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Optical and Electrical Performance Analysis of New Polymer Layer in Organic Solar Cell

Pavithra Gattu Subramanyam[1,2*], Venkatesha Muniswamy[1,2], Chaya Bangalore Muniraju[1,2], Sharat Hiremath[1,2] and Sarvepalli Sri Krishna[1,2]

[1]*Department of Electronics and Communication Engineering (ECE), Sai Vidya Institute of Technology (SVT), Bengaluru, Karnataka, India*
[2]*Visvesvaraya Technological University (VTU), Bengaluru, Karnataka, India*

***Correspondence to:**
Pavithra Gattu Subramanyam
Department of Electronics and Communication Engineering,
Sai Vidya Institute of Technology,
Bengaluru, Karnataka, India.

Visvesvaraya Technological University (VTU),
Bengaluru, Karnataka, India.
E-mail: pavi.svit@gmail.com

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Abstract

The main objective of this work is to analyze the optical and electrical performance of an organic solar cell (OSC) that uses the novel organic material PM6_D18_L8-BO as its photoactive layer. The proposed organic solar cell's efficiency was examined using the J-V curve from the GVPDM (General Photovoltaic Purpose Device Model). Bipolar drift diffusion equations are used in this application's photovoltaic modelling to analyze the electrical characteristics of the suggested polymer solar cell. It has been demonstrated that the proposed OSC structure improves sun-light absorption in the device's photoactive layer, which in turn improves the polymer solar cell's efficiency.

Keywords

Organic Solar cells, performance analysis, solar energy, GVPDM simulation.

Introduction

Solar energy is the dominant source of practically all energy on earth, including wind, fossil fuels, food production and warmth. People indirectly convert solar energy to electricity when they produce it by employing various forms of energy. Radiant energy from the sun is a considerably higher abundant resource compared to what is required to supply all of the world's energy demands.

From the sun, the amount of energy the earth obtains in one hour is equal to the amount of energy we use in one year, according to a simple mathematical calculation. This energy produces less pollutants and has less of an impact on the environment than fossil fuels like oil and gas. The benefits result in a number of interesting products such as thin film structures, flexible substrate processing at the room temperature, and lightweight equipment [1, 2].

There are several different types of solar cells depending on the materials used to make them; nevertheless, efficiency, longevity, cost, and the accessibility of the resources for production are issues for solar cells [3-5]. A promising renewable energy source for the next generation, polymer-based organic solar cells offer many appealing characteristics among the various types of solar cells and have undergone significant research [6, 7].

One method to increase power conversion ability in OSCs is to increase the quantity of photo-light absorbed by photoactive layer. In 1968, the concept of light-trapping in semiconductor devices was patented [8]. Losses can be minimised by shrinking the photoactive layer, which is made feasible by increasing effective absorption. This needs to be taken into account in organic photovoltaics in particular since active layer thickness has a significant impact on internal quantum efficiency. Surface plasmon, buried nanoelectrodes [9], and soft embossed grating architecture are methods to boost light absorption in the photoactive layer.

Experimentation

Basic principle of OSC

The organic photovoltaic cell (OPVs), which is formed of organic (polymer) materials as a thin fine layer and offers the primary methods in electricity generating through sun's radiation, will transmit and be drawn out through the junction else will be inserted through contacts.

Solar energy is transformed into electricity through OPV devices. A typical OPV device is made up of two electrodes having one or many photoactive materials between them. A typical bilayer organic photovoltaic device is represented in figure 1.

In a bilayer OPV cell, photocurrents are produced by absorbing sunlight in the active region consisting of semiconducting organic substances as donor and acceptor. The acceptor material (A) retracts electrons and primarily transports electrons, whereas the donor material (D) offers electrons and primarily transports holes. These photoactive materials, as seen in figure 2, absorb photons from sun's radiation to create excitons, that excite electrons to enter the conduction band from valence band (Light absorption). The excitons flow to the donor/acceptor contacts due to the concentration gradient, where they divide into loose holes (+ve charge carriers) and electrons (-ve charge carriers), which is termed as Charge Separation. Once the holes and electrons go to appropriate electrodes by moving via the donor phase or the acceptor phase, which is called Charge Extraction, a photovoltaic is produced.

