The impact of the buffer layer material and active layer thickness on the performance of a fullerene-free organic solar cell

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Abstract – This paper presents a step-by-step study of an organic solar cell structure by simulation. The study focuses mainly on the effect of buffer layer material on the performance of a fullerene-free organic solar cell. The studied structure composed of PBDB-T: ITIC polymer donor/small molecule acceptor blend active layer, was selected based on its considerably good power conversion efficiency compared to its peers, it has been proven that the small molecular compound ITIC performed better than the fullerene PC71BM. [1] Compared to available experimental data of the studied structure, simulation results showed an error of 2.05%, and based on that, starting from a power conversion efficiency of 11.44% we continued our study by varying buffer layer materials, and thicknesses of the active layer and interlayers thus achieving an efficiency of 12.25%.

Keywords – Fullerene-Free Organic Solar Cells, OPV, Organic Photovoltaics, Polymer Solar Cells, Buffer Layer

I. INTRODUCTION

Producing clean energy from our renewable resources has become of the utmost importance due to energy demands increasing rapidly and the fact that fossil fuels depleting. Compared to other renewable energy resources the energy bestowed upon the earth by the sun is without any doubt the most abundant natural energy available to be harvested. Photovoltaic technologies have been developing rapidly from 1% efficiency in 1884 to about 22% efficiency for residential use. [2] Yet considering the growing need for renewable energy, we need more variant ways to harvest solar radiation to allow accessibility to solar energy in public, first-generation solar cell fabrication consumes a massive amount of energy and involves toxic emissions, which makes silicon-based solar panels expensive for residential use in addition to their big size and weight.

Many alternatives emerged in the third-generation solar cells presenting interesting advantages to widen the usage of solar energy in the world. One of the promising solar technologies namely organic photovoltaics is cost-effective, easy to produce, flexible, and lightweight, but it is still necessary to improve the power production efficiency of these photovoltaic systems as they show inferior efficiency values compared to first-generation solar cells.

An organic photovoltaic system is mainly composed of an active layer, a Transparent Conductive Oxide TCO most often an Indium Tin Oxide (ITO) glass as an electrode (anode), and a second electrode made of a metal catalyst such as Aluminum or Silver. A mixture of a polymer donor that is responsible for exciton generation blended with a polymer acceptor represents the active layer. This layer is where the photovoltaic effect takes place thanks to the donor/acceptor interface, which is responsible for charge separation.

Organic photovoltaics are commonly fabricated with an active layer thickness of 100nm up to 150nm, [3] and based on the continuous investigations on the relationship between the thickness of the active layer, and the overall performance of organic photovoltaics, it was

concluded that the value of active layer thickness depends mainly on the morphology, structure, and materials present in the device.

In this study, we will demonstrate and explore the effect of buffer layer material and thickness of the active layer on the device's performance.

II. Materials and Method

We applied a simple simulation approach that begins with testing the output of our simulated power conversion efficiency (PCE) and comparing it with the experimental value, [1] then we made changes to the active layer thickness to get the most suitable active layer thickness for each device, we next tuned the thickness of buffer layers and selected the best-performing structure.

As shown in figure 1 energy levels of different layers in the studied structure. Acting as the donor is a conjugated polymer (PBDB-T: poly[(2,6-(4,8-bis(5-(2 ethylhexyl)thiophen-2-yl)-benzo[1,2-b:4,5-b']dithiophene))-alt-(5,5-(1',3'-di-2-thienyl-5',7'-bis(2-ethylhexyl)benzo[1',2'-c:4',5'-c']dithiophene-4,8-dione))]) that is blended with the small molecule acceptor ITIC to form the active layer. ZnO and MoO3 are used as the interlayers, with Aluminum and ITO as electrodes as demonstrated in the experimental reference, this structure showed up to 11.21% power conversion efficiency. [1]

Figure 2 describes details about the studied structures as we simulated each structure using a unified layer's thickness, the electrode ITO was set to 130nm and Al electrode was set to 100nm, and the active layer and anode buffer layer was set to 100nm, and the cathode buffer layer was set to 10nm, taking into account that in the structure S3 we set anode buffer to 10nm to make a variation in the thickness starting point.

Compared to the PCE of 11.21% from experimental data our simulation for the same structure yielded a PCE of 11.44% with an error of 2.05%, the active layer blend morphology affects the results because of the interfacial contact between the donor and acceptor increasing or decreasing leading to different efficiency values.
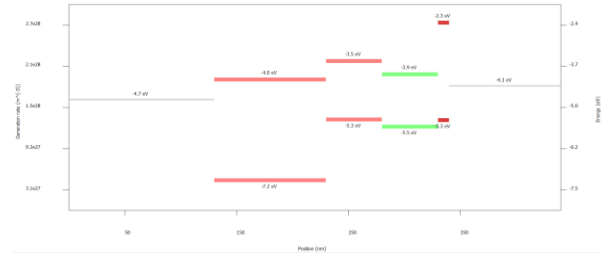

Fig. 1 Energy levels for the OPV system

Fig. 2 Studied OPV structures

Table 1 lists the obtained simulation results for each structure, we can see that structure S3 showed the best PCE compared to other structures.

Table 1: Obtained properties by simulation for the studied structures

Structure	Isc mA/cm2	Voc (V)	FF (%)	η(%)
Exp [ref]	16.81	0.90	74.20	11.21
S0	17.67	0.85	76.02	11.44
S1	15.35	0.85	76.39	9.95
S2	18.36	0.85	75.94	11.89
S3	18.54	0.85	75.88	12.01
S4	18.48	0.85	75.93	11.98

III. Results

A. Active layer

Figure 3 and Table 2 show the effect of active layer thickness upon the power conversion efficiency, a thickness higher than 100nm leads to lower efficiency due to charge collection speed and carrier mobility based on the materials used of the buffer layer as 100nm is the best distance for charge carriers to get collected and transferred to the electrodes before recombination could occur. Higher thicknesses will increase the probability of recombination thus causing a loss in charge carriers and reducing efficiency.

