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Comparative Simulation-Based Study on Different Active Layers of Organic Solar Cell via GPVDM

Yasir Usman[2,3], Khizar Jahangir[1], Assad U llah Shah[4], Muhammad Noman Yousaf[1], Abdul Samad[1] , Allao Ud Din[1] , Ghazi Aman Nowsherwan[1,2*]

[1]Centre of Excellence in Solid State Physics, University of the Punjab, Lahore, 54590, Pakistan
[2]Department of Physics, University of the Punjab, Lahore, 54590, Pakistan
[3]Department of Physics, Comsats University, Lahore, 54000, Pakistan
[4]SEECS, NUST University, Islamabad, 44000, Pakistan

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***Corresponding author:** Ghazi Aman Nowsherwan

Abstract **Review Article**

The high strength of organic photovoltaic cells lies in the variety of organic ingredients that can be built and synthesized for absorbers, receptors, and boundaries. Still, we need further development for better performance and existence of the system. In this research study, electrical simulations of different active layer materials have been performed via GPVDM software to observe the outcomes of a solar cell. Furthermore, the electrical simulation has been performed at different active layer thicknesses from 50 nm to 300 nm with active material P3HT: PC70BM. We analyzed by performing simulations with different parameters to observe the best parameters for organic solar cell performance. We observed that absorber layer thickness of 200 nm, hole transport layer of Cu_2O, pair of ITO/Al electrodes, and exponential DOS exhibit superior outcomes. At the same time, the highest power conversion efficiency was reported with active layer PTB7:PCB70BM due to its efficient optical properties. Organic solar cells are versatile and gaining popularity for a broad range of applications to keep up with the increasing energy demand and comparatively lower energy payback time.

Keywords: photovoltaic cells, GPVDM software, Organic Solar Cell, energy.

1. INTRODUCTION

Solar cells are devices or cells that convert sunlight into electric current or voltage. They're also known as photovoltaic cells (PV) or devices. Organic solar cells are classified as third-generation solar cells based on the material configuration rather than the year of development. Organic photovoltaic devices have gotten a lot of press in the recent decade for their potential as non-conservative, renewable energy sources [1].

Becquerel [2] identified the photovoltaic effect in 1839 when platinum electrodes covered with silver halogen were lit in an aqueous solution, and a photocurrent was seen. After a couple of years, Smith [3] discovered photoconductivity in selenium in 1873, and Pochettino [4] reported the first finding of photoconductivity in an organic molecule anthracene in 1906. Calvin created the first organic solar cell based on magnesium phthalocyanine (MgPc) in 1958, achieving a 200 mV open-circuit voltage [5]. Later, using an Al/MgPc/Ag cell, a 0.01 percent energy conversion efficiency was reported at a wavelength of 690 nm [6]. Conjugated polymers have also used this form of a solar cell. The energy conversion efficiency using polyacetylene as the absorber layer was 0.3 percent, and the open-circuit voltage was 0.3 V [7]. G *et al.*, proposed an organic solar cell based on Al/poly(3-methyl-thiophene)/Pt with open-circuit voltage, fill factor (FF), and external quantum efficiency of 0.4 V, 0.3 percent, and 0.17 percent, respectively [8]. Later, PPV/C60-based organic had a QE of 9% and a PCE of 1%, with a fill factor of 0.48 [9]. Halls, J. J. *et al.*, built an organic cell having an electron donor layer (EDL) of bis-perylene over which a PPV layer was formed, giving a peak external QE of 6% and a PCE of 1% [10]. In the 1970s and 1980s, poor power conversion efficiencies were attained due to the low concentration and mobility of free charge carriers [11, 12]. However, after 2000, numerous advances in structure and design enhanced power conversion efficiency dramatically. Till now PCE is reported as 20%, according to current improvements, which are due at these unique non-fullerenes acceptors [13-15].

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GPVDM is a three-dimensional tool for simulating optoelectronic devices such as OLEDs, OFETs, and various solar cell types such as OSC, perovskite solar cells, CIGS, and CdTe [16-21]. Singh *et al*., created a blend of an organic photovoltaic cell with various charge carrier mobilities and examined how efficiency changed as the charge carrier mobility changed by GPVDM [22]. The perovskite-based solar cell was modeled by Abdulsalam *et al*., They discovered that the thickness of the absorber layer has a significant impact on the performance and outcomes of cells. The greatest PCE was reached at a thickness of 3 x 10^7 m [23]. Hima *et al*., used the GPVDM software to investigate the effect of various settings on the efficiency of power conversion in a planner hetero-junction solar cell using $CH_3NH_3PbI_3$ as an absorbing layer, achieving a PCE of 12.9% [24]. GPVDM software was also used by Talib *et al*., to investigate the layer thickness effect on hetero-junction solar cells. They got the best results with a 100 nm active layer thickness and to short-circuit current density of 6.60 mA/cm^2, and simulation data shows that the mix arrangement gave the best results at 200 nm [25].