This work is focusing on analysis on efficiency of OSC based on PM6_D18_L8-BO active layer. Most of the research work is focused on OSC with photoactive layer P3HT:PCBM and PTB7:PC70BM material. The proposed device structure is simulated utilizing the GPVDM software.

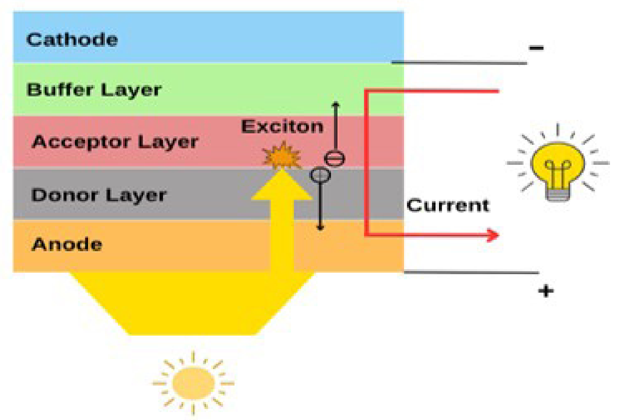

Figure 1: Basic architecture of bilayer OSC.

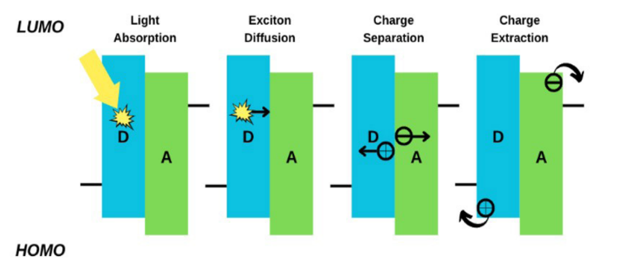

Figure 2: Functional operation of bilayer OSC.

Modeling of the proposed OSC device and materials

The fundamental architecture of polymer solar cells consists of a photo-light captivating layer, a back-electrode for collecting electrons produced by photons, a glass coated with indium-tin-oxide (ITO), which is utilized as the front-electrode and is referred to as an anode. A blend of organic substances that serve as both donors and acceptors made up the light-absorbing layer. These materials are employed to produce excitons (electron-hole pairs) and to minimize recombination of electrons (e^-) and holes (h^+) that condenses efficacy of the cell. The proposed OSC layout consists of ITO(130 nm)/PEDOT:PSS(20 nm)/PM6_D18_L8-BO(120 nm)/PNDIT_F3N(5 nm)/Ag(100 nm) layers as shown in the figure 3.

Conducting substrates that are transparent are utilized as an anode in OSC's, with glass coated with ITO being the most popular choice. As substrates for optical devices, ITO films have various advantageous qualities, such as excellent bright transparency, strong electrical conductivity, and moderate infrared reflectance. ITO is frequently used as a transparent anode in solar cells, liquid crystal displays, and light-emitting diodes because of these grounds [10, 11]. Due to extreme transparency in visible range, excellent heat resistance, excellent mechanical resilience, significant hole affinity and higher work function, PEDOT: PSS, a successful conductive polymer solution, have been employed as a hole-transport layer on a large scale in photovoltaic cell systems.

The morphological optimization of the ternary mix PM6:D18:L8-BO was the emphasis for optimal efficiency. Figure 4a and 4b depicts the bond arrangement and absorption spectrum of the substances employed in this study.

As depicted in figure 4b the highest occupied molecular orbital energies for PM6, D18 and L8-BO are -5.20 eV, -5.24 eV and -5.67 eV, respectively. The lowest unoccupied orbital energies of PM6, D18 and L8-BO are -3.06 eV, -2.95 eV and -3.92 eV, respectively.