We also note that a thickness lower than 100nm reduces the density of excitons and even with a faster collection we end up with lower exciton density thus lowering device performance.

This simple active layer thickness simulation allowed us to select the best suitable active layer thickness for further improvement.

Table 2 : Impact of active layer thickness on the PCE for studied structures

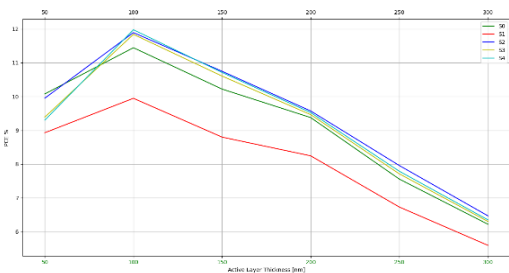| PCE%					
Active Layer Thickness [nm]	S0	S1	S2	S3	S4
50	10.075	8.927	9.949	9.389	9.298
100	11.443	9.946	11.891	11.839	11.975
150	10.219	8.798	10.746	10.604	10.711
200	9.376	8.244	9.572	9.463	9.524
250	7.556	6.729	7.957	7.711	7.788
300	6.219	5.595	6.468	6.301	6.349

Fig. 3 A graphical representation of the active layer thickness effect on the PCE

B. Buffer Layer

The buffer layer is selected based on the energy level. To give a better performance, the highest occupied molecular orbital HOMO for the anode buffer layer must lay lower as close as possible to the conduction band energy level edge of the electrode for better hole transport and collection, and the lowest unoccupied molecular orbital LUMO must lay higher than the conduction band energy edge of the cathode electrode for better collection and transfer of electrons and this was further validated by the results obtained by further modifying the buffer layer thickness to reach up to 12.25% PCE, hence the best-performing structure S4 complies with the aforementioned conditions for energy levels (Figure 4 and Figure 5).
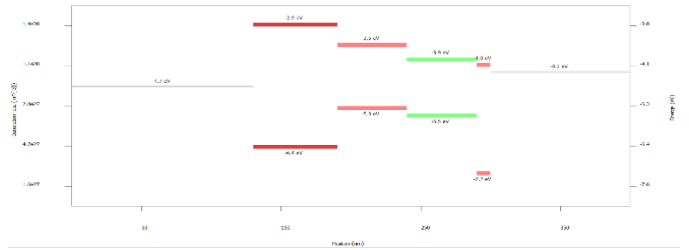

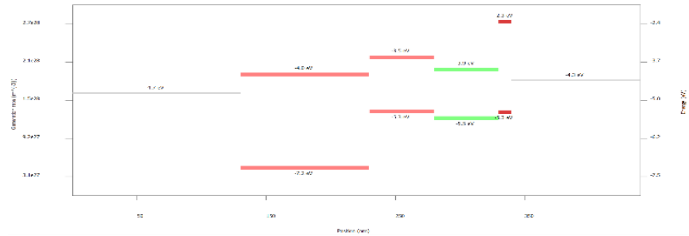Fig. 4 Energy levels for structure s4 pce12.25%

Fig. 5 Energy levels for structure s0 pce11.44%

Table 3 and Figure 4 illustrate the variation of anode buffer layer thickness versus the change in power conversion efficiency. Structures S0, S1 a thickness of 10nm showed the highest efficiency of 11.95% and 11.85% respectively, due to similar performing properties of ZnO and PEDOT:PSS lower thickness of 10nm acts better due to the low carrier mobility.

Structures S3 and S4 containing Bphen and MoO3 with higher carrier mobility showed better performance at larger thicknesses of 60nm.

Table 3: Impact of anode buffer layer thickness on the pce for studied structures.

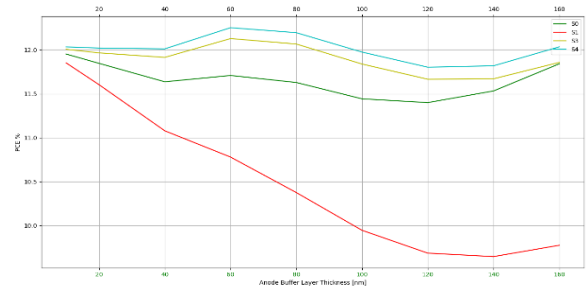| Anode Buffer Layer Thickness	S0	S1	S3	S4
10	11.953	11.852	12.007	12.034
20	11.847	11.604	11.966	12.021
40	11.637	11.079	11.915	12.012
60	11.709	10.78	12.129	12.253
80	11.629	10.376	12.067	12.196
100	11.443	9.946	11.839	11.975
120	11.4	9.686	11.666	11.803
140	11.533	9.647	11.671	11.819
160	11.842	9.776	11.858	12.035

Fig. 6 A graphical representation of the anode buffer layer thickness effect on the PCE.

IV. CONCLUSION

This study allowed us to theoretically improve the efficiency of the studied device structure by modifying buffer layers and thicknesses. With the small molecule Bphen as an anode buffer layer and ZnO as a cathode buffer layer taking into account a 100 nm thick (PBDB-T: ITIC) active layer we achieved a power conversion efficiency of 12.25% starting from a PCE of 11.44% by simulation only.

We considered an experimental reference that employed ZnO as an anode buffer layer and MoO3 as a cathode buffer layer reaching a PCE of up to 11.21%. [2]

By providing that the simulation yielded a low error of 2.05% for the PCE we can say that these results should comply with experimental data.

REFERENCES

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