followed by a decrease, yielding a maximum PCE of 5.023%, consistent with the literature. The effect of temperature on PCE was also examined, demonstrating an increase in PCE with decreasing temperature in the range of 150–320 K, with a performance of 6.371% at 150 K. Furthermore, the impact of the optical bandgap on PCE was explored, showing that the PCE increased with a decrease in the optical bandgap of the P3HT:PCBM solar cell, reaching 9.94% when the optical bandgap was 1.5 eV. These findings provide valuable insights into the optimization of the performance of organic solar cells by manipulating key parameters, such as the HOMO-LUMO offset, active layer thickness, temperature, and optical bandgap.

Keywords-organic bulk heterojunction solar cell; P3HT:PCBM; AMPS-1D; power conversion efficiency; open-circuit voltage; optical bandgap

I. INTRODUCTION

Organic Photovoltaics (OPVs) is a promising renewable energy and sustainable technology that has attracted considerable interest in recent years. The Bulk Hetero-Junction (BHJ) structure consists of a mixture of p-type and n-type organic semiconductors that have increased the Power Conversion Efficiency (PCE) of OPV cells. The BHJ active layer is usually composed of electron-donor conjugated polymers and electron-accepting fullerenes [1-3]. The most studied BHJ OPVs employ poly(3-hexylthiophene-2,5-diyl),

commonly known as P3HT, and 1-(3-methoxycarbonyl)propyl-1-phenyl-[6,6]C_{61}, commonly known as PCBM.

The PCE of single-junction BHJ organic solar cells was investigated in [4], and it was demonstrated that attaining a PCEs of over 15% requires low voltage losses. Abdallaoui et al. presented a comparative study of conventional and inverted P3HT:PCBM organic solar cells [5]. They used the current-voltage characteristics (J-V) to extract the main electrical outputs of the solar cell. The importance and advancements in employing P3HT/PCBM BHJ solar cells lie in their good impact on the field of photovoltaic technology. This includes high absorption in the visible range of the solar spectrum, low-cost processing, and fabrication, which have shown good stability compared to other organic photovoltaic materials. They can be deposited on flexible substrates, and they are tunable [6-9].

P3HT:PCBM is among the most intensively studied polymer solar cells because of its promising and reasonably simple device processing [10-15]. The performance of P3HT:PCBM is strongly influenced by thermal annealing conditions [16, 17]. Recently, researches have focused on controlling the morphology of the P3HT:PCBM, which can led to higher PCE [18, 23].

The AMPS-1D simulation program used in this study is capable of investigating the relationship between many key parameters of solar cells, such as V_{oc} and the Highest Occupied Molecular Orbital - Lowest Unoccupied Molecular Orbital (HUMO-LUMO) offset, in addition to analyzing the PCE for various parameters.

II. AMPS-1D SOFTWARE DESCRIPTION AND DEVICE STRUCTURE

Professor Stephen Fonash from Pennsylvania State University and his team wrote AMPS-1D software. For the analysis and design of transport in microelectronic and photonic systems, it is a fairly generic software [19]. The AMPS-1D uses the Newton-Raphson method and finite differences. AMPS-1D is a powerful tool that provides information on device physics and responses to various biases such as light, voltage, and temperature. The software allows users to explore and compare different scenarios, which is essential for understanding the complex interactions in the solar cell structure. However, the simulation process using AMPS-1D presents several challenges. An important limitation is that the software requires precise input parameters to simulate the behavior of the device, and any inaccuracy in these parameters can lead to deviations in the simulation results. In addition, simulations can be computationally exhaustive, especially when dealing with complex device geometries [20, 21].

The structure of the BHJ studied in this work consists of P3HT as the electron donor and PCBM as the electron acceptor. The active layer P3HT:PCBM is sandwiched between two electrodes of Indium Tin Oxide (ITO) and Aluminum (Al). The P3HT and PCBM polymer blend as active layer is still quite promising [22, 23].

III. RESULTS AND DISCUSSION

The parameters used in the simulation of the P3HT:PCBM solar cell device were collected from the available literature [24-26] and are listed in Table I.