As an alternative to the inorganic PV cell, OPVs are seen as boosting green energy sources. We primarily concentrated on different absorber layers (active materials) that play a key role in improving its performance in this research work. This study also included a detailed simulation-based research investigation on organic solar.

2. GPVDM Device Design and Simulation

2.1 Device Design

To represent the movement of charge carriers in the device, the model solves all electrons, drift-diffusion holes, and carrier continuity equations in location space. “The model also solves the Poissons equation to estimate the electrostatic potential. The model's recombination and carrier trapping are expressed using the Shockley-Read-Hall (SRH) formalism, and the distribution of trap states can be flexibly specified [26]”. The basic equations used in this model are as follows:

Gauss’s Law: $\nabla_{\epsilon_0 \epsilon_r} . \nabla_{\emptyset} = q . (n - p)$ ……………….. (1)

Electron driving terms: $J_n = q\mu_e n \nabla E_c + qD_n \nabla_n$ …….. (2)

Hole driving terms: $J_p = q\mu_h p \nabla E_v - qD_p \nabla_p$ …………. (3)

Electron continuity Equation: $\nabla . J_n = q\left(R_n + T_n + \frac{\partial n_{free}}{\partial t}\right)$ ……………..... (4)

Hole continuity Equation: $\nabla . J_p = -q\left(R_p + T_p + \frac{\partial p_{free}}{\partial t}\right)$ ……………..… (5)

The electrical simulation has four different layers, including the active layer just like as from bottom to top Al/ P3HT: PC70BM/Spiro-MeOTAD/ITO as shown in Fig.1 and Fig 2. Al is serving as a back electrode, Spiro-MeOTAD is used as a hole transport layer, and ITO (indium tin oxide) is a transparent electrode and acts as transparent conducting oxide. PC70BM is an electron acceptor, and P3HT is an electron donor, and a combination of both acts as a light-collecting layer. An active layer is responsible for photon absorption, charge separation, and electrical conduction to the electrode.

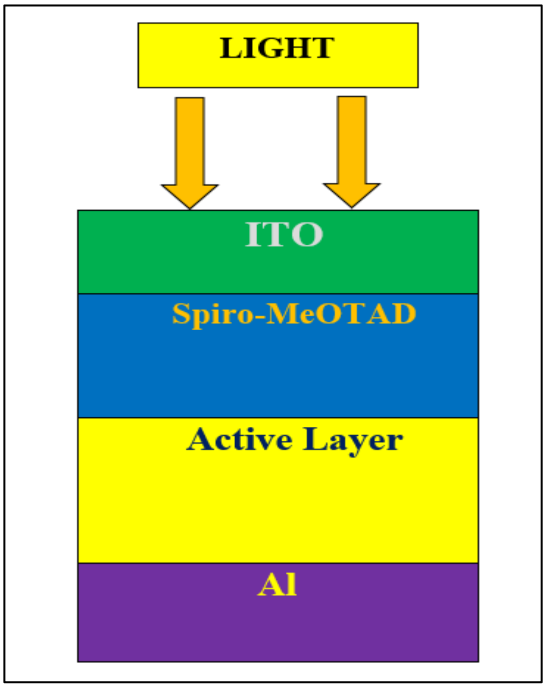

Fig 1: Structure of designed organic solar cell (OSC)

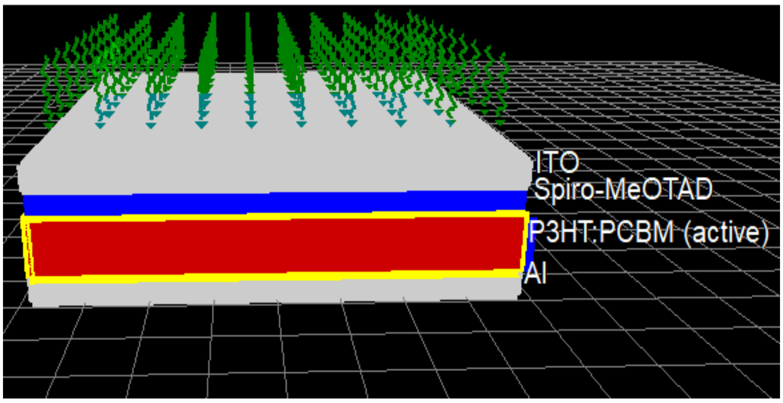

Fig 2: Schematic view of OPV in GPVDM

2.2 Device Simulation Parameters

All simulation settings for the active layer in the structure were derived from various research [13, 22-25]. In terms of trap densities, tail slope, relative permittivity, carrier mobilities, the effective density of states, and photonic bandgap, the specific material parameters for the photoactive layer are entered. For the simulation of the device, all of the prime parameters listed in Table.1 are used. The operating temperature is 300 degrees Celsius. Under these conditions, all simulations are executed.