Material L8-BO primarily absorbs light between 550 and 900 nm. In order to manipulate material crystallization and absorb short-wavelength photons between 400 and 700

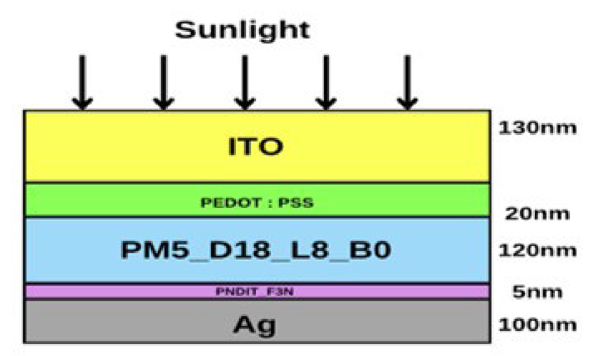

Figure 3: Proposed layout of OSC.

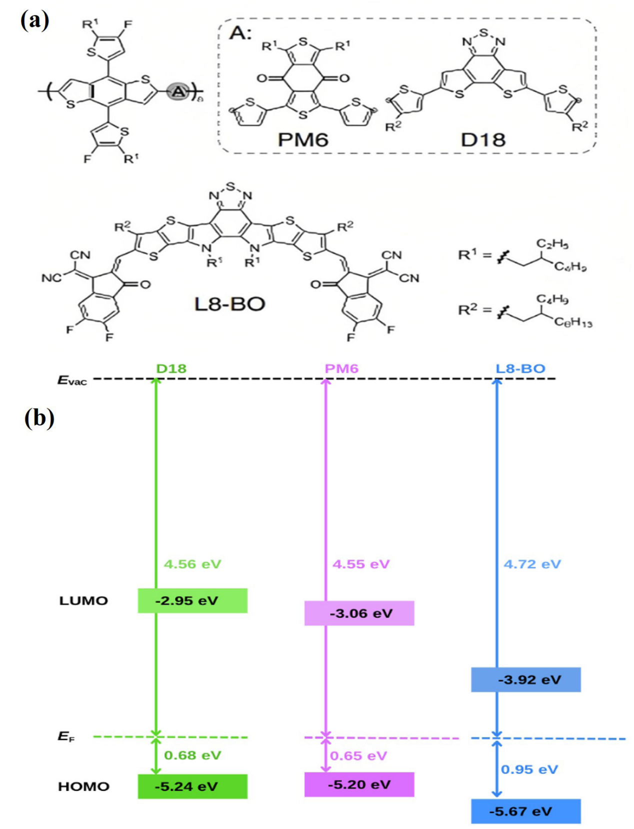

Figure 4: (a) Chemical structure of PM6:D18:L8-BO material acting as an active region. **(b)** Energy level diagram.

nm, PM6 are utilized in combination as donors to create a high-quality crystalline donor phase.

Poly[(9,9-bis(30-(N,N-dimethylamino)pro-pyl)2,7-fluorene)-alt-5,50-bis(2,20-thiophene)-,6-naphthalene1,4,5,8-tetracabox-ylic-N,N0-di(2-ethylhexyl)imide] (PNDIT-F3N) which acts as an electron-transport layer in contact with the cathode electrode made up of silver (Ag).

Results and Discussion

The analysis of proposed OSC have been presented. Simulation is done to obtain and plot the relation between J-V curve, absorbed photon density and generation rate in each layer of the defined structure. Sunlight encompasses a wide range of light wavelengths, from ultraviolet to visible to infrared. Just a small portion of the light released by the sun can be seen by the human eye. GPVDM software has a replica of the sun's spectrum in order to run simulations therefore AM 1.5. Figure 5 shows wavelength vs light intensity plot.

The splitting of an exciton into a hole and an electron by a photon in a donor-acceptor combination, which releases energy. GPVDM software, contains detailed information on the electric and the optical properties of the substances employed in the proposed OSC configuration.

GPVDM application for photovoltaic modelling explains electron and hole shift in 1D using bipolar drift diffusion equation 1 and 2.