TABLE I. MATERIALS AND DEVICE PARAMETERS USED AS INPUT FOR THE SIMULATION

Parameter	Value	
Active layer thickness (d)	100 nm (variable)	
Relative permittivity ($\varepsilon/\varepsilon_0$)	3.4	
Electron mobility (μ_e)	0.002 cm^2/Vs	
Hole mobility (μ_p)	0.0002 cm^2/Vs	
Effective density of states in the conduction band (N_c)	2.2×10^{18} cm^{-3}	
Effective density of states in the valence band (N_v)	1.8×10^{19} cm^{-3}	
Donor doping (N_D)	7.38×10^{14} cm^{-3}	
Acceptor doping (N_A)	6.0×10^{15} cm^{-3}	
Band gap of the effective medium (E_{gi})	LUMO(A)-HOMO(D) = 1.0 eV	
Electron affinity (χ)	3.8 eV	
Absorption coefficient (α)	1.0×10^5 cm^{-1}	
Optical band gap (E_g(opt))	2.0 eV	
General device parameters	Front	Back
Barrier height (φ_b)	Φ_{bn} = 0.9 eV	Φ_{bp}= 0.2 eV
Surface recombination speed of electrons (S_e)	1×10^7cm/s	1×10^7cm/s
Surface recombination speed of holes (S_h)	1×10^7cm/s	1×10^7cm/s
Reflectivity	0.1	0.9

A. The Open Circuit Voltage

1) HOMO - LUMO Offset

The variation in V_{oc} with the HOMO – LUMO offset was studied using AMPS-1D software. The interface energy bandgap in organic solar cells is defined as the energy difference between the HOMO of the donor (H_D) and the LUMO of the acceptor (L_A). The effect of the interface energy bandgap on V_{oc} is shown in Figure. 1.

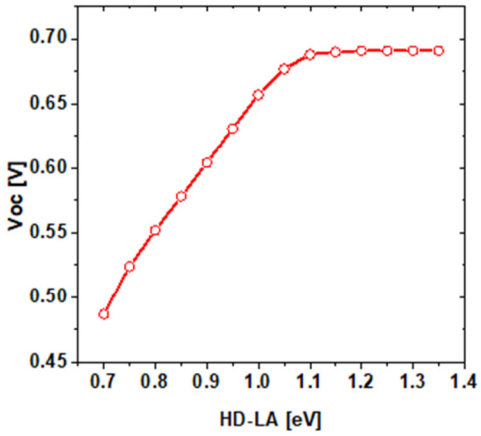

Fig. 1. Dependence of V_{oc} on the HOMO-LUMO offset. The red line has been added as a guide to the eye.

There is a correlation between V_{oc} and the H_D-L_A offset up to a value of 1.1 eV, after which V_{oc} remains constant. A

theorem based on the quasi-Fermi level was employed to better understand the V_{oc} profile [27]. The quasi-Fermi level method has been used to directly measure the internal electron quasi-Fermi level in dye-sensitized solar cells using a Ti secondary electrode [28]. This method was also used in a study of the relationship between the open-circuit voltage and quasi-Fermi level splitting in perovskite solar cells [29]. The quasi-Fermi levels are related to the electron and hole concentrations, as follows:

$$E_{Fn} = E_C + \frac{kT}{e} ln\left(\frac{n}{N_C}\right) \quad (1)$$

$$E_{FP} = E_V - \frac{kT}{e} ln\left(\frac{p}{N_P}\right) \quad (2)$$

E_{Fn} is the electron quasi-Fermi level, E_{Fp} is the hole quasi-Fermi level, E_C is the conduction band level, E_V is the valence band level, n and p are the mobile electron and hole densities, respectively, N_C is the conduction band density of states, N_V is valence band density of states, k is the Boltzmann constant, T is the absolute temperature, and e is the electron charge. Assuming ideal electrodes, the V_{oc} can be expressed as:

$$eV_{OC} = E_{Fn} - E_{Fp} \quad (3)$$

$$V_{OC} = \frac{E_g}{e} - \frac{kT}{e} ln\left(\frac{N_C N_V}{np}\right) \quad (4)$$

which can be rewritten as:

$$V_{OC} = \frac{E_g}{e} - \frac{kT}{e} ln\left(\frac{b_r N_C N_V}{G}\right) \quad (5)$$

$$np = \frac{G}{\gamma} \quad (6)$$

γ is the Langevin recombination constant [30], and G and R are the rates of generation and recombination, respectively.