Table 1: Active Layer Parameters set in simulation

Parameters name	Values	SI units
Electron trap density	3.8×10^{26}	$m^{-3}eV^{-1}$
Hole trap density	1.45×10^{25}	$m^{-3}eV^{-1}$
Electron tail slope	40×10^{-3}	eV
Hole tail slope	60×10^{-3}	eV
Electron mobility	2.48×10^{-7}	$m^{2}V^{-1}s^{-1}$
Hole mobility	2.48×10^{-7}	$m^{2}V^{-1}s^{-1}$
Energy bandgap (Eg)	1.10	eV
Relative permittivity	3.8	Au
Number of traps	20	Bands
Free electron to trapped Electron	2.5×10^{-20}	m^{-2}
Trapped electron to free Hole	1.32×10^{-22}	m^{-2}
Trapped hole to free electron	4.67×10^{-26}	m^{-2}
Effective density of free Electron states (300K)	1.28×10^{27}	m^{-3}
Effective density of free Hole states (300K)	2.86×10^{25}	m^{-3}
Free hole to trapped hole	4.86×10^{-26}	m^{-2}

2.3 Device Model Authentication

GPVDM is an 3-D opto-electronic software that may be used to model solar cells, LEDs, diodes, FETs, and other solar-related components. It was originally designed to replicate organic solar cells, but it has since been expanded to include OLEDs, OFETs, and a variety of additional 1st, 2nd, and 3rd generation solar cells. Organic solar cells, organic LEDs, organic field-effect transistors (OFETs), crystalline silicon solar cells, a-Si solar cells, and CIGS solar cells are currently being simulated by the software [16-21]. The software correctness has been demonstrated in published studies [22-25]. As a result, it can, to some extent, verify the feasibility and accessibility of cell formation and material properties. It also assessed the device performance, from actual experimental characterization to theoretical results.

3. RESULTS AND DISCUSSIONS

3.1 Influence of photoactive Layer thickness

Active layer or light-collecting layer organic solar cell plays a very important role in the enhancement of device performance. In this study, GPVDM software investigated the result of various layer thicknesses on the power conversion efficiency of a planar heterojunction solar cell using P3HT: PC70BM as an absorber layer. Organic bulk hetero-junction solar cell consists of the mixture of electron donor (P3HT) and electron acceptor (PC70BM) materials as an active layer, ITO (indium tin oxide) is a transparent electrode, Spiro-MeOTAD is electron blocking layer and hole transporting layer and Al is a back electrode. Electrical simulation has been done at different active layer thickness ranges from 50 nm to 300 nm, as shown in Table 2. The active layer thickness of 50 nm is considered very thin for an OSC, whereas the active layer of 300 nm is considered very dense (too dense for the efficient activity of the device).

In the thickness vs Jsc graph (Fig 3B), with the increase in thickness, short circuit current density increases and reaches the optimum value of 125.6 A/m^2. As light is incident on active material, it generates electron-hole pairs. With the increase in thickness, excess carrier concentration increases, and more carriers are extracted towards the respective electrodes, which ultimately leads to high Jsc. In Voc vs thickness graph (Fig 3A), with the increase in thickness, Voc increases due to high generation rate and low recombination rate, but when the thickness exceeds 100 nm it starts to decrease due to the probability of high recombination rate and low generation rate. The optimum value of Voc is obtained at a thickness of 100 nm. While in the thickness vs PCE graph (Fig 3C), with the increase in thickness, PCE increases and reaches a maximum value of ~5.6 %. It is due to accumulation of excess charge carriers and high generation rate, and in thickness vs FF graph (Fig 3D), with the increase in thickness fill factor drops down from 79.72 % to 75.28 % due to rise of internal power depletion, as fill factor is measured as the ability of the device to transfer maximum obtainable power to a generated load. As thickness increases, the effect of the built-in electric field enhances that degrades the FF of the device.