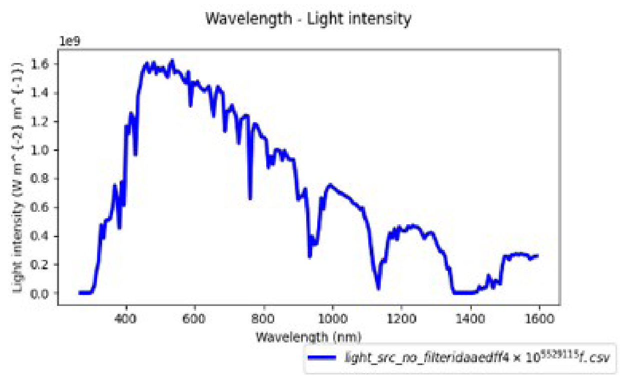

Figure 5: Wavelength vs Light intensity plot.

$$J_n = q\mu_e n \frac{\partial E_{LUMO}}{\partial x} + qD_n \frac{\partial n}{\partial n'} \quad (1)$$

$$J_p = q\mu_p n \frac{\partial E_{HOMO}}{\partial x} + q\mu_p \frac{\partial p}{\partial x} \quad (2)$$

Figure 6 depicts the current density vs voltage plot which shows improvement in the current density compared to other OSC devices using P3HT:PCBM and PTB7:PC70BM as an photoactive layer [12].

In each part of the device's design, the density of photon absorbers ITO/PEDOT:PSS/PM6 D18 L8-BO/PNDIT F3N/Ag is shown in the aforementioned figure 7, which also shows the highest absorption spectrum edges that correspond to the visible photon wavelength spectrum. The active layer's higher photon absorption density may contribute to the production of extra excitons that enhance cell performance.

Excitons are generated when the photoactive layer absorbs energy at the donor (D) – acceptor (A) interface and continuously separates the charge carriers into holes and electrons. Figure 8 illustrates how the position of the device's components affects the rate of electron and hole creation (a-c).

As a result, in the bulk-heterojunction blending of donor (D) and acceptor (A), both charge carriers have large generation rates (Figure 9). As a result, the bulk heterojunction utilised as a photoactive layer act as a significant role in optimizing polymer photovoltaic cell efficacy. Furthermore, this device

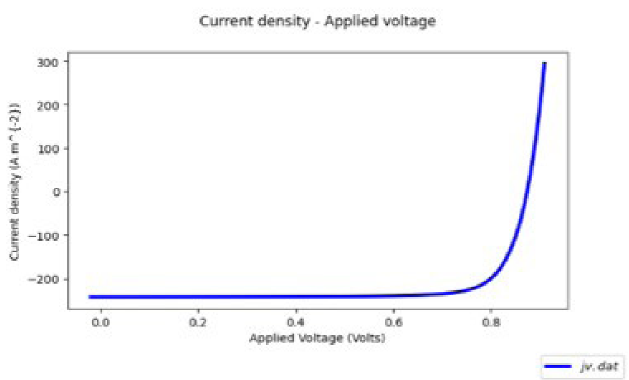

Figure 6: J-V characteristic for PM6:D18:L8-BO active layer.

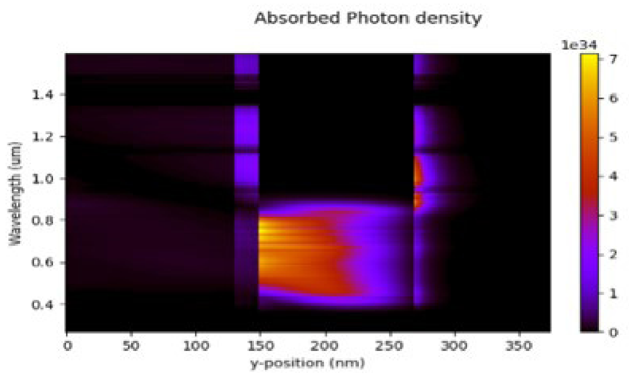

Figure 7: Absorption of photon density in several device architectural components of ITO/PEDOT:PSS/PM6_D18_L8-BO/PNDIT_F3N/Ag.