A modified expression for V_{oc} of the bulk heterojunction solar cells takes the form [31]:

$$V_{OC} = \frac{E_g}{e} - \frac{kT}{e} ln\left[\frac{\gamma(1-P)N_C^2}{PG}\right] \quad (7)$$

P represents the dissociation probability of a bound electron-hole pair into free charge carriers. Previous experiments revealed that P is approximately 0.52. Upon substitution of E_g =1.0 V (corresponding to the energy difference between the HOMO of the donor P3HT and the LUMO of the acceptor PCBM), with the generation rate corresponding to AM1.5, G_{max}= 8×10^{21} $cm^{-3}s^{-1}$, and Langevin recombination constant, $\gamma = 1.17\times10^{-9}cm^3s^{-1}$. Equation (7) gives a V_{oc} of 0.64 V at room temperature. This agrees very well with the computer simulation value of 0.68 V (Figure 1) [32, 33].

2) Effect of Back Contact Potential Barrier on V_{OC}

In this study, we also tested the influence of the potential barrier between the LUMO of the acceptor and the negative electrode work function, φ_{bl} on the V_{oc} of P3HT:PCBM bulk heterojunction solar cell. The simulation results are shown in Figure 2. For Ohmic contact ($\varphi_{bl} \leq 0.2$ eV), the V_{oc} does not depend on the back contact potential barrier. However, for non-Ohmic contact ($\varphi_{bl} > 0.2$ eV), V_{oc} is linearly reduced by the back contact potential barrier, which agrees with the results published in the literature [34].

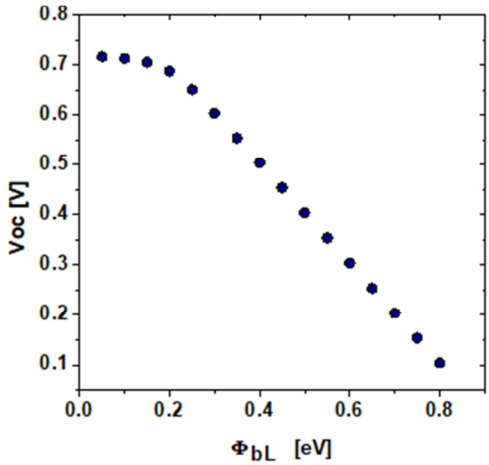

Fig. 2. The V_{oc} as a function of the back contact potential barrier.

B. The Power Conversion Efficiency

1) Effect of Thickness on PCE

The relationship between the PCE and the thickness of the active layer is depicted graphically in Figure. 3, which shows that increasing the thickness up to 0.40 μm the efficiency increases. However, thicker P3HT:PCBM films resulted in lower-efficiency solar cells. At the optimum thickness, the PCE increased to 5.023%, which agrees with similar studies [35].

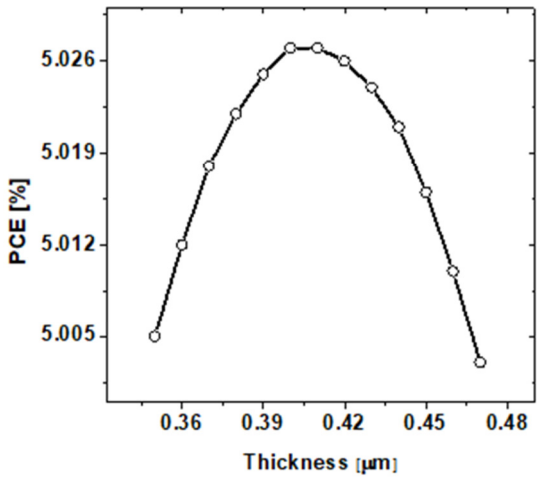

Fig. 3. The dependence of the PCE on the P3HT:PCBM active layer thickness. The black line is added as a guide to the eye.

2) Effect of Temperature on PCE

The relationship between PCE and temperature was investigated in our study. Figure 4 demonstrates that as the temperature decreased, the PCE increased. We obtained a correlation between the PCE and T in the range of 150–320 K in steps of 10 K. Good linear regression was achieved using the straight-line equation:

$$PCE = 7.66\pm0.019 + (-0.0088\pm7.5\times10^{-5})T \quad (8)$$

Note that the PCE at T =150 K is 6.371% is in agreement with the results published in the literature [3, 36].