Table 2: Device performance at a different photoactive layer thickness

Thickness (nm)	Voc(V)	Jsc (A/m^2)	FF (%)	PCE (%)
50	0.581	48.93	79.72	2.26
100	0.598	91.94	78.86	4.34
150	0.595	94.48	78.03	4.39
200	0.595	108.68	77.14	4.99
250	0.594	120.57	76.25	5.46
300	0.591	125.60	75.28	5.60

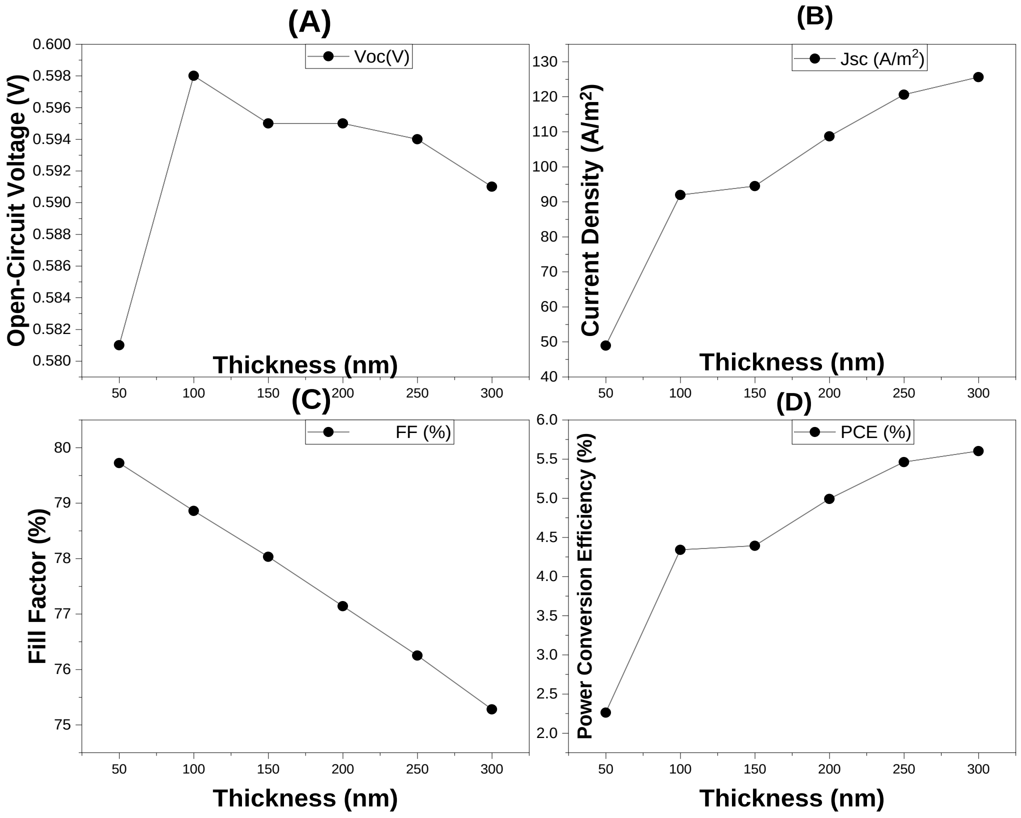

Fig 3A: Open-circuit voltage (Voc) vs, Active layer thickness (nm), Fig 3B: short-circuit current density (Jsc) vs. Active layer thickness (nm), Fig 3C: PCE (%) vs. Active layer thickness (nm) and Fig 3D: FF (%) vs. Active layer thickness (nm)

3.2 Influence of different electrodes pairs on device performance

As electrodes in any kind of solar are responsible for conduction and start conductivity in external circuit connected to device. In this study, we have taken pairs of different electrodes to analyze the performance of the device, which is elaborated in Table.3. And observed, the pair of ITO/Al gives the highest efficiency compared to the other electrodes, but the outcomes of all electrodes are close to each other. The very less difference can be seen in device performance by changing electrodes. The electrodes whose work function goes best with the absorber and charge transport layer will show the superior outcome. Work function is basically the minimum energy required by the charge carrier to eject from the Fermi level to the vacuum. All the simulation is carried out at a thickness of 250 nm and keep all other parameters constant.