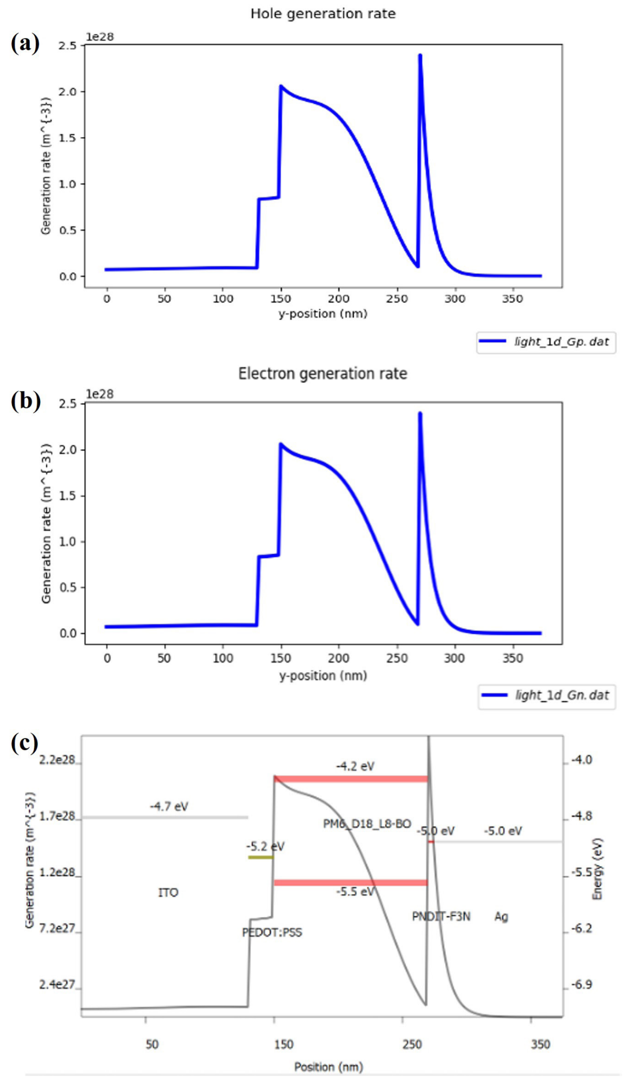

Figure 8: **(a)** Hole generation rate, **(b)** Electron generation rate, and **(c)** Generation rate in the proposed device structure.

maybe employed in the analysis of absorption-based sensing for various application [13, 14].

Conclusion

The results obtained are evident that there is a better

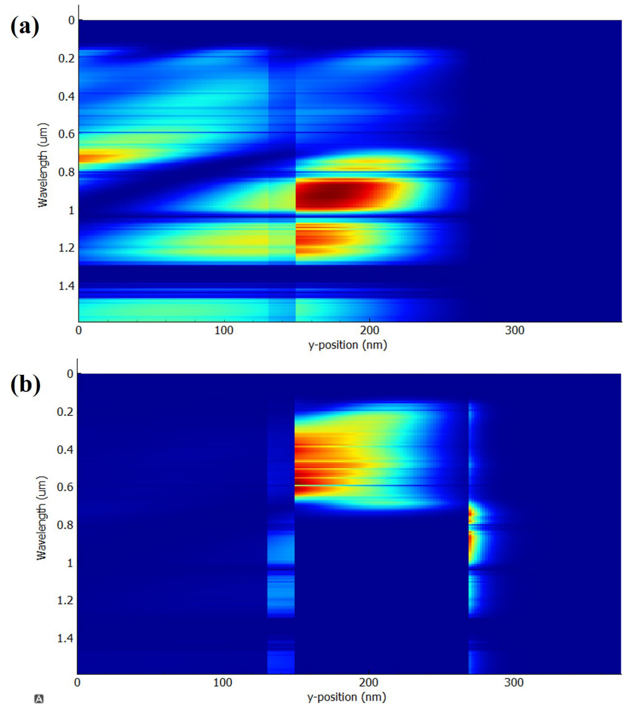

Figure 9: **(a)** Photon distribution and **(b)** Absorbed photon distribution in the OSC structure.

performance in OPVs with newly introduced material PM6_D18_L8-BO as an active layer in comparison with the P3HT:PCBM and PTB7:PC70BM based OSCs. The maximum absorption is in the visible wavelength range. Further investigation can be performed to optimize the device for further performance enhancement of the polymer solar cell.

Acknowledgements

None.

Conflict of Interest

None.

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