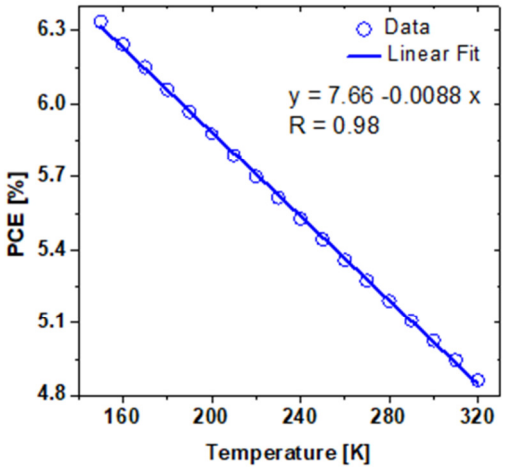

Fig. 4. Variation in PCE with temperature of P3HT:PCBM BHJ solar cell. The blue line represents the linear fit.

3) Effect of Optical Bandgap on the PCE

The effect of the optical band gap on the PCE is shown in Figure 5. The PCE increased with a decrease in the optical bandgap of the P3HT:PCBM BHJ solar cell. Note that the efficiency reaches 9.94% when the optical bandgap is 1.5 eV, which agrees with results published in the literature [37].

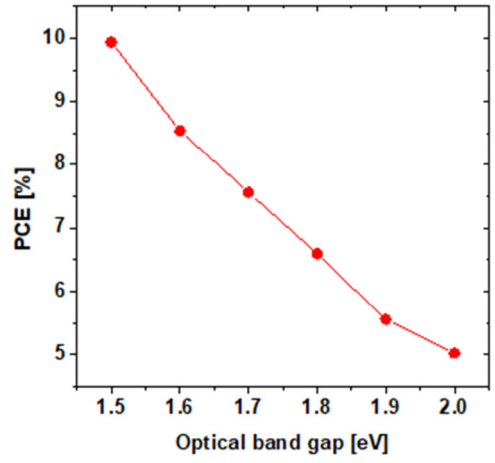

Fig. 5. Relation between PCE and optical band gap. The red line is added as a guide to the eye.

IV. CONCLUSIONS

In this study, we utilized the AMPS-1D software to explore the relationship between the open-circuit voltage (V_{oc}) and the energy difference between the Highest Occupied Molecular Orbital (HOMO) of the donor and Lowest Occupied Molecular Orbital (LUMO) of the acceptor in P3HT:PCBM heterojunction organic solar cells. Our findings revealed a clear correlation between V_{oc} and the HOMO-LUMO offset up to 1.1 eV, beyond which V_{oc} stabilized. This behavior was further clarified using a quasi-Fermi level theorem, which provided a theoretical V_{oc} value of 0.64 V, closely matching our simulated value of 0.68 V. This correlation is important because it directly affects the maximum voltage that can be generated by the solar cell under open-circuit conditions, which is a key factor in determining the overall Power Conversion Efficiency (PCE). The analysis of PCE for active layer thickness showed an initial increase in PCE up to 0.40 μm, followed by a decrease, resulting in an optimum PCE of 5.023%, consistent with previous studies. The effect of temperature on the PCE demonstrated an increase in efficiency with decreasing temperature, with a PCE of 6.371% at 150 K, consistent with earlier studies. The agreement between the simulated results and previously published data was good. Furthermore, the impact of the optical bandgap on PCE was significant, with a maximum efficiency of 9.94% achieved at an optical bandgap of 1.5 eV, corroborating existing literature. Overall, this work provides valuable insights into the optimization of organic solar cell performance by manipulating key parameters such as the HOMO-LUMO offset, active layer thickness, temperature, and optical bandgap. These findings will contribute to the development of more efficient and reliable organic photovoltaic technologies.

This study uncovered several routes for future research. This may include the study of new materials with optimized HOMO-LUMOs that can improve V_{oc} and PCE, exploring different device architectures, such as tandem structures, to benefit from the results of the HOMO-LUMO difference and optical band gaps, and the study of long-term stability and performance under different operating conditions (e.g., light intensity, temperature, and humidity).

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