Table 3: Device performance with different electrode pairs

Electrode	Voc (V)	Jsc (A/m^2)	FF (%)	PCE (%)
ITO/Al	0.59	120.57	76.25	5.46
FTO/Ag	0.59	120.50	76.25	5.45
FTO/Au	0.59	119.74	76.24	5.41

3.3 Influence of different active layers on device performance

In organic or any kind of solar cell active layer plays a very major role in device performance. As active material is responsible for efficient light absorption. And we have studied the effect of different active layers in this simulation and concluded which active layer exhibits the best device performance. Also, If the quality of films is good, then there are fewer traps and recombination centers are present, and the performance of the device is generally high. But if the quality of films is not good, then traps and recombination centers eventually degrades the device performance. All the simulated results are taken with GPVDM software.

As P3HT: PC70BM exhibits the PCE of 6.74%, PIF8BT: PDI gives PCE of 6.35%, and PTB7:PC70BM gives the maximum productivity among all active layers discussed above as PTB7:PC70BM have very fine optical properties and has high absorption coefficient and conductivity with respect to other active layers. Due to which it absorbs light more efficiently comparatively other light-harvesting layers and transport more charge carriers towards respective electrodes.

Table 4: Device performance with different active layers

Active Layers	Voc(V)	Jsc (A/m^2)	FF (%	PCE (%)
P3HT:PCBM	0.64	132.95	78.82	6.74
PTB7:PC70BM	0.64	159.11	79.56	8.12
PIF8BT:PDI	0.63	125.51	79.86	6.35

3.4 Influence of different DOS of Active Layer on performance cell

We also checked the influence of DOS of the active layer on the performance of the cell, which is also shown in Table.5. The power conversion efficiency for both densities of state was quite different. We observed there is a significant effect of exponential DOS of the active layer on device outcomes. The efficiency of cells with exponential DOS of the active layer is 6.10 %. It is high because, in exponential DOS, carrier movement and transport are better and less scattering occurs as compared to simple DOS. Which leads to high mobility eventually, which leads to high outcomes for the device.

Table 5: Device performance with different DOS

DOS of Active Layer	Voc (V)	Jsc (A/m^2)	FF (%)	PCE (Efficiency) %
Simple	0.59	120.71	76.25	5.46
Exponential	0.63	120.66	80.12	6.10

3.5 Influence of different hole conductive materials on performance cell

As hole transport layer plays a very important role in device performance. We checked out the influence of different high conductive materials at a thickness of 250 nm. The power Conversion efficiency of different high conductive materials was found different, but we observed that the Cu_2O has high power conversion efficiency at a thickness of 250 nm, elaborated in Table 6. As Cu_2O exhibits superior outcomes due to its superior interaction and strong communication with the absorber layer. As it was high p-type conductivity, wide bandgap, high relative stability, and less cost. It can also be used as an alternative to Spiro-MeOTAD and PEDOT: PSS in various kinds of the solar cell.

Table 6: Device performance with hole conductive materials

Diff. Conductive Materials	Voc (V)	Jsc (A/m^2)	FF (%)	PCE %
PEDOT:PSS	0.59	110.47	76.50	4.99
SPIRO-MeOTAD	0.59	120.71	76.25	5.46
Cu_2O	0.60	127.01	76.09	5.76

3.6 Optimized Performance of OSC with Different Active Layer

As we have observed that what are the best parameter for OSC performance, and we analyzed by performing simulations with different parameters while other parameters are kept at default values. We observed absorber layer thickness of 200 nm, hole transport layer of Cu_2O, pair of ITO/Al electrodes, and exponential DOS exhibits the superior outcomes. We have taken all these parameters into account and observed the quite significant effect on device performance & outcomes.

Table 7: Device performance with optimized parameters with different active layers

Active Layer	Voc(V)	Jsc (A/m^2)	FF (%)	PCE (%)
P3HT:PCBM	0.64	132.95	78.82	6.74
PTB7:PC70BM	0.64	159.11	79.56	8.12
PIF8BT:PDI	0.63	125.51	79.86	6.35

As shown in Table 7, PTB7:PCB70BM exhibits the highest efficiency of 8.12% with optimized parameters as compared to other active layers due to its strong optical properties.

4. CONCLUSION

The organic solar cell is designed by using GPVDM software and is organized as ITO/Spiro-MeOTAD/ Active / Al. The PTB7:PC70BM as an active layer exhibits the highest power conversion efficiency, which results due to its superior optical and electrical properties that make it's a strong candidate to act as an absorber layer. Further, the impact of absorber layer thickness, hole transport layers, and DOS on device performance was also investigated. The hole transport layer of Cu_2O and exponential DOS display the maximum outcomes by an active layer of PTB7:PC70BM at a thickness of 200 nm, according to our findings. This research suggests a potential route toward the effectual implementation of OPV by altering their characteristics, which are pointedly reliant on the outcomes of organic solar cells.

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